

# STN<sup>®</sup> Screen Dictionary

## *for Structure Searching*

### *3<sup>rd</sup> Edition*

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# STN<sup>®</sup> Screen Dictionary for Structure Searching

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**Introduction** This dictionary replaces the *CAS Online Screen Dictionary for Substructure Search, 2<sup>nd</sup> Edition*, published in 1981. The STN structure search environment has changed greatly since that time, so a new version of the screen dictionary is valuable. The screen frequency data was collected in May 2005.

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**The Screen Dictionary Today** The primary use of the screen dictionary in today's search environment is to:

- Document the total list of available screens
- Support the addition of screens to enable a structure search query to run to completion within existing system limits
- Represent structural information that cannot be represented by structures

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**What is a Screen?** A screen, also called a filter, is a numerical code, 1-4 digits in length, which represents a structural feature of a chemical substance.

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**Screens** This introduction explains the various types of screens and how to find them in the dictionary.

A query screen set is automatically generated from a structure query in the STN search command. The search strategy may be enhanced by manually adding additional screens.

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**Structure Search Queries** In the STN structure search system, a search query may be defined by using STN Express<sup>®</sup>, with the Structure Query Search Assistant of STN<sup>®</sup> on the Web<sup>SM</sup>, or with the online STRUCTURE command. From the search query, STN creates a set of screens.

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**Screen Set Refinement**

In a structure search, the query screen set is refined by keeping only those screens that have a very low frequency of occurrence in the search file and therefore assist in uniquely representing the search query.

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**Structure Search Process**

The search process uses this refined screen set in the first step (SCREENING) of the structure search to retrieve a set of candidate answers<sup>1</sup> for the query. The candidate answers are then verified against the query using an atom-by-atom and bond-by-bond comparison (ITERATION) of the query and the candidate answers. Candidates that pass iteration are entered into the answer set (represented by an L-number).

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**Adding Screens to STN Structure Searches**

Details concerning the addition of the screens from this dictionary to your query may be found in *A Guide to Adding Screens in STN Structure Searching*, available at [www.cas.org](http://www.cas.org).

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**Screen-Only Searches**

Details on building “screen-only” search queries are found in Appendix I (*Substructure Profile Development*, page 43) and Appendix II (*Tautomer and Alternating Bonds*, page 83).

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**Screen Capable Databases**

Screens may be used with any STN structure search except in the MARPAT<sup>®</sup> and LMARPAT<sup>SM</sup> databases. At present, databases that support the use of screens are:

- CAS REGISTRY<sup>SM</sup>/ZREGISTRY/LREGISTRY<sup>SM</sup>
  - CASREACT<sup>®</sup>/LCASREACT<sup>SM</sup>
  - CHEMINFORMRX
  - DJSMONLINE
  - DRUGU/LDRUG
  - GMELIN97
  - PS
  - REAXYSFILE
  - WPINDEX/WPIDS/WPIX (Derwent World Patents Index<sup>®</sup>)
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<sup>1</sup> Candidate answers may be viewed with the EXTEND option for the structure search. For more details, enter HELP EXTEND at an arrow prompt (=>).

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**Topics in the Introduction**

This introduction explains the various types of screens and how to find them in the dictionary. These discussions are organized into the following sections:

- Types of screens
  - Structure fragments and search screens
  - The screen dictionary
  - Using the screen dictionary
  - STN Substructure Search Query Development
  - Appendixes
- 

**Screen Authority List**

The *STN Screen Dictionary for Structure Searching* is the master list of all screens recognized by the STN structure search system.

- The appropriate dictionary screens are added during the search file-building process to provide an easily searchable database.
  - You can use the dictionary to refine a search query, enabling the search to run to completion within system limits.
  - You can use the screens to specify search parameters that cannot easily be represented by structural fragments.
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**Dictionary Organization**

The *STN Screen Dictionary for Structure Searching* is organized by:

- The type of screens and ordered within that grouping so that it can be used to find the appropriate screen
  - Screen number order so that any given screen number may be found to ascertain its structure
- 

**Structure Fragments**

Most of the structure fragments are derived from what is termed the “graph” of the structure query connection table.<sup>2</sup> This describes the non-hydrogen atoms and the bonds between them that comprise the basic structure of the substance.

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<sup>2</sup> A connection table is an atom-bond matrix that mathematically represents the substance structure within the database.

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**Hydrogens and  
Connection  
Tables**

The term “hydrogen” will be used throughout this introduction to mean H, D, T, and higher hydrogen isotopes (e.g.,  $^4\text{H}$ ,  $^5\text{H}$ , etc.), and “non-hydrogen” to mean any other element and isotope.

“Normal” hydrogen atoms (i.e., monovalent H) are not described explicitly in the connection table, but only implicitly. Hydrogen count data is not carried in the structure record, but calculated when needed (the number of hydrogen atoms present on a given atom is equal to its valence less bonding requirements and the absolute value of any charge present).

The presence of “normal” hydrogen atoms is ignored by all substructure search screens except the Hydrogen Augmented Atom (HA) and Twin Augmented Atom (TW) screens. These screens consider all hydrogen atoms (H, D, or T) as H.

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**Deuterium and  
Tritium**

The presence of deuterium is indicated through the Graph Modifier (GM) “deuterium” screen (2045), and tritium and higher isotopes (e.g.,  $^4\text{H}$ ,  $^5\text{H}$ , etc.) through the GM “tritium” screen (2046).

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**Unusual  
Hydrogen  
Atoms**

“Unusual” hydrogen atoms are explicitly described in the connection table record and are effectively treated just as non-hydrogen atoms. These are predominantly hydrogen atoms with a valence greater than one, as needed to comply with structuring conventions for “bridge” hydrogens in boron cage compounds or the hydrogens in metal hydrides. They also include the atoms in hydrogen molecules where the hydrogen–hydrogen bonds must be described in the connection table.

The presence of “unusual” hydrogen is indicated only by their inclusion in the AC counts and in DC and CS connectivity values. There is no Element Composition (EC) screen corresponding to “unusual” hydrogen described in the connection table (i.e., an EC H screen). (The GM EC H screen specifies the presence of hydrogen ions described as single atom fragments.)

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**Screens and  
Structure  
Components**

A basic structure and simple derivatives of a basic structure (i.e., hydrates and simple metal or acid salts) that are described via the single atom fragment (SAF) portion of the structure record are considered to be one-component substances. A SAF (single non-hydrogen element, e.g., HCl or Na) leads to the generation of Graph Modifier Element (GME) fragments. More complex derivatives involving multiatom fragments are multicomponent substances and each component has its own connection table and screen set.

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**Number of  
Occurrences**

Each screen includes a count or number of occurrences that specifies the number of times that the fragment appears in the structure;<sup>3</sup> a count of one, though, is not explicitly shown in the dictionary listings. This count is a minimum value, not an exact value. A count of 2, for example, means that the fragment appears two or more times. A structure that contains five oxygen atoms, for example, is retrieved by a search query that specifies, via the EC 3 O element count screen, that three or more oxygen atoms must be present.

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<sup>3</sup> In the discussions that follow, “fragment” refers to an item of search data generated for a substance, and “screen”, to a search term listed in the dictionary. The distinction is made because some screens indicate the presence of any number of different fragments, due to screen number sharing.

# Types of Screens

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## Introduction

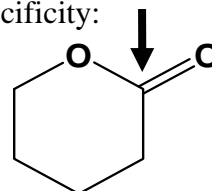
There are 12 types of screens, three describing “clusters” of atoms, three describing linear strings of atoms, and six describing other structural features.

- AA Augmented Atom Screens
  - HA Hydrogen Augmented Atom Screens
  - TW Twin Augmented Atom Screens
  - AS Atom Sequence Screens
  - BS Bond Sequence Screens
  - CS Connectivity Sequence Screens
  - AC Atom Count Screens
  - DC Degree of Connectivity
  - EC Element Count Screens
  - RC Ring Count Screens
  - TR Type of Ring Screens
  - GM Graph Modifier Screens
- 

## Augmented Atom (AA) Screens

The **augmented atom (AA) screen** is the most important of the three “cluster” classes. It describes an atom and its immediate non-hydrogen attachments, with the screen description citing the central atom first and then its attachments in element symbol order; bonds to the central atom are described in the more specific AA screens, while more generic screens use less specific bond descriptions. The indicated carbon atom, for example, could thus be described at three different levels of specificity:

AA	1	C	*1	C	*1	O	-2	O
AA	1	C	*	C	*	O	-	O
AA	1	C		C		O		O



where the AA indicates the screen type and the “1” that the screen occurs one or more times;<sup>4</sup> the bond symbols \*1 and -2 represent a single ring bond and a double chain bond, respectively, while \* and - represent simply ring and chain bonds of any value and a blank represents any bond.

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## Augmented Atom (HA and TW) Screens

The other members of this family are the **hydrogen augmented atom (HA)** and **twin augmented atom (TW)** screens, which add hydrogen count specifications to the basic AA description. HA screens give the hydrogen count for the central atom, TW screens for the central atom and one attached atom.

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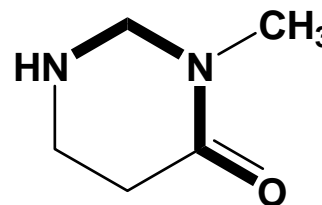
<sup>4</sup> The counts of “1” are shown here for clarity; normally, only counts of 2 or higher are explicitly shown.



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**Linear  
Sequence (AS)  
Screens**

The **linear sequence** family of screens describes linear 4- to 6-atom strings and includes three classes of screens, each describing an atom string in a different manner. The example screens shown below are describing the same 5-atom string (NCNCO) indicated in the structure given here.



An **atom sequence (AS)** screen specifies the element values of the atoms in the string and the types of bonds between them (i.e., whether these bonds are ring or chain), as in:

**AS 1 N \* C \* N \* C - O**

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**Linear  
Sequence (BS,  
CS) Screens**

A **bond sequence (BS)** screen specifies both type and value for the bonds between the string atoms but uses only dummy “A” element symbols to represent the atoms, as in:

**BS 1 A \*1 A \*1 A \*1 A -2 A**

A **connectivity sequence (CS)** screen specifies the connectivity values (the number of non-hydrogen attachments) of the atoms in the string and the types of bonds between them, as in:

**CS 1 2 \* 2 \* 3 \* 3 - 1**

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**Other Classes  
(AC, DC, EC,  
RC, TR, GM)  
Screens**

Other classes of screens describe other aspects of structures.

- Atom count (AC) screens specify the number of atoms present.
  - Degree of connectivity (DC) screens specify the minimum number of atoms having at least a specified number of non-hydrogen atoms attached to them.
  - Element count (EC) screens specify the number of atoms present of specified elements that are present.
  - Ring count (RC) and type of ring (TR) screens specify the rings that are present.
  - Graph modifier (GM) screens specify special structural features and substance classes.
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**Summary**

In general, augmented atom (AA) and atom sequence (AS) screens are the most precise screens. Effective screen profiles can be developed using only these two types of screens.

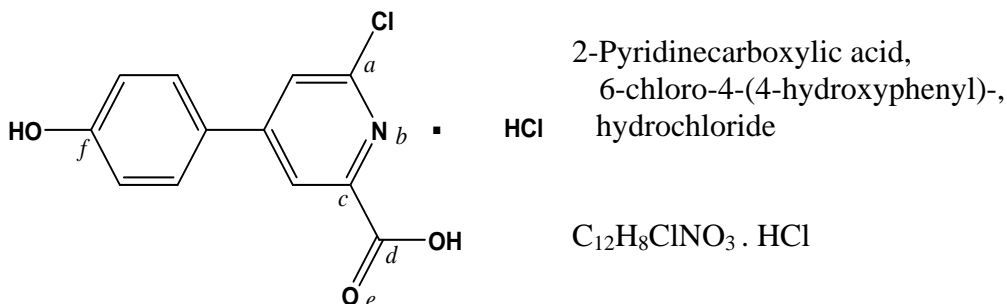
When analyzing a query to determine which screens are most helpful, concentrate on AA and AS fragments that contain several heteroatoms or unusual bonding patterns, since these fragments are the most likely to give useful (i.e., highly specific) screens.

The types of structural fragments that generally lead to useful AA and AS screens are discussed later. The other types of screens are generally less useful, but can still often provide good selectivity for those queries where they are applicable.

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**Screen Types**

Screen types are discussed and illustrated via examples for the following structure:

**Note**

The hydrochloride fragment is described in the structure record as a single atom fragment (SAF); as such, the appropriate screen to describe it is a Graph Modifier Element (GME) screen.

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**Atom and Bond Symbols** The **augmented atom** and **sequence** families of screens, to be discussed next, describe groups of atoms and the bonds between them. The bond symbols used in their screen definitions are the following:

- \* = any ring bond (value not defined)
- = any chain bond (value not defined)
- \*1 = single ring bond
- 1 = single chain bond
- \*2 = double ring bond
- 2 = double chain bond
- \*3 = triple ring bond
- 3 = triple chain bond
- \*4 = alternating (aromatic or completely conjugated) or tautomeric or delocalized ring bond<sup>5</sup>
- 4 = tautomeric or delocalized chain bond<sup>5</sup>

In addition to these bond symbols, a “blank” symbol is used to represent any bond, ring or chain, of any value.

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**Note** Bond value specifications are exact. A **\*2** symbol, for example, represents only a double ring bond, not a double or alternating ring bond.

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**Augmented Atom (AA) Screens** AA screens are descriptions of atoms and their non-hydrogen attachments. Bonds may be unspecified, specified just as ring or chain type, or completely specified, using the bond symbols shown in the table given earlier. The level of bond specificity used for AA screens in the screen dictionary depends on the elements involved:

- Screens for the frequently occurring **C–N** bond, for example, usually completely specify bonds, as in **AA C -1 N**, **AA C -2 N**, etc.
- Screens for the less common **C–P** bonds cite only bond types, as in **AA C \* P** and **AA C - P**.
- Screens for the uncommon **P–P** bond is simply **AA P P**, with no bond specification at all.

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<sup>5</sup> Appendix II (page 83) discusses the definition of tautomer and alternating bonds, how they are handled in CAS REGISTRY, and how tautomer and alternating bonds must be considered when a search query is defined.

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**AA Screens**

In the description of an AA fragment, the central atom is cited first, followed by its attachments in element symbol order. If bonds are specified, a secondary ordering cites \* ring bonds before - chain bonds, and complete bond specifications in the order \*1 \*2 \*3 \*4 -1 -2 -3 -4.

Thus, in the example structure, carbon atom *C* could be described by a number of AA fragments including AA C C C N, AA C \* C - C \* N, and AA C \*4 C -1 C \*4 N.

AA's using out-of-order attachment citations, such as AA C N C C or AA C - C \* C \* N, are not valid and cannot be found in the dictionary.

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**Note**

An augmented atom fragment may be a complete description of a central atom and its environment, as in AA C \*1 C \*1 C -2 O, or just a partial description, as in AA C -1 C -2 O or AA C \* C \* C - O.

In the latter case, additional attached atoms may or may not be present in structures containing the fragment; there is no way to prohibit additional attachments to the central atom without completely describing it, through use of a HA or TW screen, for example, or several AA screens combined with OR logic.

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**Hydrogen Augmented Atoms (HA)**

These screens are augmented atoms whose definitions include a specification of the hydrogen attached to the central atom. The HA fragments used as screens are only those that occur relatively frequently, most having carbon, nitrogen, or oxygen central atoms.

For the example structure, the HA O H -1 C fragment is used to describe the hydroxy group attached to atom *f*.

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**Twin Augmented Atoms (TW)**

These screens are augmented atoms whose definitions include the specification of the hydrogen attached to the central atom and to one of its attached atoms. Only a few TW screens are present in the screen dictionary, to describe common occurrences of -CH<sub>3</sub>, -NH<sub>2</sub>, -OH, and -SH groups.

For the example structure, the TW C \*4 C \*4 C -1 O H fragment is used to describe atom *f*.

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**Notes**

Several points should be noted about HA and TW fragments and the specification of hydrogen atoms:

- HA and TW screens are the only screens that may be used to specify the presence of “normal” hydrogen atoms (i.e., monovalent  $^1\text{H}$ ). All other search screens simply ignore them:
  - The AC screen specifies a count of non-hydrogen atoms.
  - There are no EC screens for H.
  - H atoms are not cited in AA or AS screens.
  - Only bonds between non-hydrogen atoms are cited in BS screens.
  - Non-hydrogen connectivity values are used in DC and CS screens.
- Hydrogen specification is an exact count of the number of attached hydrogens (including D or T, if present), not an “or more” count. These counts follow the atom’s element symbol and appear as follows: “C” indicates a carbon atom with no attached hydrogens; “C H”, a carbon atom with one hydrogen; “C H2”, a carbon with two hydrogens, etc.
- HA and TW screens cannot be used to specify the presence of hydrogen on nitrogen or chalcogen (O, S, Se, or Te) atoms involved in tautomeric situations.

Unlike AA screens, the HA and TW screens present in the screen dictionary completely describe the central atom, so that it may have no additional attachments beyond those shown in the screen definition. This is due, however, to the choice of definitions to be included in the dictionary and is not a requirement implicit in the nature of HA and TW screens.

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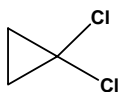
**Atom Sequence (AS)** These screens are descriptions of linear sequences of 4, 5, or 6 atoms. Bond types may be specified for the more common AS fragments, but bond values are not used.

In a query for the example structure, the *b-c-d-e* atom sequence is described by **AS N \* C - C - O** or the equivalent **AS O - C - C \* N**.

As a user aid, screen dictionary entries for AS screens, as well as BS and CS screens, are “double posted”. If the screen definition is not symmetrical, both the “forward” and “reverse” definitions are entries. Both definitions for the AS example given here appear in the dictionary.

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**Note** These sequences, as well as those in BS and CS screens, are linear, so that an atom cannot appear twice in any given sequence. The screen **AS Cl - C \* C \* C \* C - Cl**, for example, could not be used to describe 1,1-dichlorocyclopropane, since the disubstituted carbon atom is cited twice in the sequence.



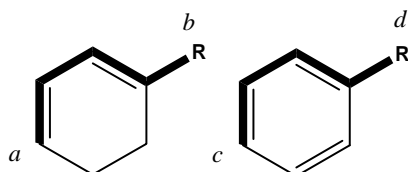
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**Bond Sequence (BS)** These screens are descriptions of linear sequences of 3, 4, or 5 bonds, always specifying the bond types and often the bond values. For clarity, the BS descriptions include “A” dummy atom symbols between the bond symbols.

In a query for the example structure, the BS screen used to describe the *a-b-c-d-e* bond sequence is **BS A \*4 A \*4 A -1 A -4 A** or the equivalent **BS A -4 A -1A \*4 A \*4 A**.

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**Note** Bond sequence definitions are exact and do not imply alternative bond specifications. Where tautomer or alternating bonds exist, \*4 and -4 bond symbols must be used in BS descriptions, not the usual “fixed” \*1 and -1 single and \*2 and -2 double bond symbols. Thus, for example, the BS screen **BS A \*2 A \*1 A \*2 A -1 A** is used to describe the indicated bond path (*a – b*) in the structure containing a cyclohexadiene ring but not in the structure (*c – d*) containing the benzene ring; the screen **BS A \*4 A \*4 A \*4 A -1 A** is used to describe the path in that substance.



**Connectivity Sequence (CS)** These screens are descriptions of non-hydrogen connectivities for linear sequences of 4, 5, or 6 atoms, often including bond types but never bond values. The connectivity values here are the exact number of non-hydrogen attachments, not the usual “or more” specification, so that, for example, a “1” always indicates a terminal atom and a “2” an atom with exactly two non-hydrogen attachments.

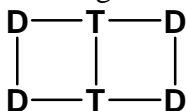
For the example structure, the CS fragment used to describe the *a-b-c-d-e* 5-atom sequence is **CS 3 \* 2 \* 3 - 3 - 1** or the equivalent **CS 1 - 3 - 3 \* 2 \* 3**.

**Ring Count (RC)** These screens specify the minimum number of rings present in the structure. Technically speaking, this is a count of the ring closure pairs present in the structure record, which is equal to the minimum number of bonds that have to be broken to open all rings.

The RC 2 screen is used to describe the example structure.

**Type of Ring (TR)** These screens describe the node sequences of rings of 3-7 atoms. The symbol “D” is used to indicate a non-fused ring atom (an atom attached to exactly two other ring atoms), and “T”, to indicate a fusion point or bridgehead atom with three or more bonds to other ring atoms.

The “smallest set of smallest rings” definition is used to define a “ring” here, so that the “envelope” rings circumscribing smaller rings are not considered. In the simple bridged ring shown here, there are two DDTT rings but no DDTDDT ring; the 6-membered envelope ring is not recognized by the TR screen generation procedure.



There is also a TR screen that simply provides an indicator that an 8-membered or larger ring is present.

For the example structure, if you were to specify that the two 6-membered rings were to be isolated (i.e., could not be part of larger ring systems), the **TR 2 DDDDDD** screen is used to describe them.

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<b>Note</b>	Both D and T are exact node symbols. If you were to allow fusion to the benzene ring in a query for the example structure, then all fusion node possibilities have to be specified or a loss of retrieval occurs.
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<b>Atom Count (AC)</b>	<p>These screens are used to specify the minimum number of non-hydrogen atoms present in the graph (i.e., excluding any atoms described as single atom fragments).</p> <p>The <b>AC 17</b> screen is used to describe the example structure.<sup>6</sup></p>
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<b>Degree of Connectivity (DC)</b>	<p>These screens specify the minimum number of atoms having at least a specified number of non-hydrogen atoms attached to them. DC screens are provided which specify non-hydrogen connectivities from three or more to six or more.</p> <p>The <b>DC 6 3</b> screen, specifying the presence of six or more atoms having non-hydrogen connectivities of three or more, is used to describe the example structure.</p>
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<b>Element Composition (EC)</b>	<p>These screens specify the minimum number of atoms of each element (except H, D, and T) present in the CT graph (i.e., again excluding atoms described in SAFs). The common elements have EC screens with specific counts; carbon, for example, has 13 EC screens ranging from <b>EC 4 C</b> to <b>EC 40 C</b>, and sulfur has <b>EC S</b> to <b>EC 5 S</b>.</p> <p>The EC screens for the less common elements such as gold or lead all have counts of one, specifying simply the presence of one or more atoms of the elements.</p> <p>The <b>EC 12 C</b>, <b>EC Cl</b>, <b>EC N</b>, and <b>EC 3 O</b> screens are used to describe the example structure, whose molecular formula is C<sub>12</sub>H<sub>8</sub>ClNO<sub>3</sub> . HCl.</p>
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<sup>6</sup> Actually, since the **AC 17** screen does not appear in the screen dictionary, the **AC 16** screen is used in its place.



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<b>Note</b>	The Cl EC screen is <b>EC Cl</b> , not <b>EC 2 Cl</b> . The Cl atom of the HCl SAF is <u>not</u> described via an EC screen.
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<b>Graph Modifier (GM)</b>	Most GM screens are Graph Modifier Element (GM E) screens that are used to describe the elements cited in the Single Atom Fragment (SAF) portion of the structure record.
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In a query for the example structure, the GM E Cl screen is used to specify the presence of the hydrochloride salt.

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<b>Other GM Screens</b>	<p>Other GM screens are used to specify the following:</p> <ul style="list-style-type: none"><li>• Unusual structural features Unusual mass, valence, or charge attributes of atoms in the graph of the connection table or the SAF portion of the structure.</li><li>• Multicomponent substance data The presence of two or more to four or more components and the presence of SAFs.</li><li>• Chemical substance class identifiers, classification of substances as:<ul style="list-style-type: none"><li>– Alloys</li><li>– Incompletely described substances</li><li>– Minerals</li><li>– Mixtures</li><li>– Multicomponent substances</li><li>– Polymers</li><li>– Radical ions</li></ul></li></ul> <p>with further subclassifications for incompletely described substances and polymers.</p>
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<b>Screen Generation in Structure Search</b>	The procedure that generates the 12 types of fragments just discussed and builds the screen search files for the STN search system performs an analysis of each structure. The procedure is briefly summarized here as background information.
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**Structure  
Search File  
Building**

These are the steps taken to create substructure search screens for a substance:

- A fragment generation step, in which structure fragments and other search data are generated from the substance connection table
- A subsequent screen generation step to check the generated fragments against a dictionary, since the generation procedure is exhaustive, creating all possible structure fragments
- Recording of the presence of structure fragments that are cited in the dictionary (Those fragments not cited are ignored.<sup>7</sup>)

Most of the structure fragments are generated from what is termed the graph of the connection table; this describes the atoms and bonds that comprise the basic structure of the substance.

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**Multi-  
component  
Structures**

Simple derivatives of this basic structure (i.e., hydrates and simple metal or acid salts) that are described via the single atom fragment (SAF) portion of the record lead to the generation of GME fragments. In more complex derivatives involving multiatom fragments, each multiatom fragment is described by a connection table (from which structure fragments are generated) and single-atom fragments are described as SAFs.

A search screen includes a count or number of occurrences that gives the number of times that the fragment appears in the structure. This is a minimum value, not an exact value. A count of 2, for example, means that the fragment appears two or more times. The “or more” ability is implemented during the screen generation step that creates the bit string used in searching.

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**Example**

If the structure contained five oxygen atoms, for example, the fragment generation step creates an **EC 5 O** fragment. The screen generation step then sets all EC O fragments with a count of five or less (i.e., the screens **EC O** through **EC 5 O**), so that, for example, the structure is retrieved by a search query specifying, via the **EC 3 O** screen, that three or more oxygen atoms must be present.

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<sup>7</sup> These fragments are for the most part very frequently occurring and thus of little selectivity, or else are so rare that they will not be used enough in searching to justify their inclusion in a dictionary of limited size.

The fragment generation procedure generates all possible fragments, using exhaustive procedures. (While this might seem inefficient, it is both easier and faster than the generation of only those fragments that appeared in the screen dictionary.) The augmented atom generation procedure, for example, generates AA fragments for each non-hydrogen atom in the graph, using an exhaustive procedure that considers all possible combinations of attached atoms and bond specification levels. For the carboxy group carbon (atom **d**) of the example structure shown earlier, the procedure begins with the most specific **C -1 C -4 O -4 O** fragment and generates 14 others, yielding the fifteen fragments shown below:

$$\begin{array}{rcl}
 C & C & C \quad -1 \quad C \quad -4 \quad 0 \\
 C & - \quad C & C \quad C \quad 0 \quad 0 \\
 C & -1 \quad C & C \quad - \quad C \quad - \quad 0 \quad - \quad 0 \\
 C & C \quad 0 & C \quad -1 \quad C \quad -4 \quad 0 \quad -4 \quad 0 \\
 C & - \quad C \quad - \quad 0 & C \quad 0 \\
 & & C \quad - \quad 0 \\
 & & C \quad -4 \quad 0 \\
 & & C \quad 0 \quad 0 \\
 & & C \quad - \quad 0 \quad - \quad 0 \\
 & & C \quad -4 \quad 0 \quad -4 \quad 0
 \end{array}$$

The subsequent screen generation step checks the screen dictionary for each of the generated fragments, and finds only six of them, shown underlined above, to be present. The bits for these fragments are set in the screen search record bit string.

It should be pointed out that the AA fragment generation procedure creates **only one** AA fragment of each specific type possible for each central atom. For the sample structure, for example, there are three O C fragments generated (i.e., an **AA 3 O C**) but only two C O fragments. Although there are three oxygen atoms attached to carbon atoms, there are only two carbons (atoms *d* and *f*) attached to oxygens. As a consequence, when using AA screens for which counts greater than one are provided, you should take care that the count selected does correspond to the number of different central atoms.

# The STN Screen Dictionary

---

## Introduction

In the STN search system, your query is defined by the system in terms of screens and sets of screens combined with Boolean logic. The more frequently occurring screens are automatically removed from the query to facilitate a timely search process. This screen dictionary allows you to locate screens for manual addition to the search query to bring the predicted results within system limits. The dictionary is an ordered listing of the screens used in the STN structure search system.

Two different orderings are provided:

- **Screen order** groups screens by type, in the order AA, HA, TW, AS, BS, CS, RC, TR, AC, DC, EC, and GM. Within each type grouping, screens are ordered by screen definition, then by number of occurrences, and finally by screen number.
- **Screen number order** – Under each screen number, entries are ordered first by screen type and then by screen definition.

Use the screen order dictionary to locate screens to add to a search query. Use the screen number order dictionary primarily for checking the screen number definitions.

---

## Screen Definition Order

The specification of screen definition order is dependent upon the type of screen.

AA, HA, TW, AS, and BS screens are listed in increasing alphabetic order of element symbols, then bond symbols, with the bond order as shown:

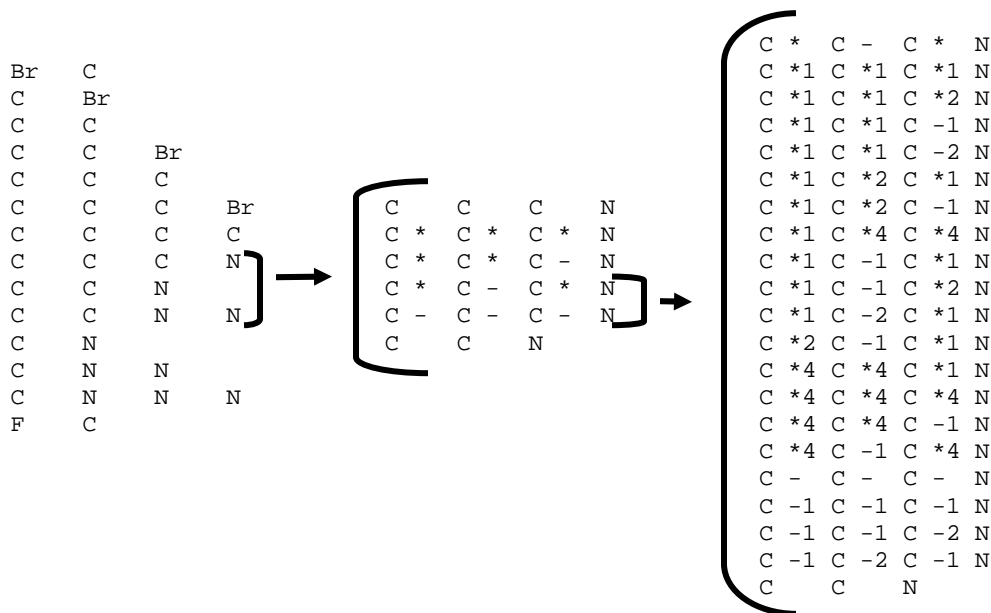
**(none) \* \*1 \*2 \*3 \*4 - -1 -2 -3 and -4**

---

---

## Screen Order

This is not a strict left-to-right alphabetical ordering, but one that imposes a hierarchy. It groups screens first by the elements cited and then by bond type and value, as shown by the example:



- CS screens are listed in increasing numeric order of connectivity values, and then bond symbols. Again, this is not a strict left-to-right ordering.
  - RC screens are listed in increasing order of number of occurrences, which is simply the ring count.
  - TR screens are listed in increasing order of ring size, and then in increasing alphabetic order of definition.
  - AC screens are listed in increasing order of number of occurrences, which is simply the atom count.
  - DC screens are listed in increasing numeric order of connectivity values, and then in increasing order of number of occurrences.
  - EC screens are listed in increasing alphabetic order of element symbol.
  - GM screens describing “unusual” structural features appear at the beginning of the GM screen listing. The GME screens describing the presence of elements as single atom fragments (SAFs) are then listed in increasing alphabetic order of element symbol.
-

---

**Screen  
Dictionary  
Format**

Each line in the screen dictionary is formatted as shown:

```
961    AA    C    Br    Cl    #    0.25
ssss    tt  nn  ddddddddddddddd x    ffff
```

where the line fields provide the following data:

- s** Screen number (leading zeros are not used)
- t** Screen type
- n** Number of occurrences (“or more”): In all cases where multiple numbers of occurrences are used for a screen, the entries are grouped together in increasing order of number of occurrences. Note that counts of one are not shown, nor are leading zeros used.
- d** Definition
- x** Multiple-use flag: In the screen order dictionary listing, a “#” indicates that the screen number is shared by two or more different screens, as discussed below, while a blank indicates that the screen number is unique to the screen. In the screen number order listing, the “#” flag is not used, since multiple usage is obvious from the screen groupings.
- f** Frequency of appearance in the total CAS REGISTRY search file (as of May 2005): If the screen number is shared, the frequency is for structures containing any of the screens. Note that these frequencies are truncated to 0.01%, so that a frequency of 0.00% means that fewer than 0.01% of the structures contain the screen, not that no structures are present that contain the screen.

Sample pages from the screen number order and screen order dictionaries are shown as the next two pages of this section.

---

Sample Page in  
Screen Number  
Order

Screen Number Order

Screen Number	Fragment Definition	Freq. %
1 AS	C * C - C * C	13.51
2 AS AS	C * C - C - C C - C - C * C	34.96
3 AS	C - C * C - C	14.19
4 AS	C - C - C - C	32.65
5 AS	C * C * C * C * C	78.62
6 AS AS AS AS AS AS AS AS AS AS AS AS AS AS AS AS	Br- C * C - C * C C * C - C * C - Br C * C - C * C - C C - C * C - C * C C * C - C * C - Cl C * C - C * C - F C * C - C * C - I C * C - C * C - N C * C - C * C - O C * C - C * C - S Cl- C * C - C * C F - C * C - C * C I - C * C - C * C N - C * C - C * C O - C * C - C * C S - C * C - C * C	7.08
7 AS AS AS AS AS AS AS AS AS AS AS	C * C - C * C - C C - C * C - C * C C * C - C - C * C - C C - C * C - C - C * C C - C * C - N - C * C C - C * C - O - C * C C - C * C - S - C * C C * C - N - C * C - C C * C - O - C * C - C C * C - S - C * C - C	6.85
8 AS	C * C - C - C * C	6.91
9 AS AS	C * C - C - C - C C - C - C - C * C	17.57
10 AS	C - C * C * C - C	12.64

Sample Page in  
Screen Type  
Order

Augmented Atoms

Screen Number	Fragment Definition	Freq. %
935 AA	A *2A	34.69
937 AA	A *3A	0.14
936 AA	A *4A	72.06
938 AA	A -2A	59.17
939 AA	A -4A	39.02
940 AA	A * A * A	41.18
941 AA	A * A - A - A	12.51
942 AA 2	A * A - A - A	3.34
943 AA 3	A * A - A - A	1.07
944 AA	A - A - A - A	73.89
945 AA	A * A * A * A	7.17
946 AA 2	A * A * A * A	1.92
947 AA	A * A * A - A	7.64
948 AA 2	A * A * A - A	3.57
949 AA 3	A * A * A - A	1.36
1820 AA	As As	# 0.35
1820 AA	As B	# 0.35
1552 AA	As * C	# 1.15
1558 AA	As M	# 3.13
1391 AA	As * M	# 6.30
1392 AA	As - M	# 6.25
1667 AA	As -4N	# 2.86
1820 AA	As P	# 0.35
1820 AA	As Se	# 0.35
1820 AA	As Si	# 0.35
1820 AA	As Te	# 0.35
952 AA	As X	# 0.53
1820 AA	B As	# 0.35
1820 AA	B B	# 0.35
1552 AA	B * C	# 1.15
953 AA	B - C	0.39
1558 AA	B M	# 3.13
1391 AA	B * M	# 6.30
1392 AA	B - M	# 6.25
954 AA	B N	0.22
1667 AA	B -4N	# 2.86
955 AA	B * O	# 0.30
955 AA	B - O	# 0.30
1820 AA	B P	# 0.35
1820 AA	B Se	# 0.35
1820 AA	B Si	# 0.35
1820 AA	B Te	# 0.35
952 AA	B X	# 0.53
956 AA	Br C	4.36
1552 AA	C * As	# 1.15



---

**2127 Screen Numbers**

Although there are only 2127 screen numbers, there are almost 6000 different screen definitions in the dictionary. To increase the number of screens available, many screen numbers are associated with two or more definitions. Screen number 961, for example, is used for six AA screens describing the presence of two unlike halogen atoms on a carbon:

AA	C	Br	Cl	AA	C	Cl	F
AA	C	Br	F	AA	C	Cl	I
AA	C	Br	I	AA	C	F	I

The screen order dictionary entries for these six AA screens are all flagged with the “#” multiple-use marker. The frequency of appearance cited is 0.16%, and is the same for all six screens; 0.16% of the file is structures containing at least one of any of the six different fragments.

---

**Selectivity**

Since the addition of such a screen number to a search query seems to limit the query to retrieve only structures containing any of the associated fragments, it might seem that this approach does not benefit the selectivity of the search. In practice, there is actually selectivity observed, since other features in the structure assist in the selectivity.

---

## Screen Number Sharing Schemes

Several different schemes have been used to set up multiple screens sharing a screen number:

- There are many cases where several related AA screens share a screen number. The six possible AAs describing a carbon atom attached to two different halogen atoms (e.g., **AA C Br Cl**) are specified by 961, for example. To narrow down retrieval to a specific fragment, you combine (“AND”) 961 with additional AA screens, **956 AA Br C** and **1347 AA C Cl**, for example, to select the bromo–chloro species.
- Most elements do not have specific screen numbers for either EC or GME screens, nor is there a distinction made between the element appearing in the connection table (CT) and appearing as a single atom fragment (SAF).<sup>8</sup> The approach taken assigns screen numbers to groups<sup>9</sup> and series of elements, as shown by the table on the next page, so that a specific element is selected by combining two screens with AND logic, one screen specifying a vertical group from the periodic table and the other screen a horizontal series, silver, for example, is pinpointed by screens 1920 AND 1921 (specifying group Ib and transition series II, respectively).
- The most common elements, such as Al or Br, have specific screen numbers assigned to them, while the least common elements, such as Ac, can be accessed only via a generic screen specifying a group or series.
- As a consequence of this approach, the screen dictionary listings for EC and GME screens have been replaced with a table specifying the screen number(s) to be used to specify any particular element, as shown by the sample table entries which follow:

“Or-more”		Element Count	Graph	Modifier	EC or GM
Count	(CT Graph)		(SAF)		(CT + SAF)
Ac	1				1919 0.19% max.
Ag	1				1920 AND 1921 0.57% max.
Al	1				1922 1.27%
Br	1		2030	0.55%	1938 5.30%
	2	1939	1.12%		
	3	1940	0.30%		
	4	1941	0.18%		

<sup>8</sup> The less common elements occur so infrequently that the CT/SAF distinction is of little practical value. The CT/SAF distinction is made only for nine common elements (Br, Ca, Cl, H, I, K, N, Na, and O), which appear frequently enough as SAFs that distinct GME screens are beneficial.

<sup>9</sup> Group designations in the tables are those used in Europe, not the U.S.

**Generic  
Element Count  
and Graph  
Modifier  
Screens**

Screen	Freq.	Description	Elements
1918	14.84%	"metals"	all except Ar As At B Br C Cl F H He I He I Kr N Ne O P Rn S Se Si Te Xe
1967	2.00%	group Ia	Cs Fr K Li Na Rb
1936	1.24%	group IIa	Ba Be Ca Mg Ra Sr
1988	0.53%	group IIIa	La Sc Y
1984	1.39%	group IVa	Hf Ti Zr
2001	1.12%	group Va	Nb Ta V
1966	2.44%	group VIa	Cr Mo W
1991	1.96%	group VIIa	Mn Re Tc
1965	6.72%	group VIII	Co Fe Ir Ni Os Pd Pt Rh Ru
1920	2.10%	group Ib	Ag Au Cu
1956	1.03%	group IIb	Cd Hg Zn
1923	2.93%	group IIIb	Al B Ga In Tl
1983	5.61%	group IVb	Ge Pb Si Sn
1925	6.12%	group Vb	As Bi P Sb
2003	86.62%		O S
• • •			
2029	0.61%	"SAFs"	all except Br Ca Cl H I K N Na O

**Screen  
Number  
Sharing**

In many cases, related AS, BS, or CS screens share a screen number. With BS screens in particular, there are sets of related screens describing two rings linked by a short chain, and each specific BS fragment appears in two sets of screens, one set having fragments with the same ring bonds but different combinations of chain bonds, and the other set having fragments with the same chain bonds and differing ring bonds. Screen 834, for example, specifies two rings linked by three -1 bonds, while 845 specifies two rings with \*4 bonds linked by different combinations of three chain bonds. The fragment BS A \*4 A -1 A -1 A -1 A \*4 A appears in both screen sets and is pinpointed by 834 AND 845.

**Implicit  
Screen  
Number  
Sharing**

Finally, there is an implicit screen number sharing accomplished through the use of three generic element symbols, "A" representing any atom, "M" representing any metal, and "X" representing any halogen.

The 937 screen AA A \*3 A thus represents any two atoms connected by a cyclic triple bond, while the 1390 screen AA C M specifies any carbon-metal bond and the 1364 screen AA C X X X specifies a carbon atom attached to three halogen atoms in any combination.

# Using the Screen Dictionary

---

## Introduction

The screen dictionary enables you to add screens to your search strategy by using the tables in this document. In some cases, this simply requires locating the desired screen in the dictionary. In other cases, when the desired screen is not in the dictionary, you will need to identify the best screen or screens that are available. This section discusses how screens are found in the dictionary, with emphasis on the **augmented atom** and **sequence** families of screens.

---

## Finding AA, HA, and TW Screens

The augmented atom (AA), hydrogen augmented atom (HA), and twin augmented atom (TW) screens are relatively easy to locate in the screen dictionary listing, once you have become accustomed to the *hierarchical ordering* used for these screens. In the description of an augmented atom:

Step	Action
1	Cite the central atom first.
2	Cite its attachments in element symbol order.
3	If bonds are specified, a secondary ordering cites * <b>ring bonds</b> before - <b>chain bonds</b> .
4	Cite complete bond specifications in this order: <b>*1 *2 *3 *4 -1 -2 -3 -4</b>

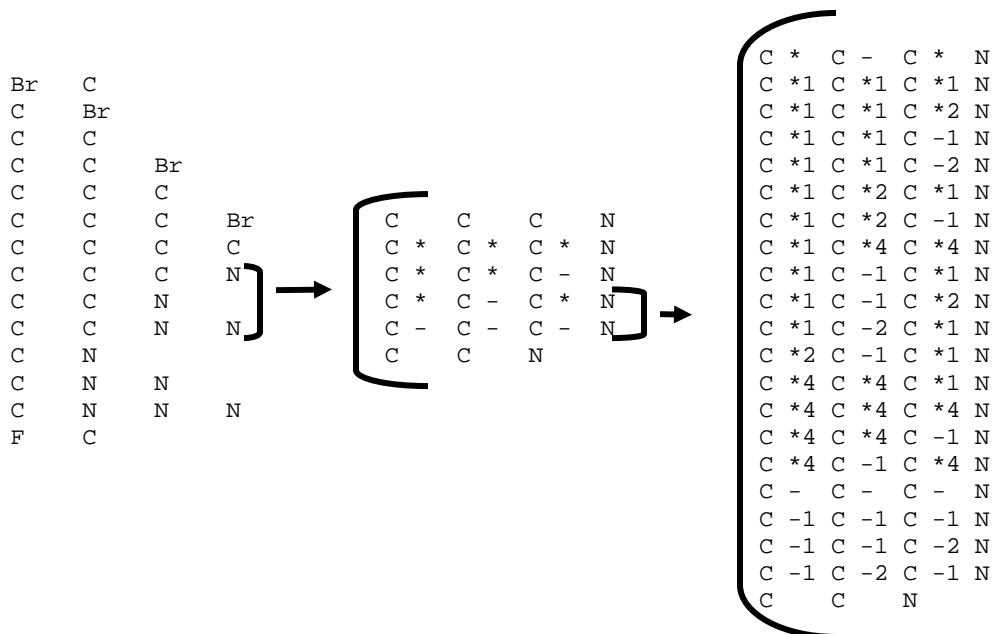
You should thus look for **AA C \*1 C \*4 C \*4 N**, for example, and not for AA's using out-of-order attachment citations, such as **AA C \*4 N \*1 C \*4 C** or **AA C \*4 C \*1 C \*4 N**.

---

---

**Screen  
Descriptions**

These descriptions are listed in increasing order of element symbols, and then bond symbols, resulting in the hierarchical ordering as illustrated here:



---

**Screen  
Specificity**

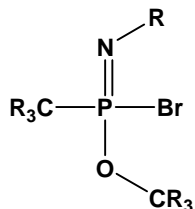
When an AA screen describing an atom is sought, check for the most specific screen possible under the constraints imposed by the query structure – a screen describing the central atom and all of its attached atoms, with bond type and value specified. If the most specific screen, the “target” screen, is not present in the dictionary, then check for less specific screens. These screens are derived from the “target” screen by decreasing the number of attached atoms and by reducing the level of bond specificity.

---

---

**Example**

As an example, consider the structure shown below. The most specific AA fragment based on P as the central atom is **P -1 Br -1 C -2 N -1 O**, and this “explodes” into a total of 57 AA fragments of various degrees of specificity:<sup>10</sup>



$\text{R}_3 = \text{anything including H}$

P -1 Br -1 C -2 N -1 O	P - Br - C - N - O	P Br C N O
P -1 Br -1 C -2 N	P - Br - C - N	P Br C N
P -1 Br -1 C -1 O	P - Br - C - O	P Br C O
P -1 Br -2 N -1 O	P - Br - N - O	P Br N O
P -1 C -2 N -1 O	P - C - N - O	P C N O
P -1 Br -1 C	P - Br - C	P Br C
P -1 Br -2 N	P - Br - N	P Br N
P -1 Br -1 O	P - Br - O	P Br O
P -1 C -2 N	P - C - N	P C N
P -1 C -1 O	P - C - O	P C O
P -2 N -1 O	P - N - O	P N O
P -1 Br or Br -1 P	P - Br or Br - P	P Br or Br P
P -1 C C -1 P	P - C C - P	P C C P
P -2 N N -2 P	P - N N - P	P N N P
P -1 O O -1 P	P - O O - P	P O O P

---

<sup>10</sup> Note that the two-atom AA fragments may be represented in two distinct forms, and these forms are not equivalent. The fragment **AA P -1 Br**, for example, describes a central P atom with an attached Br atom, while the fragment **AA Br -1 P** describes a central Br atom with an attached P atom. The distinction occurs when numbers of occurrences are considered, the  $-\text{SO}_2$  sulfonyl group has the fragments **AA S -2 O** and **AA 2 O -2 S**, for example, since only one fragment is created for the S central atom, but two are created for the two different O central atoms.

---

**AA Fragments** By checking the screen dictionary, you will find only seven of these AA fragments, shown underlined in the illustration, and one is redundant (1688 implies 1686):

1533	<u>AA</u>	C	-	P		2.98%
1686	<u>AA</u>	N	-	P		0.60%
1688	<u>AA</u>	N	-2	P		0.09%
1722	<u>AA</u>	O	-1	P		2.22%
1743	<u>AA</u>	P		C	N	0.29%
1744	<u>AA</u>	P		C	O	1.25%
1752	<u>AA</u>	P		N	O	0.49%

The six AA screens together (omitting 1686) define almost the entire desired augmented atom, but do not describe the P-Br bond. Two additional screens are needed: the generic **P X** screen specifying a phosphorus-halogen bond (either ring or chain) and an EC screen to specify the presence of Br in the connection table:

1561	<u>AA</u>	X	P	0.42%
1938	<u>EC</u>	Br		5.30%

Thus, the you would seek the desired specific AA fragment via a set of eight screens combined with AND logic:

1533 1561 1688 1722 1743 1744 1752 1938

Maximum retrieval is 0.09%, the retrieval of screen 1688, the rarest screen.

---

**Worst Case** This example of using AA screens represents a “worst case”, more involved than usually encountered in practice. It was chosen so that a number of screens are needed to describe the desired AA fragment, to illustrate the techniques needed to handle difficult cases. Most AA fragments needed in typical substructure searches can either be found in the screen dictionary or be handled by specifying two or three smaller AA screens; only those AA fragments containing several of the less common heteroatoms have to be analyzed as shown in the preceding example.

---

---

**HA Screens**

You can seek hydrogen augmented atom (HA) screens in the same manner as AA screens. Note that the selection of HA screens is rather limited:

- All HA screens have at least one hydrogen attached to the central atom.
  - Only a limited set of elements may be specified as attached atoms:
    - C central atom: C, N, O, S, or X (generic halogen) attached atoms
    - N central atom: C, N, O, or S attached atoms; two generic screens are also provided for N–“hetero” (As, B, O, P, S, Se, Si, or Te)
    - O central atom: C or N attached atoms; two generic screens are provided for O–O or O–S and for O–“hetero” (As, B, P, Se, Si, or Te)
    - Al, As, B, Ge, P, S, Sb, Se, Si, Sn, or Te central atom: C attached atoms only
- 

**TW Screens**

You can seek twin augmented atom (TW) screens in the same manner as AA screens. The selection of TW screens is very limited. The central atom is always a carbon atom with zero, one, or two attached hydrogens. Attached atoms are limited to carbon atoms and one atom with H specified: a CH<sub>3</sub>, NH<sub>2</sub>, OH, or SH.

---

**AS Screens**

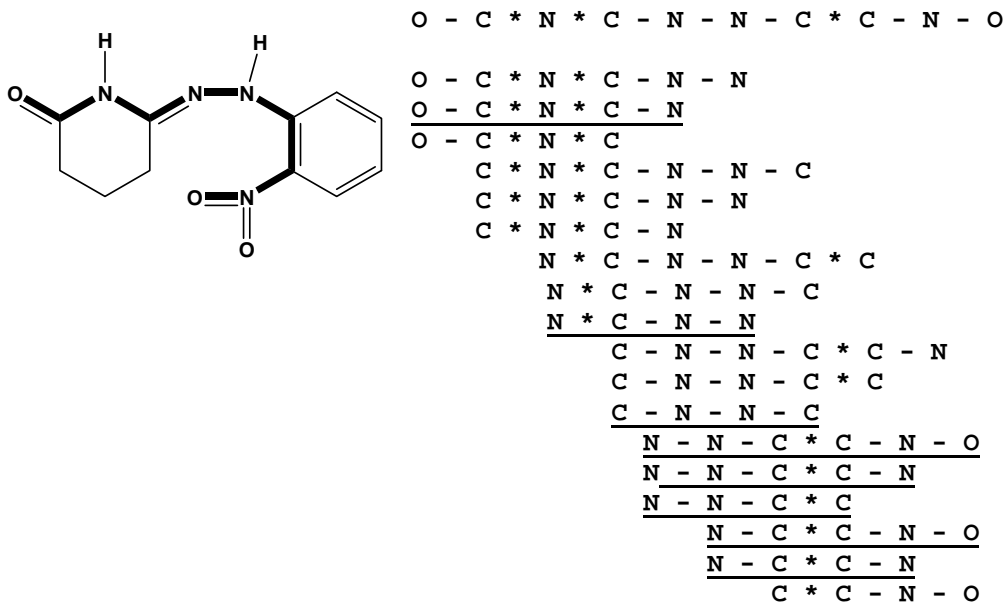
When you need atom sequence (AS) screens, check for long paths through heteroatoms and through links between rings and chains. Then break down each path into overlapping 4- to 6-atom sequences to be located in the screen dictionary. Note that an atom should not appear twice in any given path, since the sequence screens describe only linear sequences. (There is, of course, no restriction on an atom appearing in two or more different paths.)

---



### AS Example

Consider the structure shown below, where a 10-atom path containing six heteroatoms can be traced from the oxo substituent on the left to the nitro group on the right. Break down this 10-atom sequence into smaller 4- to 6-atom fragments to be located in the dictionary, since the sequence screens are “double posted”, with an a-b-c-d sequence also entered in the screen dictionary as d-c-b-a. The breakdown of the 10-atom sequence can be done on a simple left-to-right basis.



### AS Screens

By checking the screen dictionary, you will find nine of these AS fragments, shown underlined in the illustration, resulting in seven AS screens with bond types specified and four more generic AS screens without bond types specified.

174	AS	C * C - N - O	#	6.36%
248	AS	C - N - N - C		4.27%
386	AS	N - C * C - N		1.42%
394	AS	N C C N O	#	3.00%
396	AS	N - C * C - N - O	#	0.72%
431	AS	N C N N		5.69%
433	AS	N * C - N - N		0.55%
167	AS	N - N - C * C		2.67%
393	AS	N N C C N		3.65%
450	AS	N N C C N O	#	0.51%
429	AS	O - C * N * C - N	#	1.44%

---

**Redundant  
Screens**

Check the coverage of the 10-atom sequence by these 11 screens. Five screens are found to be unnecessary: four are contained in longer sequences and one is a less specific generic screen.

O - C * N * C - N - N - C * C - N - O										
O - C * N * C - N										429
	N	C	N	N						431
		N	* C - N - N							433
			C - N - N - C							248
				N - N - C * C						167
				N	N	C	C	N		393
				N	N	C	C	N	O	450
					N - C * C - N					386
					N	C	C	N	O	394
					N - C * C - N - O					396
						C * C - N - O				174

Eliminating these five screens leaves six screens to be used to describe the 10-atom path.

O - C * N * C - N - N - C * C - N - O										
O - C * N * C - N										429
	N	* C - N - N								433
		C - N - N - C								248
			N - N - C * C							167
			N	N	C	C	N	O		450
				N - C * C - N - O						396

Combine these screens with AND logic. Maximum retrieval is 0.51%, the retrieval of screen 450, the rarest screen in the set.

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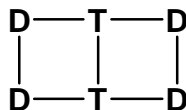
## BS and CS Screens

You can find bond sequence (BS) and connectivity sequence (CS) screens in a similar manner. Keep in mind two special aspects of these two screen types:

- Many BS screens appear in two sets of related screens, and it is necessary to use both screen numbers connected with AND logic to specify the desired screen.
  - These are generally sets of related screens describing two rings linked by a short chain, with each specific BS fragment appearing in two sets of screens: one set has fragments with the same ring bonds but different combinations of chain bonds, and the other set has fragments with the same chain bonds and differing ring bonds. Screen 834, for example, specifies two rings linked by three -1 bonds, while screen 845 specifies two rings with \*4 bonds linked by different combinations of three chain bonds. The fragment **BS A \*4 A -1 A -1 A -1 A \*4 A** appears in both screen sets and is pinpointed by 834 AND 845.
  - In CS screens, the connectivity values are the exact number of non-hydrogen attachments, not the usual “or more” specification, so that, for example, a “1” always indicates a terminal atom and a “2” an atom with exactly two attachments.
- 

## TR Screens

The type of ring (TR) screens describe rings of 3-7 atoms as node sequences and also provide an indicator that an 8-membered or larger ring is present. The symbol “D” is used to indicate a non-fused ring atom (attached to exactly two other ring atoms), and “T” is used to indicate a fusion point or bridge-head atom with three or more bonds to other ring atoms. The “smallest set of smallest rings” definition is used to define a “ring” here, so that “envelope” rings circumscribing smaller rings are not considered. In the simple bridged ring shown here, there are two DDTT rings but no DDTDDT ring, since the 6-membered envelope ring is not recognized by the screen generation procedure.



---

**TR Screen  
Permutations**

For the 3- to 7-membered rings, screens for all possible unique D and T combinations are present in the dictionary listing, ordered alphabetically within groupings by ring size. For a given D and T combination, there are usually several possible representations. The 4-membered ring of the example above might be cited as DDTT, DTTD, TDDT, or TTDD. The dictionary entry will always be the representation that is first if the alternative representations were ordered alphabetically, here DDTT.

---

**AC, RC, and  
DC Screens**

The atom count (AC), ring count (RC), and degree of connectivity (DC) screens are all very easy to locate and use because these screens are simply counters. The lookup process merely finds the desired count in the number of occurrences column of the dictionary listing. If the desired count is not present, the next lower count that is present should be used. (Remember that the numbers of occurrences are “or more” specifications and state that the feature appears n or more times in the structure; the DC connectivity values are also “or more” specifications.)

---

**EC and GM E  
Screens**

The element count (EC) and graph modifier element (GME) screens are likewise easy to use, provided that you refer to the screen tables and not to the EC and GM screen listings themselves. The tables are provided to facilitate the use of the EC and GM screens, since most elements do not have dedicated EC and GM screen numbers and must be specified by combining two generic screens with AND logic.

Three tables of screens are provided in the screen dictionary, instead of the EC and GME screen listings:

- Table I – Specific Element Count and Graph Modifier Screens
  - Table II – Generic Element Count and Graph Modifier Screens
  - Table III – Generic Element Count and Graph Modifier Screens in Screen Number Order
-

**Table I**

Lists EC and GM screens in element order. These screens fall into three classes, as shown by these example entries from the table:

<u>“Or-more” Count</u>		<u>Element Count (CT Graph)</u>	<u>Graph Modifier (SAF)</u>	<u>EC or GM CT + SAF</u>	
Ac	1			1919	0.19% max.
Ag	1			1920 AND	
				1921	2.10% max.
Al	1			1922	1.27%
Br	1		2030 0.551.%	1938	5.30%
	2	1939	1.12%		
	3	1940	0.30%		
	4	1941	0.18%		

**Elements**

Most elements can be specified only as present in the structure as a whole, either in the connection table (CT) itself or in a single atom fragment (SAF). These screens appear in the column headed “**EC or GM (CT + SAF)**”.

**More Common Elements**

The **more common elements**, such as Al or Br in the example entries above, have a dedicated screen number to specify the presence of one or more atoms of the element in the CT and/or as a SAF.

**Less Common Elements**

The **less common elements**, such as Ag, are specified by combining two generic screens with AND logic, one screen specifying the elements in a vertical group<sup>11</sup> from the periodic table and the other those in a horizontal series. These screens are listed in Tables II and III. Note that the frequency of occurrence cited for such an element is a maximum value, not an actual value, and is the lower of the frequencies for the two AND’ed screens. As a reminder, the frequency cited is followed by the abbreviation “max.”

<sup>11</sup> Group designations in the tables are those used in Europe, not the U.S.

---

**Rarest Elements**

The **rarest elements**, such as Ac, can be specified only via a generic screen for a periodic series. The frequency of occurrence cited for such an element is a maximum value, not an actual value, and is simply the frequency of occurrence of structures containing one or more atoms of any element in the series. Again, the frequency cited is followed by the abbreviation “max.”

---

**Very Common Elements**

The **very common elements**, such as Br in the examples above, can be specified as present in the connection table or as present as an SAF. Here, the screen for a count of 1 (“one or more”) is always a composite CT + SAF screen, while screens for counts of 2 or higher, in the column headed “**Element Count (CT Graph)**”, refer to atoms of the element present in the connection table graph itself.

The nine elements that most frequently occur as SAFs have dedicated screens specifying the presence of the element as an SAF. These screens are in the column headed “**Graph Modifier (SAF)**” and are provided for Br, Ca, Cl, H, I, K, N, Na, and O.

---

**Note**

Table I also provides screens for the specification of “halogen” in the CT graph. These screens, found under the generic halogen element symbol “X”, specify the total “or more” count of halogen atoms present in the CT, whether F, Cl, Br, or I.

---

**Table II**

Lists the generic EC/GM screens by category. These screens simply record the presence of one or more atoms of any of the cited elements, whether in CT or SAF. Two special generic screens should be mentioned:

- 1918 “metals” specifies the presence of any metal atom.
  - 2029 “SAFs” specifies the presence as a single atom fragment of any element except Br, Ca, Cl, H, I, K, N, Na, and O, the nine elements with specific SAF screens.
-

---

**Table III**

Lists the generic EC/GM screens in screen number order, and is provided for your convenience.

The GM “unusual features” screens are also quite easy to use, should they be needed. These screens describe the following:

- Unusual structural features: unusual mass, valence, or charge attributes of atoms in the graph of the connection table or the SAF portion of the structure
- Multicomponent substance data: the presence of 2-4 or more components and the presence of SAFs
- Chemical substance class identifiers

Classification of substances as:

- |                                     |                             |
|-------------------------------------|-----------------------------|
| – alloys                            | – multicomponent substances |
| – incompletely described substances | – polymers                  |
| – minerals                          | – radical ions              |
| – mixtures                          |                             |

with further subclassifications for incompletely described substances and polymers

A complete list of these screens is provided on the following page.

---

Special Purpose  
GM Screens

Screen	Description	Freq.
<b><u>Structural feature screens</u></b>		
2039	abnormal mass - all isotopic specifications	0.97%
2045	deuterium isotope	0.49%
2046	tritium and higher H isotopes (e.g., <sup>4</sup> H, <sup>5</sup> H, etc.)	0.06%
2047	isotope at unknown location (IUL)	0.05%
2041	abnormal valence	32.34%
2040	charge - all charges: fixed, tautomeric or delocalized	12.50%
2042	delocalized charge only	0.10%
2076	tautomer	39.88%
<b><u>Multicomponent substance screens</u></b>		
2127	2 or more components	18.61%
2077	3 or more components	7.24%
2078	4 or more components	4.55%
2079	single atom fragment (SAF)	6.69%
<b><u>Chemical substance class identifier screens</u></b>		
Note that these screens are not mutually exclusive. A substance may belong to as many classes as are appropriate.		
2050	alloy	3.22%
2082	CASREACT	14.04%
2049	coordination compound	8.16%
2048	incompletely defined (ID) substance	1.43%
2071	ID - unknown structure (ID molform)	0.21%
2072	ID - unknown point of attachment	0.99%
2073	ID - ester	0.14%
2074	ID - hydrogen (bond)	0.10%
2053	manual registration	221.62% <sup>12</sup>
2052	mineral	0.05%
2051	mixture (substance named as "mixt. with" in CA/CAPLUS)	0.29%
2043	polymer (general category)	4.18%
2067	homopolymers and copolymers [(A) <sub>x</sub> , (A.B) <sub>x</sub> , etc.]	3.20%
2068	polymers defined as structural repeating units (SRUs)	1.48%
2069	SRU with end groups [X-(-Y-) <sub>n</sub> -Z]	0.52%
2070	SRU without end groups [-(-Y-) <sub>n</sub> -]	1.00%
2054	radical ion	0.23%

<sup>12</sup> The value greater than 100% is due to sequence registrations. The percentage is based on the total number of structure connection tables.



# STN Substructure Search Query Development

---

## Introduction

Your substructure search query may be created using the structure drawing tools provided by STN. The factors usually considered in creating a structure query are:

- What is the basic substructure desired
- Whether an “open” (SSS) or “closed” (CSS) substructure search will retrieve the desired answers
- Will screens be necessary or desirable

The latter point may not be known until a SAMPLE search has been completed and results and Full File Projections analyzed. If screens (filters) are needed or desirable, they should be added as a separate set of L-numbers and then combined using Boolean operators (usually AND or NOT) with the structure L-number(s).

---

## Note

Structure L-numbers and screen L-numbers may not be enclosed within the same set of parentheses.

A detailed discussion with examples of adding screens to a query may be found in *A Guide to Adding Screens in STN Structure Searching*, available at [www.cas.org](http://www.cas.org).

---

## The SCREEN Command

The SCREEN command provides for the input of a single screen or a set of screens combined using Boolean operators (AND, OR). More complex screen combinations may be handled using the QUERY command.

- AND logic connects a set of screens to specify that all of the screens must be present.
- OR logic specifies that at least one of the screens must be present.

To use this command, at an arrow prompt (=>), enter “SCREEN” or “SCR” and the screen expression. The system assigns an L-number to the screen expression.

---

## AND and OR Operators

A screen expression consists of screen numbers, separated by AND or OR. When both AND and OR are used in a list of screen numbers, the AND is executed first. If no operators separate the screen numbers, AND is assumed. Parentheses and NOT logic are not allowed in the SCREEN command.

---

---

**NOT Operator**     Since the NOT operator is not allowed in the SCREEN command and your total screen expression requires parentheses or NOT logic, first use the SCREEN command to build several smaller sets of screen L-numbers. Then combine these L-numbers with the QUERY command. The QUERY command does allow parentheses and NOT logic.

---

**SCREEN Command Example**

```
=> SCREEN  
    ENTER SCREEN EXPRESSION OR (END): 2127 OR 2043  
    L2      SCREEN CREATED
```

```
=> S L1 NOT L2 SSS FULL  
(where L1 is a structure query)
```

---

**Query Command Example**

```
=> SCR 2043 AND 2077  
    L3      SCREEN CREATED
```

```
=> SCR 2078  
    L4      SCREEN CREATED
```

```
=> QUERY  
    ENTER LOGIC EXPRESSION OR (END): L3 NOT L4  
    L5      QUE L3 NOT L4
```

```
=> S L1 AND L5 FULL  
(where L1 is a structure query)
```

---

## Appendix I: Substructure Profile Development

---

**Introduction** STN structure searchers do not normally build screen-only structure queries. This appendix is presented to illustrate the techniques used in building screen-only structure queries in case such is desired.

---

**Initial Profiling Steps** Follow these steps:

1. Analyze the query to determine the basic structural components.
2. Develop an overall encoding strategy for the components.
3. Identify “key” structural fragments to encode the components.
4. Obtain the screen (fragment) numbers from the screen dictionary.
5. Develop the Boolean logic strategy to combine the selected screens using the SCREEN and QUERY commands.

---

**Screen Query Analysis** The analysis of the search question into its structural components is carried out to the extent that the structural fragments corresponding to each component can be connected in a simple Boolean expression (i.e., an un-nested expression formed without the use of parentheses to group sets). This is necessary because the SCREEN command provides only for the input of either a single screen (fragment) number or a series of screen numbers connected by Boolean operators in an un-nested expression. More complex logic expressions must be handled via the QUERY command.

---

**Screen Query Boolean Expressions** The Boolean expressions that are accepted by the SCREEN command are thus limited to the following, where ### is used to represent a screen number:

- **### AND ### ... AND ###**  
AND logic is used to connect a set of screens to specify that all of the screens must be present.
- **### ### ... ###**  
If no operator is present, AND logic is assumed.
- **### OR ### ... OR ###**  
OR logic is used to specify that at least one of the screens must be present.
- **### AND ### OR ### AND ### ... AND ### OR ### etc.**  
Alternative sets of screens may be specified via the SCREEN command, since the AND operator has priority over the OR operator. The screens connected with AND logic are grouped before the OR operator is applied, effectively resulting in (### AND ###) OR (### AND ### ... AND ###) OR ###, etc.

---

---

**Simple Query Strategy**

The encoding strategy for a simple query containing no structural variables is naturally also simple. Just select fragments, obtain screen numbers for the fragments, and combine the screens with AND logic.

---

**Uncommon Structural Features**

It might even be unnecessary to describe the entire query. If a portion of the structure being sought is very uncommon, encoding only that portion might provide sufficient specificity. Then you could simply browse through the retrieved substances to select those substances that meet the query specification and to review for possible interest those related substances containing the uncommon structural feature, but not meeting the full query specification.<sup>13</sup>

---

**Example**

For example, if a search query includes the substructure:



Three screens describe the C—C—C—N moiety:

914	BS	A	-3A	-1A	-3A	0.09%
1019	AA	C	-1C	-3C		1.00%
1243	AA	C	-1C	-3N		4.12%

The bond sequence screen specifying the chain triple–single–triple bond path is so selective that it fully defines the C—C—C—N moiety. The two AA screens can be omitted from the search. In addition, a test search on the BS screen alone may retrieve so few structures that it is not necessary to add screens to define the “R” portion of the query.

---

---

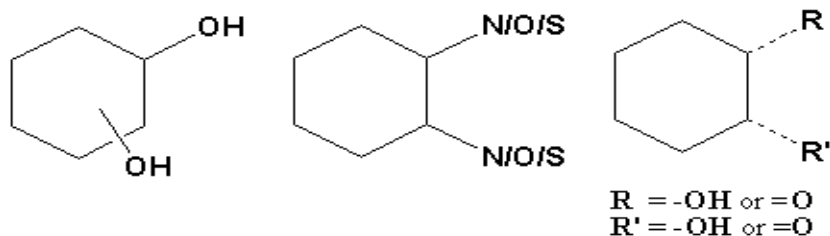
<sup>13</sup> This approach might decrease the precision of the search, but it does not affect the recall. If only a portion of the query structure is encoded and searched, the retrieved substances include any and all substances on file that contain the specified screens, so possible answers are never lost due to a partial specification of the query structure.

Note, however, that when a search query specifies alternatives for some portion of the substructure, you must describe either all of the alternatives in the encoded query or none at all. If some but not all of the alternatives are described in the encoded query, the result is likely to be missed answers and a loss of recall.

---

**Structural Variables**

Once structural variables are introduced into a search query, encoding strategies become more complex. A search query may specify alternatives for the graph (topology), nodes (element values), or bonds of the substructure being sought, as illustrated below with three queries for substituted cyclohexanes:



Alternative Graph

Alternative Nodes

Alternative Bonds

When a search query contains such variables, you are combining a number of searches for different substructures into a single search. This can often be done with little effort, and more complex queries can be created as you become more experienced. Only a few quite complex queries will need to be broken down and searched as multiple queries with less complex structural variables.

---

**Strategy Development**

The discussions that follow first consider how to develop overall encoding strategies for the three example queries shown earlier. After a discussion of “key” structural fragments, those structural fragments most important to a search query, the analysis of these three example queries continues.

---

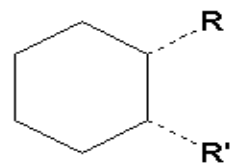
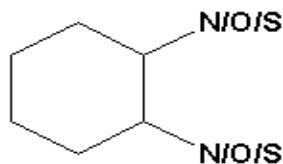
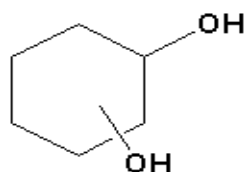
**“Fixed” and “Variable”**

When a search query specifies alternatives for the graph, nodes, or bonds of the substructure, the initial analysis of the query should break the substructure down into “fixed” and “variable” portions:

- The “**fixed**” portion(s) of the query *must always be present* and is in every relevant substance that is an answer to the query.
  - The “**variable**” portion(s) of the query describe sets of alternatives, and *one alternative from each set must always be present* in any substance that is an answer.
-

**Fixed and  
Variable  
Examples**

For the three example queries, the rings are assumed to be isolated cyclohexane rings (i.e., rings not part of a larger ring system). The fixed and variable portions of the queries are as follows:



$R = -OH \text{ or } =O$   
 $R' = -OH \text{ or } =O$

Alternative Graph

Fixed:

- cyclohexane ring
- two –OH groups on ring

Variable:

- position of –OH groups (1,2 1,3 or 1,4)

Alternative Nodes

Fixed:

- cyclohexane ring
- position of substituents
- single bonds to ring

Variable:

- N/O/S elements

Alternative Bonds

Fixed:

- cyclohexane ring
- two O's on ring in fixed positions

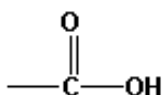
Variable:

- R & R' –OH or =O

---

**“Key”  
Structural  
Fragments**

“Key” structural fragments are the most specific fragments available in the screen dictionary to describe a substructure. These are the low-frequency screens. Since the screen dictionary is set up to allow encoding of a wide range of search queries, from very specific to very general, the screens likewise range from the specific to the general. The general screens are found with higher frequency in the substances present in the search file. For example, the following screens from the dictionary, listed in order of increasing specificity, can be used to encode a carboxylic acid group:



2005	EC	2	O				70.64%
1518	AA		C	—	O	— O	29.91%
1526	AA		C	—4	O	—4O	11.09%

- Screen 2005 simply specifies the presence of at least two oxygens.
- Screen 1518 is more precise, specifying the presence of at least one carbon atom having two oxygens attached by chain bonds of any value.
- Screen 1526 is the most precise, specifying the presence of at least one carbon atom attached to two oxygens by equalized chain bonds.

Clearly, the most precise screen for “carboxylic acid” is 1526. The other screens can be omitted, since these specifications are implied in the 1526 screen.

---

---

## Two Query Aspects

Most key structural fragments describing a query substructure can be identified by concentrating on two aspects of the query:

- Fully defined portions of the substructure: When bond values can be specified, useful low-frequency screens can often be found even for substructures that seem to be common, as shown by the AA screens listed below describing a carbocycle with an oxygen substituent:

1275	AA		C	*	C	-	O	45.33%	1135	AA		C	*	C	*	C	-	O	35.34%
1276	AA	2	C	*	C	-	O	23.50%	1136	AA	2	C	*	C	*	C	-	O	17.07%
1279	AA		C	*1	C	-1	O	10.84%	1138	AA		C	*1	C	*1	C	-1	O	8.84%
1280	AA	2	C	*1	C	-1	O	4.74%	1139	AA		C	*1	C	*1	C	-2	O	5.34%
1281	AA	3	C	*1	C	-1	O	2.71%	1140	AA	2	C	*1	C	*2	C	-2	O	1.31%
1282	AA	4	C	*1	C	-1	O	1.93%	1142	AA	2	C	*1	C	*2	C	-1	O	1.32%
1283	AA		C	*1	C	-2	O	16.45%											
1286	AA		C	*2	C	-1	O	1.67%											
1290	AA		C	*4	C	-1	O	25.19%											
1291	AA	2	C	*4	C	-1	O	10.71%											
1292	AA	3	C	*4	C	-1	O	3.45%											
1293	AA	4	C	*4	C	-1	O	1.58%											

- “Unusual” portions of the substructure containing several heteroatoms, uncommon elements, several multiple bonds, uncommon ring sizes (rings of 3, 4, 7, 8, or more atoms), or large polycyclic ring systems

Anything unusual is likely to be of low frequency and thus useful, even if the feature can only be described by a generic (but still uncommon) screen.

---

## Using Low-Frequency Screens

The screen dictionary has been designed, by a careful selection of the screens that are provided, to assist you in defining a search query with low-frequency screens wherever possible.

A look at the AA screen section, for example, shows almost 1000 screens with carbon as the central atom. Most of these screens include one or more heteroatoms among the attached atoms, and most have bond values specified.

Carbon is the most common element in a file of organic substances, and this depth of detail is necessary to get screens specific enough to be useful. Phosphorus, on the other hand, is relatively uncommon in the file substances, and only a few more than 50 AA screens have it as their central atom, with bonds specified for only a few. The most common of these generic screens has a frequency of only 6.30%, and most of them have frequencies under 2.00%.

---



---

**Most Precise Screens**

In general, augmented atom (AA) and atom sequence (AS) screens are the most precise screens. Effective screen profiles can be developed using only these two types of screens. You can concentrate on AA and AS fragments that contain several heteroatoms or unusual bonding patterns, initially looking at larger fragments and longer sequences. The fragments most likely to give useful screens include the following:

- AA fragments with carbon as a central atom and several attached heteroatoms
  - AA fragments with carbon as a central atom and an attached heteroatom, where bond values can be specified
  - AA fragments with a central heteroatom
  - AA fragments with carbon as a central atom and three or four attached atoms (describing a ring fusion point or bridgehead atom, a ring atom with one or two acyclic substituents, or a chain branch point)
  - AS sequences containing several heteroatoms
  - AS sequences containing both ring and chain bonds (describing a chain–ring–chain or ring–chain–ring path)
- 

**Larger Structure Fragments**

If the larger fragments and longer sequences cannot be found in the screen dictionary, you can break them down into smaller and more generic fragments and sequences:

- Large and specific AA fragments can be made smaller by specifying fewer attached atoms (removing carbon atoms first, then heteroatoms), and more generic by removing bond value specifications and, if necessary, bond type specifications.
  - Specific 6-atom AS sequences used to cover a path through the substructure can be made smaller simply by covering the path with 4- and 5-atom sequences, and more generic by removing the bond type specifications.
- 

**Other Screens**

The other types of screens are less generally useful but can provide good selectivity when they are applicable. These screens and their uses, along with some cautionary notes, are illustrated in the following sections.

---

---

**HA and TW Screens**

Hydrogen augmented atom (HA) and twin augmented atom (TW) screens are useful when the presence of hydrogen on an atom must be specified. The selection of screens is a bit limited:

- Most HA screens have C, N, or O as their central atom, with only very generic screens available for other central heteroatoms.
  - TW screens have carbon central atoms and C, N, O, or S as the attached atom with hydrogen specified.
- 

**HA and TW Limitations**

Several limitations on the use of HA and TW screens should be noted:

- The hydrogen specifications in these screens are exact counts of the number of attached hydrogens, not “or more” counts.
  - The HA and TW screens present in the screen dictionary completely describe the central atoms and may have no additional attachments beyond those shown in the screen definitions.
  - HA and TW screens cannot be used to specify the presence of hydrogen on nitrogen or chalcogen (O, S, Se, or Te) atoms involved in tautomeric situations.
- 

**TR Screens**

Type of ring (TR) screens are primarily useful when describing the following:

- Isolated rings or systems that are large polycyclic ring systems
  - Rings with 3, 4, 7, 8, or more nodes, or spiro systems
  - When describing structures that contain several isolated 6-membered rings
- 

**D and T Symbols**

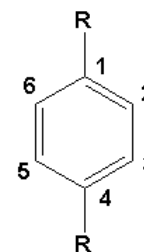
The D and T symbols are used to encode TR definitions and are exact specifications. You must be cautious when using TR screens to encode queries where the ring systems are allowed to have additional rings fused to them or to have bridges, for example, when a ring system in a query may be part of a larger system (e.g., a substituted benzene ring is described, but a properly substituted naphthalene or other polycyclic system is acceptable).

---

---

**TR Limitation** TR screens are not used to describe the ring unless all of the possible TR screens are used and grouped with OR logic. For a query specifying a 1,4-disubstituted benzene ring, six TR screens are needed.

<u>fusion points</u>					
	1867	TR	DDDDDD	64.12%	none
OR	1874	TR	DDDDTT	31.00%	2,3 or 5,6
OR	1878	TR	DDDTDT	1.04%	2,6 or 3,5
OR	1883	TR	DDTDDT	0.53%	2,5 or 3,6
OR	1884	TR	DDTDTT	0.64%	2,3,5 or 2,3,6 or 2,5,6 or 3,5,6
OR	1889	TR	DTTDTT	3.09%	2,3,5,6



(Screens 1878, 1883, and 1884 retrieve structures containing benzene rings with large macrocycle bridges, structures that are unlikely but still possible.)

---

**RC Screens** Ring count (RC) screens are useful only for describing either structures containing five or more rings or very generic structures.

---

**BS Screens** Bond sequence (BS) screens are useful when the query structure contains chain–ring–chain or ring–chain–ring paths with specified bond values or paths containing multiple bonds.

Note that bond sequence definitions are exact and do not imply alternative bond specifications. Where tautomer or alternating bonds exist, \*4 and -4 bond symbols must be used in BS descriptions, not the usual \*1 and \*2 or -1 and -2 single and double bond symbols. You must use several BS screens, grouped with OR logic, to describe a bond path that might contain tautomeric or alternating bonds.<sup>14</sup>

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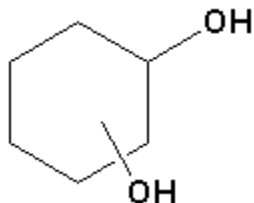
<sup>14</sup> Appendix II discusses the definition of tautomer and alternating bonds, how they are handled in the CAS REGISTRY, and how tautomer and alternating bonds must be considered when a search query is defined.

<b>CS Screens</b>	<p>Connectivity sequence (CS) screens are useful when the query structure contains chain–ring–chain or ring–chain–ring paths through atoms with known fixed connectivities.</p> <p>Since the connectivity values cited in these screens are exact non-hydrogen connectivities (not “or more” values), CS screens are not used to describe paths through atoms with uncertain connectivities (i.e., atoms where substitution is possible but not explicitly required) unless OR logic is used to group CS screens containing all possible combinations of connectivity values for such atoms.</p>
<b>GM Screens</b>	<p>The GM “unusual structural features” screens are useful when the query structure must contain a charge or an atom of abnormal mass. The GM “abnormal valence” screen is needed only when describing a substructure where the unusual valence is not implied by an AA screen (e.g., the screen is useful when searching for a structure containing a –ClO<sub>3</sub> perchloryl group, but not for one containing an –NO<sub>2</sub> nitro group, since the latter is adequately described by the screen AA N O O).</p> <p>The GM screens provide access to multicomponent substance data and chemical substance class identifiers. These are primarily useful for special-purpose searches.</p>
<b>EC Screens</b>	<p>The element count (EC) and graph modifier element (GME) screens are useful when the query structure contains metal atoms or single atom fragments (SAFs), or when the query structure is so loosely specified that only very generic screens can be used.</p>
<b>AC Screens</b>	<p>The atom count (AC) screens are useful only when the query structure is very generic and rather large.</p>

---

**First Example**

Going back to the first of the three examples under discussion, the alternative graphs query, the analysis of the query proceeds as follows:



Fixed: – cyclohexane ring  
– two –OH groups on ring

Variable: – position of –OH groups  
(1,2 1,3 or 1,4)

- The “key” features are the two –OH groups, and these can be described by three screens. Although the third screen (1136) probably adds little selectivity over that provided by the second (1280), there is no reason not to include it with the AND’ed set of screens once it has been selected. The number of screens in the AND’ed set does not affect the performance of the search.<sup>15</sup>

1701	HA	2	O H -1 C	7.80%	
1280	AA	2	C *1 C -1 O	4.74%	Set A
1136	AA	2	C * C * C - O	17.07%	

- Only two screens are available to describe the isolated cyclohexane ring, and only one is somewhat selective:<sup>16</sup>

985	AA	6	C *1 C *1 C	12.75%	Set A
1867	TR		DDDDDD	64.12%	cont.

- For the variable portion of the structure, three AS screens can be used:

496	AS	O - C * C - O #	7.98%	
482	AS	O - C * C * C - O #	6.67%	Set B
470	AS	O - C * C * C * C - O #	7.27%	

---

*Continued on next page*

---

<sup>15</sup> Note, though, that this is not true for screen sets grouped with OR logic, nor should it be taken to mean that redundant screens (e.g., EC 6 C for the query under discussion) should ever be included in a search specification.

<sup>16</sup> An experienced searcher would be aware that many structures contain isolated benzene and pyridine rings. These common rings lead to the high frequency of the TR DDDDDD screens. The combination of 985 and 1867 is useful in specifying an isolated cyclohexane ring.

## First Example (continued)

When the search is performed, the “fixed” screens are combined in one set with AND logic and the “variable” screens are combined in another set with OR logic.

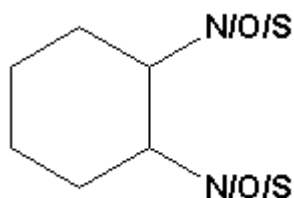
Set A: 1701 AND 1136 AND 1280 AND 985 AND 1867

Set B: 496 OR 482 OR 470

Query: A AND B

## Second Example

For the second of the three examples, the alternative bonds query, the analysis of the query proceeds as follows:



Fixed:

- cyclohexane ring
- position of substituents
- bonds are ring single

Variable: – substituent elements

- The “key” features are the N/O/S substituents. Although they are in the variable portion of the structure, their positions are fixed so that a set of three AS screens, to be combined with OR logic, can be used:

496	AS	O - C *	C - O #	7.98%	Set A
496	AS	O - C *	C - S #	7.98%	
403	AS	O - C *	C - N #	6.11%	
496	AS	S - C *	C - S #	7.98%	
403	AS	S - C *	C - N #	6.11%	
386	AS	N - C *	C - N #	1.42%	

- Two screens are available to describe the isolated cyclohexane ring:

985	AA	6	C *1 C *1 C	12.75%	Set B
1867	TR		DDDDDD	64.12%	

When the search is performed, the “fixed” screens are combined in one set with AND logic and the “variable” screens in another with OR logic, as follows:

Set A: 496 OR 403 OR 386

Set B: 985 AND 1867

Query: A AND B

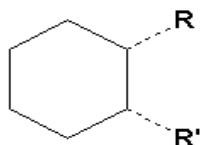
**Second  
Example  
Precision**

If the description of the variable portion of the structure is not selective enough, you can add AA screens describing the ring atoms. This makes the search logic more complex since all six alternative structures must be described:

	496	AS	O - C * C - O #	7.98%	Set C
AND	1136	AA 2	C * C * C - O	17.07%	
	496	AS	O - C * C - S #	7.98%	Set D
AND	1135	AA	C * C * C - O	35.34%	
AND	1158	AA	C * C * C - S	7.91%	
	403	AS	O - C * C - N #	6.11%	Set E
AND	1135	AA	C * C * C - O	35.34%	
AND	1097	AA	C * C * C - N	28.97%	
	496	AS	S - C * C - S #	7.98%	Set F
AND	1159	AA 2	C * C * C - S	1.93%	
	403	AS	S - C * C - N #	6.11%	Set G
AND	1158	AA	C * C * C - S	7.91%	
AND	1097	AA	C * C * C - N	28.97%	
	386	AS	N - C * C - N #	1.42%	Set H
AND	1098	AA 2	C * C * C - N	10.75%	

Query: B AND (C OR D OR E OR F OR G OR H)

**Third Example** For the last of the three examples, the alternative nodes query, the analysis of the query proceeds as follows:



R = -OH or =O  
R' = -OH or =O

Fixed:    – cyclohexane ring  
          – two O's on ring in fixed position

Variable: – R & R' -OH or =O

- The “key” features are the R and R' substituents. They are in the variable portion of the structure. Since two oxygen atoms will always be attached to the ring, two generic screens (specifying bond types but not bond values) describing the O-ring substitution will always be present, whether the R and R' groups are -OH or =O:

1136	AA	2	C * C * C - O	17.07%	Set A
496	AS		O - C * C - O #	7.98%	

- Three sets of screens are needed to describe the three possible combinations of -OH and =O substituents:

1701	HA	2	O H -1 C	7.80%	Set B
1280	AA	2	C *1 C -1 O	4.74%	
885	BS		A -1 A *1 A -1 A	23.45%	

1700	HA		O H -1 C	20.14%	Set C
1138	AA		C *1 C *1 C -1 O	8.84%	
1139	AA		C *1 C *1 C -2 O	5.34%	
886	BS		A -1 A *1 A -2 A	14.04%	

1140	AA	2	C *1 C *1 C -2 O	1.31%	Set D
891	BS		A -2 A *1 A -2 A	1.95%	

- Two screens are available to describe the isolated cyclohexane ring:

985	AA	6	C *1 C *1 C	12.75%	Set A
1867	TR		DDDDDD	64.12%	

When the search is performed, the set groupings and logic are as shown:

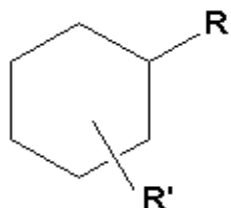
Set A: 1136 AND 496 AND 985 AND 1867  
Set B: 1701 AND 1280 AND 885                   -OH and -OH  
Set C: 1700 AND 1138 AND 1139 AND 886       -OH and =O  
Set D: 1140 AND 891                               =O and =O  
Query: A AND (B OR C OR D)



---

**Too Generic  
Query**

As an example of what might happen when a search query becomes so generic that it begins to present problems, consider the following query describing an isolated cyclohexane ring with two substituents, where the graph, nodes and bonds are all variable:



$R = -OH \text{ or } =O \text{ or } -SH \text{ or } =S \text{ or } -NH_2 \text{ or } =NH$   
 $R' = -OH \text{ or } =O \text{ or } -SH \text{ or } =S \text{ or } -NH_2 \text{ or } =NH$

Although this query might seem rather simple, it describes 54 different structures. There are three different substitution positions (1-2, 1-3, and 1-4), and 18 combinations of R and R' (six combinations of R and R' considering just the elements involved, and three combinations of R-ring and R'-ring bonding), for a total of  $3 \times 18 = 54$  possibilities. Since a search query explicitly describing all of these possibilities is obviously too complex to be practical, an easier, though less specific, approach needs to be developed.

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**Generic  
Strategy  
Development**

As before, two screens describe the isolated cyclohexane ring:

	985	AA	6	C *1 C *1 C	12.75%	Set A
AND	1867	TR		DDDDDD	64.12%	

For this query, AS screens are the key screens, since they allow the specification of both the R and R' elements and the substitution positions to be combined in a single set of screens.

A check of the screen dictionary shows that only nine different AS screens are needed. There are 18 (6 x 3) different combinations of R and R' elements and substitution positions, since the screens for combinations of O and S atoms on the ring share screen numbers. Using "O/S" to represent the generic atoms in the AS screens specifying either O or S atoms, these screens are the following:

	496	AS	O/S	-	C	*	C	-	O/S	#	7.98%				
OR	403	AS	O/S	-	C	*	C	-	N	#	6.11%				
OR	386	AS	N	-	C	*	C	-	N		1.42%				
OR	482	AS	O/S	-	C	*	C	*	C	-	O/S	#	6.67%		
OR	375	AS	O/S	-	C	*	C	*	C	-	N	#	4.45%	Set B	
OR	361	AS	N	-	C	*	C	*	C	-	N		1.84%		
OR	470	AS	O/S	-	C	*	C	*	C	*	C	-	O/S	#	7.27%
OR	348	AS	O/S	-	C	*	C	*	C	*	C	-	N	#	5.24%
OR	342	AS	N	-	C	*	C	*	C	*	C	-	N		2.33%

These nine screens are OR'ed together in one set to specify the ring substitution patterns.

---

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**Substituent Screens**

A third set of screens can be set up to describe the possibilities for the R and R' substituents. Describing the 18 different combinations of R and R' is not practical, since this requires 18 sets of screens, each containing 2-4 screens. Instead, the description specifies only the six different possibilities for one substituent. This can be done with one set of six screens OR'ed together. The screen set is as follows:

1700	HA	O H -1 C	20.14%	
OR 1139	AA	C *1 C *1 C -2 O	5.34%	
OR 1771	HA	S H -1 C	0.85%	Set C
OR 1162	AA	C *1 C *1 C -2 S #	0.44%	
OR 1568	HA	N H2 -1 C	7.57%	
OR 1255	HA	N H -2 C	4.33%	

A look at the frequencies with which these screens occur shows that the set of nine screens OR'ed together adds almost no specificity to the search. Since the substitution positions have been fairly well specified by the set of AS screens, the set of BS screens adds little more to the search than the specification of substituent-ring bonds.

---

**Splitting a Query**

A better approach for this query is to split the query into several simpler queries. An inspection of the frequencies for the set of screens that describe the substituents shows that the screens for the oxygen substituents –OH and =O are much less specific than the screens for the S and N substituents. The search query can, therefore, be divided into two queries, one searching for two O substituents (R and R' are limited to –OH and =O) and one searching for at least one S or N substituent. If recall and precision for either search remain unsatisfactory, the two queries could be divided still further. The first could be split into three queries, each looking for a particular combination of –OH and =O substituents, while the second could be split into two queries, one looking for one O substituent and one S or N substituent, the other for two S or N substituents.

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**NOT Logic**

The final aspect of substructure search profile development to be considered is the use of NOT logic, whereby you can specify a screen or set of screens that should ***not*** appear in any structure that is an answer to the search. *While this ability can be very useful, it can also be very harmful if misused, causing you to miss legitimate answers to the search query.*

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**NOT Logic Can Be Harmful**

The potential for harm arises because a substance is not included as an answer if it contains the specified fragment(s) anywhere in its structure, not just in the portion of the structure defined by the screens grouped by AND and OR logic that describe the substructure sought by the query. If you are looking for nitroso compounds, for example, use the screen for C–N=O:

1642    AA    N -1 C -2 O                    5.21%    Set A

as a key screen, and you will find that most of the retrieved answers contain nitro groups, not nitroso groups. If you used NOT logic to specify that no answer should contain screen 1680, the key screen for a nitro group.

1680    AA    N       O       O                    5.54%    Set B

By specifying A NOT B in the search logic, the number of answers retrieved by the search decreases to much less than before. However, the NOT logic rejects legitimate answers along with the undesired structures that did not contain nitroso groups, since *all* structures containing a nitro group are rejected, *including those structures that contained both a nitro and a nitroso group*.

---

**Safely Using NOT Logic**

NOT logic can safely be used when you indeed want to exclude any structure containing an undesired fragment or set of fragments. A query for polycyclic hydrocarbons, for example, shows the proper use of NOT logic, since you are not interested in any structure containing elements other than C and H. The query is then described as follows:

	1942	EC	4	C	90.13%	Set A
AND	1839	RC	2		62.14%	
	1918	"metals"			14.51%	
OR	1925	group Vb	(As Bi P Sb)		6.96%	
OR	2003		(O S)		81.49%	
OR	2019		(Po Se Te)		0.63%	
OR	1929	group VIIb	(At Br Cl F I)		29.63%	Set B
OR	1924	group 0	(Ar He Kr Ne Rn Xe)		0.01%	
OR	1932	EC	B		1.02%	
OR	1992	EC	N		62.13%	
OR	2026	EC	Si		2.63%	

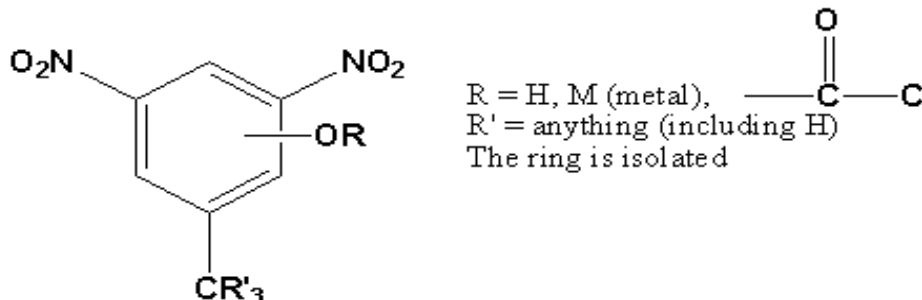
Search logic: A NOT B

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## Example of Substructure Search Profile Development

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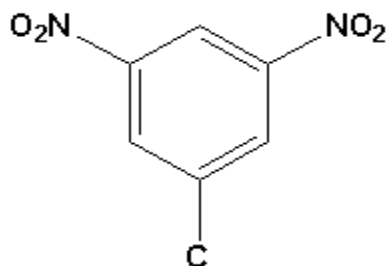
**Search Query** The steps in the development of a profile can be illustrated by using the following query:



This query, as with most substructure queries, has structural variables: the position of the –OR group and the value of R. The strategy for this query will consider both the “fixed” portion and the “variable” portion of the structure when deriving the components and their Boolean logic relationship.

---

**Query “Fixed” Portion** Every relevant substance that is an answer to the query must contain the “fixed” portion of the structure:



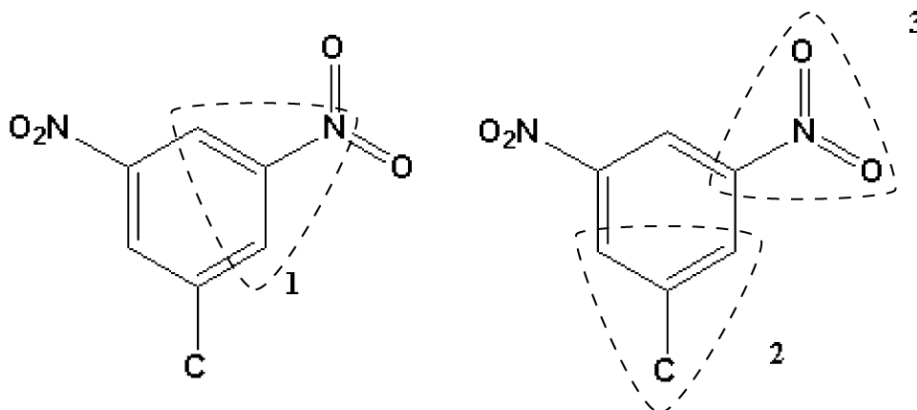
The discussion that follows describes in detail how this structure is analyzed in terms of augmented atom and linear sequence fragments and how these fragments are, in turn, analyzed in terms of search screens present in the dictionary.

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**“Fixed” Portion Analysis**

To begin the analysis of the “fixed” portion of the structure, select the best augmented atom fragments available: the substituted ring atoms and the nitrogens of the nitro groups. The AA fragments are as shown:



(1) C \*4 C \*4 C -1 N  
(2) C \*4 C \*4 C -1 C  
(3) N -1 C -2 O -2 O

Since the benzene ring is a very common ring, there is no need to describe it via AA fragments beyond that implicit in the C \*4 C \*4 C sections of fragments (1) and (2).

---

**Screen Dictionary Fragments**

Locate each of these fragments in the screen dictionary:

1121	AA	2	C	*4	C	*4	C	-1	N	8.53%	(1)
1044	AA		C	*4	C	*4	C	-1	C	53.13%	(2)
1642	AA		N	-1	C	-2	O			5.21%	(3)
1681	AA	2	N		O		O			1.28%	

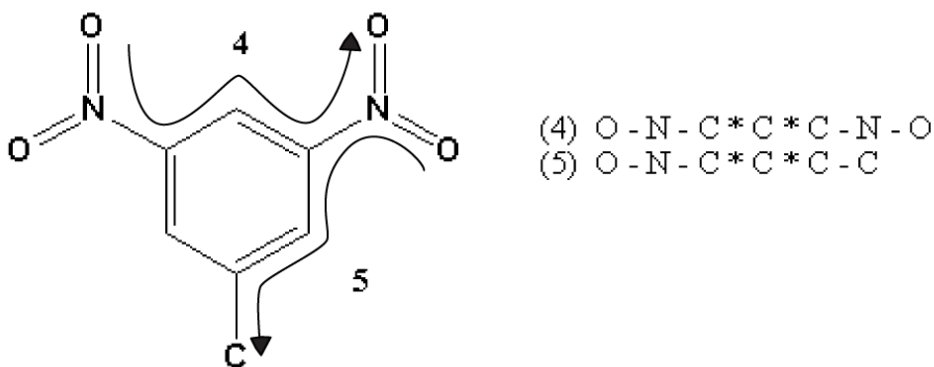
The first two fragments are exactly matched by screens in the dictionary, even the desired number of occurrences of fragment (1). The second screen, though, is quite common and does not add any significant specificity to the search. Fragment (3) describing the nitro groups cannot be found as is, but is adequately handled by two screens, the first describing a C–N=O substructure and the second effectively describing two nitro groups.

---

---

**Atom Sequence  
Fragments**

Continue the analysis of the “fixed” portion of the structure by selecting the best atom sequence fragments available: the atom sequences between the two nitro groups and between either nitro group and the carbon substituent. The AS fragments are as shown:



Locate each of these fragments in the screen dictionary:

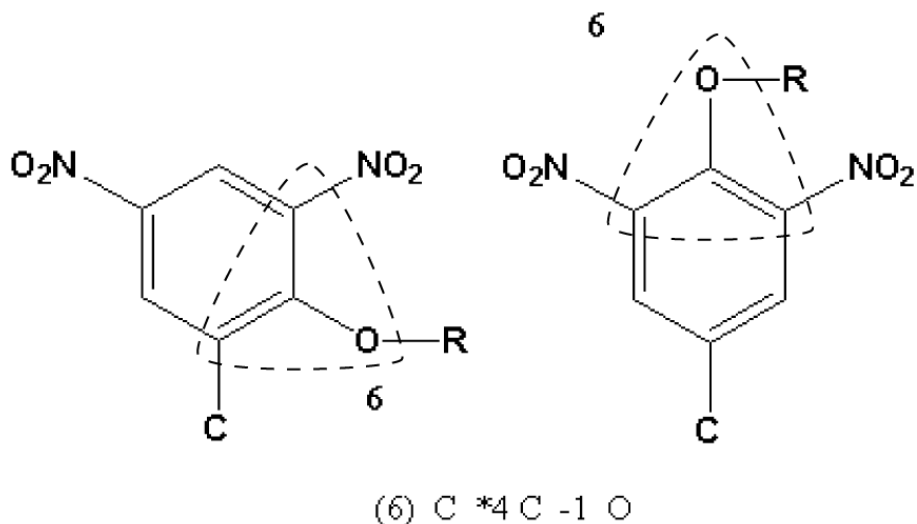
367	AS	O	-	N	-	C	*	C	*	C	-	N	1.02%	(4)
71	AS	C	-	C	*	C	*	C	-	N	-	O	1.36%	(5)

The first fragment is a symmetrical seven atom sequence, and the screen citing six of these atoms is the best available – the screen dictionary only describes sequences of 4, 5, or 6 atoms. The second fragment of six atoms is exactly matched by a screen.

---

**“Variable”  
Portion  
Analysis**

Begin the analysis of the “variable” portion of the structure by selecting the best augmented atom fragments available that describe the substitution of the –OR group on the ring. Note that either substitution position results in the same augmented atom:



Locate the fragment in the screen dictionary:

1290	AA	C	*	4	C	-1	O	25.19%	(6)
------	----	---	---	---	---	----	---	--------	-----

Although not an exact match, the screen is adequate for describing the –OR substitution on a benzene ring. Check at a more generic level without the specification of bond values, and you will find another screen to describe the fragment:

1135	AA	C	*	C	*	C	-	O	35.34%
------	----	---	---	---	---	---	---	---	--------

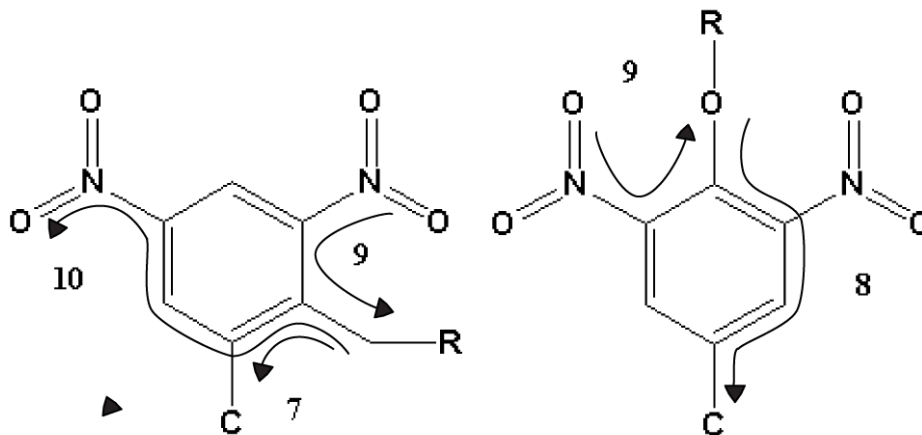
The screen is common enough, though (35.34% frequency), that it likely does not provide any additional specificity to the search.



---

**Atom Sequence  
Fragments**

Continue the analysis of the “variable” portion of the structure by selecting the atom sequence fragments that describe the substitution of the –OR group on the ring. Note that the two substitution positions result in two quite different atom sequences between the carbon substituent and the –OR group, but the same atom sequence between either nitro group and the –OR group:



- (7) O - C \* C - C  
(8) O - C \* C \* C \* C - C  
(9) O - N - C \* C - O  
(10) O - C \* C \* C \* C - N - O

Locate the fragments in the screen dictionary:

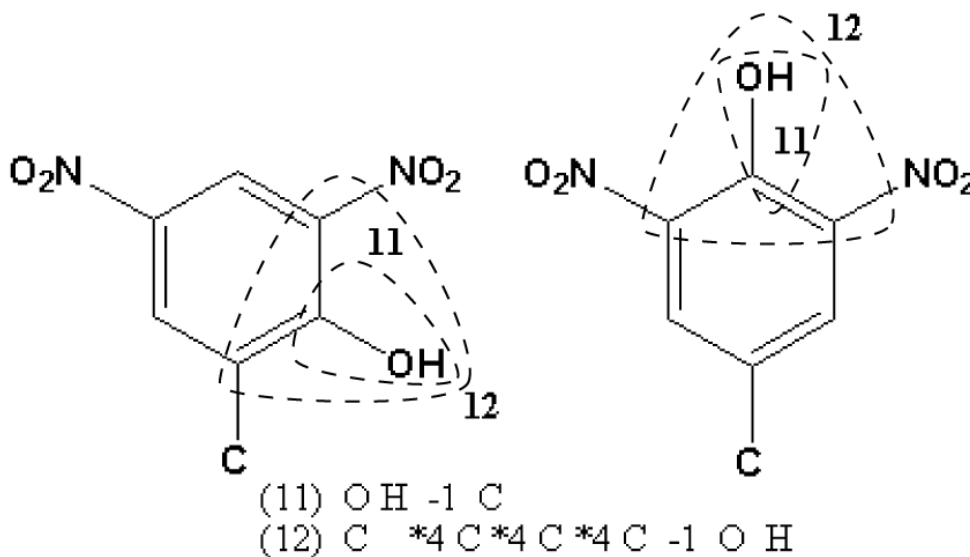
119	AS	O - C * C - C	15.43%	(7)
41	AS	O - C * C * C * C - C	15.40%	(8)
490	AS	O - N - C * C - O	1.17%	(9)
348	AS	O - C * C * C * C - N	4.48%	(10)

The first three sequences are exactly matched by dictionary screens, and a 6-atom screen describes the last sequence. Note that the 490 screen is included in the “fixed” portion of the query, since that sequence is always present in the structure. The “variable” portion of the structure here is described by (119 AND 348) OR (41).

---

**Further  
“Variable”  
Portion  
Analysis**

Continue the analysis of the “variable” portion of the structure by selecting fragments that describe the different possibilities for the –OR group. For the case of R = H, giving an –OH substituent, HA and TW fragments are the obvious choice:



Both screens are present in the dictionary:

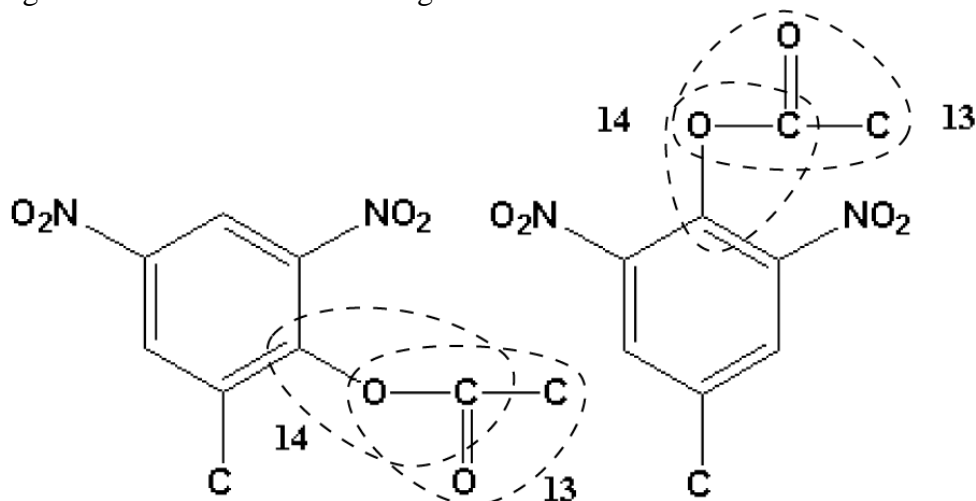
1700	HA	O H -1 C	18.20%	(11)
1832	TW	C *4 C *4 C -1 O H	5.72%	(12)

Since the more specific TW screen “contains” the HA screen, the HA screen is ignored.

---

**Second Case**

For the second case where  $R = -C(=O)-C$ , giving an  $-O-C(=O)-C$  ester linkage substituent, both AA and AS fragments are considered. Two AA fragments describe the ester linkage:



(13) C -1 C -1 O -2 O  
(14) O -1 C -1 C

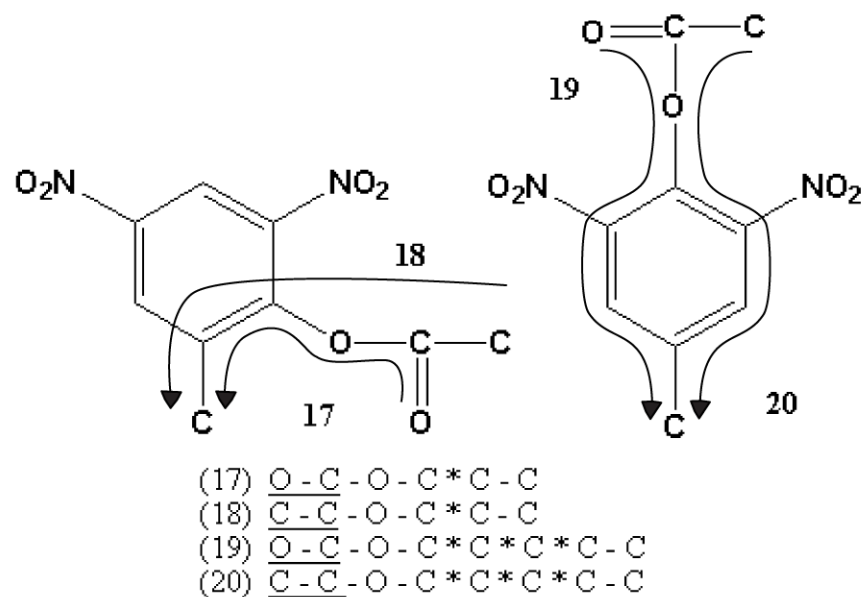
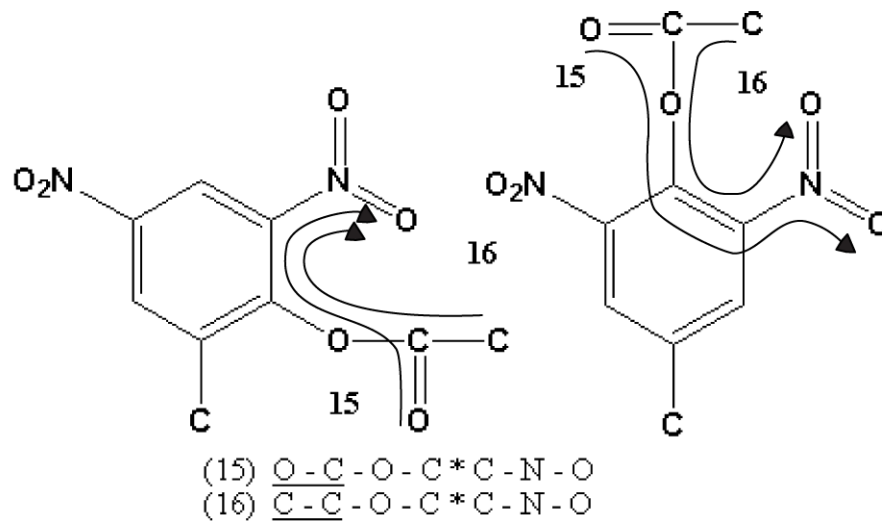
Both AA screens are present in the dictionary, the O - C - C screen being effectively equivalent to the O -1 C -1 C screen sought; neither screen is very selective.

1199	AA	C	-1	C	-1	O	-2	O	43.86%	(13)
1707	AA	O	-	C	-	C			38.39%	(14)

---

## AS Fragments

Continuing with this case, select the AS fragments, first those sequences between the  $-\text{O}-\text{C}(=\text{O})-\text{C}$  substituent and a nitro group, then those between the  $-\text{O}-\text{C}(=\text{O})-\text{C}$  substituent and the  $-\text{C}$  substituent:



---

**Selected AS  
Screens**

Since AS screens have already been selected to describe the  $\text{--OR}$  group, screens selected here do include one or more atoms of the  $\text{--C(=O)--C}$  substructure, shown underlined above. As before, the two substituent positions result in two quite different atom sequences between the carbon substituent and the  $\text{--O--C(=O)--C}$  group, but the same atom sequence between either nitro group and the  $\text{--O--C(=O)--C}$  group. Checking the dictionary results in the following screens:

409	AS	O	-	C	-	O	-	C	*	C	-	N	0.36%	(15)
271	AS	C	-	O	-	C	*	C	-	N	-	O	0.42%	(15 & 16)
183	AS	C	-	C	-	O	-	C	*	C			14.37%	(16, 18 & 20)
123	AS	C	-	O	-	C	*	C	-	C			6.93%	(17 & 18)
193	AS	O	-	C	-	O	-	C	*	C			4.71%	(17 & 19)

Screen 123 is specific to one position of substitution of the  $\text{--O--C(=O)--C}$  group and is omitted; the other four screens are applicable for either position of substitution.

---

**Third case:  
R = Metal**

For the third case, where R = (metal), the screen is simply the generic “metals” screen 1918.

1918 GM	“metals”	14.84%	(15)
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**SAMPLE  
Screen Profile**

A sample screen profile for the query, showing the various components, the screens selected to encode the components, and the Boolean logic used to group the screens is shown here. Since there are many highly selective screens available, the less selective screens with frequencies above 20% are omitted.

	1121	AA	2	C	*4	C	*4	C	-1	N		8.53%				
AND	1642	AA		N	-1	C	-2	O				5.21%				
AND	1681	AA	2	N		O		O				1.28%				
AND	367	AS		O	-	N	-	C	*	C	*	C	-	N	1.02%	Set A
AND	71	AS		C	-	C	*	C	*	C	-	N	-	O	1.36%	
AND	1290	AA		C	*4	C	-1	O							25.19%	
AND	490	AS		O	-	N	-	C	*	C	-	O			0.94%	
	119	AS		O	-	C	*	C	-	C					18.18%	Set B
AND	348	AS		O	-	C	*	C	*	C	*	C	-	N	5.24%	
	41	AS		O	-	C	*	C	*	C	*	C	-	C	19.86%	Set C
	1832	TW		C		*4	C	*4	C	-1	O	H			6.53%	Set D
	409	AS		N	-	C	*	C	-	O	-	C	-	O	0.36%	
AND	271	AS		C	-	O	-	C	*	C	-	N	-	O	0.42%	Set E
AND	183	AS		C	*	C	-	O	-	C	-	C			14.37%	
AND	193	AS			O	-	C	-	O	-	C	*	C		4.71%	
	1918	"metals"													14.84%	Set F

Screens 367, 71, and 490 are perhaps the most important screens for the query, since they are very precise ones. They retrieve a substance containing an aromatic ring with *meta* N substituents, with *meta* N and C substituents, and with *ortho* N and O substituents, respectively, and even make a partial specification for the presence of a nitro group.

---

**Structural Features**

The structural features described by these screen sets are as follows:

- Set A: The “fixed” portion of the query structure that must be present, regardless of the position of the –OR group or the nature of R
- Set B: The “variable” portion of the structure when the –OR group is attached to the ring between the carbon substituent and either nitro group
- Set C: The “variable” portion of the structure when the –OR group is attached to the ring between the two nitro groups
- Set D: The “variable” portion of the structure when the –OR group is –OH
- Set E: The “variable” portion of the structure when the –OR group is –O–C(=O)–C
- Set F: The “variable” portion of the structure when the –OR group is –O–(metal)

In the search query, group the sets as:

A AND ( B OR C ) AND ( D OR E OR F )

---

**Estimating Retrieval**

The maximum number of structures that the query will retrieve can be estimated by considering the frequencies of the search screens used and how they are grouped together. In a set of screens grouped with AND logic, the maximum retrieval is that of the most infrequent (i.e., most specific) screen, so the retrieval for the six screen sets considered individually is as follows:

Set A	Set B	Set C	Set D	Set E	Set F
0.94%	5.24%	19.84%	6.53%	0.42%	14.84%

For the full search query, the limiting factor is the most specific intermediate screen set. Here, the frequencies of sets OR’ed together is summed to maximize the retrieval for the intermediate “OR” set.

Search logic: A AND ( B OR C ) AND ( D OR E OR F )

Set A	Set (B OR C)	Set (D OR E OR F)	Search
0.94%	25.08%	21.79 %	0.94%

---

---

**Actual  
Retrieval**

The actual retrieval is somewhat lower than the maximum 0.94%, due to the coordination of a number of uncommon screens in set A. The actual retrieval of a search is usually only about half that estimated in this manner.

---

**Searching the  
Query**

Input the query profile in the STN structure search system by using the SCREEN command or STN Express or STN on the Web to describe the six screen sets and the QUERY command to describe the Boolean logic relationship between the sets.

```
=> FIL REG
=> SCREEN
ENTER SCREEN EXPRESSION OR (END):1121 AND 1642 AND 1681 AND
367 AND 71 AND 1290 AND 490
L1    SCREEN CREATED
=> SCR 119 AND 348
L2    SCREEN CREATED
=> SCR 41
L3    SCREEN CREATED
=> SCR 1832
L4    SCREEN CREATED
=> SCR 409 AND 271 AND 183 AND 193
L5    SCREEN CREATED
=> SCR 1918
L6    SCREEN CREATED
=> QUERY
ENTER LOGIC EXPRESSION OR (END):L1 AND (L2 OR L3) AND (L4 OR
L5 OR L6)
L7    QUE L1 AND (L2 OR L3) AND (L4 OR L5 OR L6)
```

You can now do a SAMPLE search to test the query, review results, and decide whether to search the full file or revise the query.

---

**“Typical”  
Search Query**

Based on the results of some developmental studies, the “typical” search query requires the input of 10-15 “good” screens to optimize the search precision. If a sample search shows that an excessive number of structures are likely to be retrieved by a full search, it may be desirable to extend the analysis of the query to derive additional search screens. For the example query, since all relevant AA and AS screens have been identified, bond and connectivity sequence (BS and CS) screens can be added.

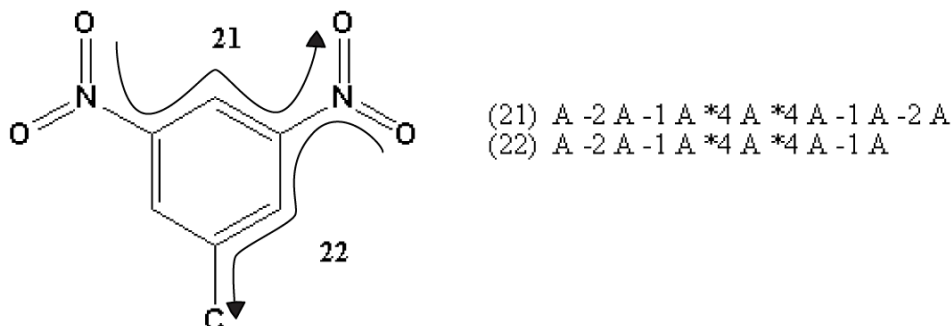
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**BS Screens**

Begin the analysis of the query to identify bond sequence (BS) screens by examining the “fixed” portion of the structure. Bond sequences between the two nitro groups and between either nitro group and the carbon substituent are as shown:



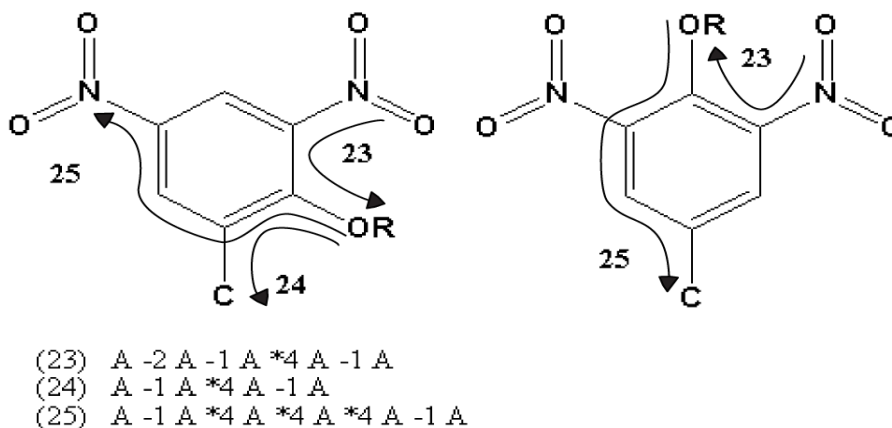
Since bond sequence screens describe sequences of 3-5 bonds, one BS screen describes both of these fragments:

882 BS A -2 A -1 A \*4 A \*4 A -1 A 7.58% (21 & 22)

---

**Further BS Screens**

Continue the analysis by selecting BS screens to describe the position of the -OR group on the ring. You will find three fragments:



Screens corresponding to all three fragments are found in the dictionary:

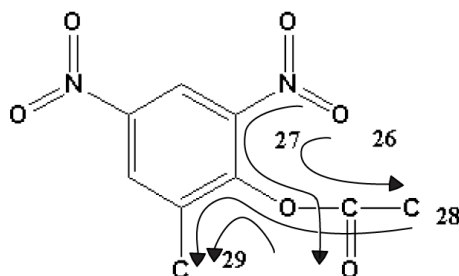
895	BS	A -2 A -1 A *4 A -1 A	7.01%	(23)
889	BS	A -1 A *4 A -1 A	24.67%	(24)
868	BS	A -1 A *4 A *4 A *4 A -1 A	35.57%	(25)

Of these three screens, only 895 is useful. Screen 889 is contained within 895, and 868 is probably too general to add any specificity to the search. Since screen 895 is present regardless of the position of the -OR group, add it to the set of “fixed” screens.

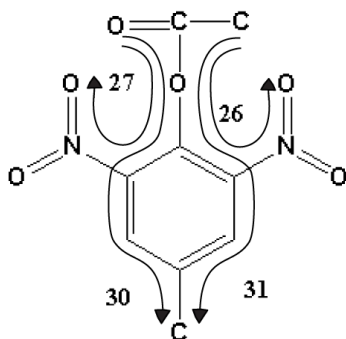
---

## Still More BS Screens

Continue the analysis of the “variable” portion of the structure continues by selecting BS fragments that describe the different possibilities for the –OR group. You will not find new fragments for the cases where R = H or metal. For the case where R = –C(=O)–C, giving an –O–C(=O)–C substituent, you will find six BS fragments, although the fragments are quite similar:



(26) A -2 A -1 A \*4 A -1 A -1 A -1 A  
 (27) A -2 A -1 A \*4 A -1 A -1 A -2 A  
 (28) A -1 A \*4 A \*4 A \*4 A -1 A  
 (29) A -1 A \*4 A \*4 A \*4 A -2 A



(30) A -1 A \*4 A \*4 A \*4 A -1 A -1 A -2 A  
 (31) A -1 A \*4 A \*4 A \*4 A -1 A -1 A -1 A

By checking the dictionary, you will find five screens describing these fragments:

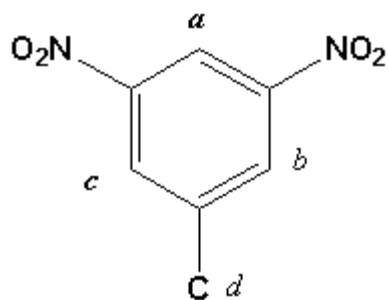
898	BS	A -2 A -1 A *4 A -1 A -1 A	4.41%	(26 & 27)
827	BS	A *4 A -1 A -1 A -1 A	32.93%	(26, 28 & 31)
828	BS	A *4 A -1 A -1 A -2 A	6.41%	(27, 29 & 30)
792	BS	A *4 A *4 A -1 A -1 A	50.44%	(30 & 31)
868	BS	A -1 A *4 A *4 A *4 A -1 A	35.57%	(30 & 31)

Of these screens, only the first three are present for both positions of the –O–C(=O)–C group, and only 898 and 828 are selective enough to be useful.

---

## CS Screens

The analysis of the query structure to identify connectivity sequence (CS) screens is more complex than the previous analyses. The difficulties arise from the specification of exact non-hydrogen connectivities in the CS screens, where a “2”, for example, stands for an atom with exactly two attachments, not an atom with two or more attachments. As a consequence, consider not only the query structure itself but also the possibility of substitution on the query structure. In the “fixed” portion of the query, there are four atoms with variable connectivity, as shown:



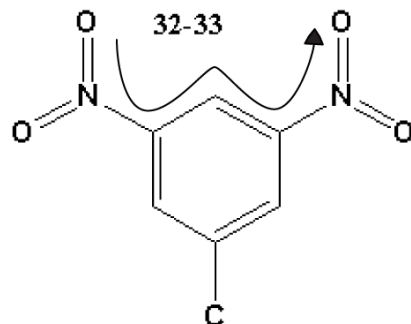
– atoms *a*, *b*, and *c* may have connectivities of either 2 or 3; at least one of these atoms will have a connectivity of 3 because of the presence of the –OR group

– atom *d* may have a connectivity of 1, 2, 3, or 4 due to its definition as –CR'<sub>3</sub>, where R' may be anything (including H)

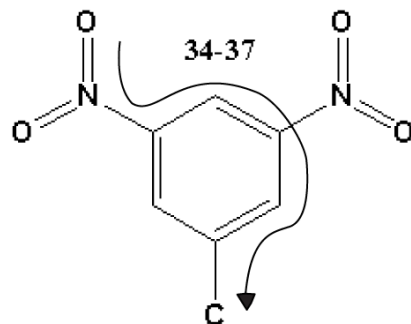
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## CS Screen Analysis

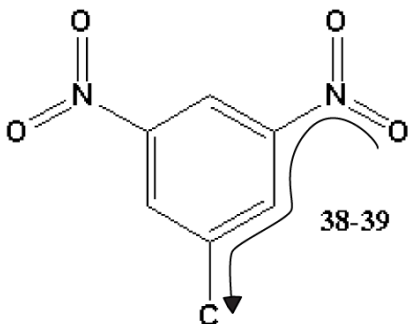
For the analysis of the structure for connectivity screens, consider three paths: the path from one nitro group to the other and the “long” and “short” paths from a nitro group to the ring atom bearing the carbon substituent.



(32) 1 - 3 - 3 \* 3 \* 3 - 3 - 1  
(33) 1 - 3 - 3 \* 2 \* 3 - 3 - 1



(34) 1 - 3 - 3 \* 2 \* 3 \* 3 \* 3  
(35) 1 - 3 - 3 \* 2 \* 3 \* 2 \* 3  
(36) 1 - 3 - 3 \* 3 \* 3 \* 2 \* 3  
(37) 1 - 3 - 3 \* 3 \* 3 \* 3 \* 3



(38) 1 - 3 - 3 \* 2 \* 3  
(39) 1 - 3 - 3 \* 3 \* 3

You will find only four CS screens to describe these paths:

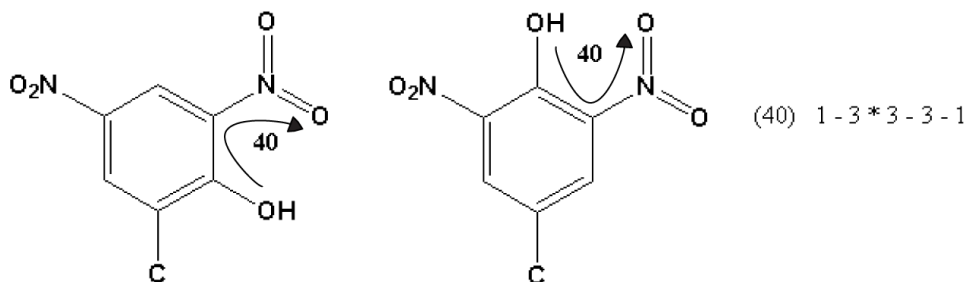
712	CS	3 - 3 * 3 * 3 - 3	2.35% (32)
700	CS	3 - 3 * 2 * 3 - 3	5.43% (33)
576	CS	1 - 3 - 3 * 3	18.41% (32, 36, 37 & 39)
571	CS	1 - 3 - 3 * 2 * 3	14.13% (33, 34, 35 & 38)

In the search profile, group these screens (712 OR 700) to describe the structure with or without a substituent on atom *a*, and (576 OR 571) to describe the structure with or without a substituent on atom *b* (or its equivalent, atom *c*).

---

**Further CS Screens**

Continue the analysis of the “variable” portion of the structure for connectivity sequence screens by selecting screens that describe the different possibilities for the –OR group. For the case of R = H, giving an –OH substituent, consider the path between the HO– and a nitro =O, since this path is independent of the position of the –OH group on the ring.



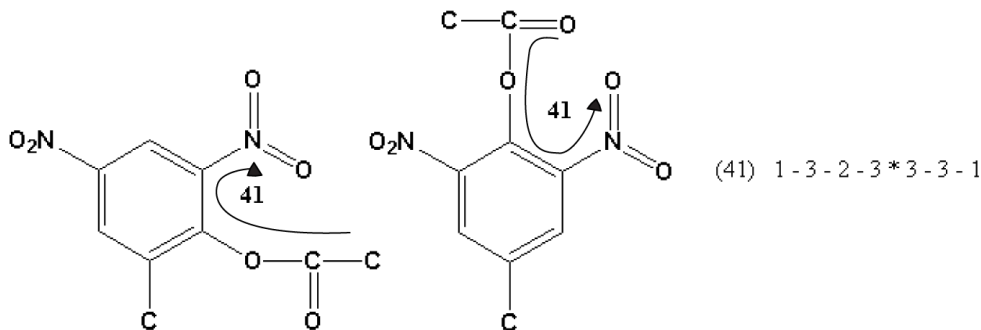
You will find two CS screens to describe this path:

575	CS	1 - 3 * 3 - 3	15.42%	(40)
576	CS	3 * 3 - 3 - 1	18.41%	(40)

---

**More CS Screens**

For the second case where R = –C(=O)–C, giving an –O–C(=O)–C ester linkage substituent, consider the path between the carbonyl =O and a nitro =O, since this path is independent of the position of the group on the ring.



You will find three CS screens to describe this path:

556	CS	1 - 3 - 2 - 3 * 3	10.21%	(41)
576	CS	3 * 3 - 3 - 1	18.41%	(41)
657	CS	2 - 3 * 3 - 3	10.72%	(41)

---

**CS Screens for Metals**

For the third case, where R = (metal), you do not need to find CS screens. This eliminates the need to check structuring conventions to determine how the O–metal bond is described.

---

## Refining the Query

Group the new BS and CS screens to describe structural features in the same fashion as in the previous examples.

- Set AA: The “fixed” portion of the query structure that must be present:

882	BS	A	-2	A	-1	A	*4	A	*4	A	-1	A	7.58%
AND	895	BS	A	-2	A	-1	A	*4	A	-1	A		7.01%

- Set BB: The “variable” portion when the –OR group is attached to the ring between the carbon substituent and either nitro group:

*no new screens*

- Set CC: The “variable” portion when the –OR group is attached to the ring between the two nitro groups:

*no new screens*

- Set DD: The “variable” portion when the –OR group is –OH:

575	CS	1	-	3	*	3	-	3	15.42%	
AND	576	CS	3	*	3	-	3	-	1	18.41%

- Set EE: The “variable” portion when the –OR group is –O–C(=O)–C:

898	BS	A	-2	A	-1	A	*4	A	-1	A	-1	A	4.41%
AND	828	BS	A	*4	A	-1	A	-1	A	-2	A		6.41%
AND	556	CS	1	-	3	-	2	-	3	*	3		10.21%
AND	576	CS	3	*	3	-	3	-	1				18.41%
AND	657	CS	2	-	3	*	3	-	3				10.72%

- Set FF: The “variable” portion when the –OR group is –O–(metal):

*no new screens*

- Set GG: The structure with or without a substituent on the ring between the nitro groups:

712	CS	3	-	3	*	3	*	3	-	3	2.35%	
OR	700	CS	3	-	3	*	2	*	3	-	3	5.43%

- Set HH: The structure with or without a substituent on the ring between a nitro group and the carbon substituent:

576	CS	1	-	3	-	3	*	3	18.41%			
OR	571	CS	1	-	3	-	3	*	2	*	3	14.13%

---

**SCREEN  
Command**

The SCREEN command can be used to define the five new screen sets, and the QUERY command can then be used to add them to the search profile as shown:

```
A AND AA AND (B OR C) AND ( (D AND DD) OR
(E AND EE) OR F) AND GG AND HH

=> FIL REG
=> SCR 1121 AND 1642 AND 1681 AND 367 AND 71 AND 1290 AND 490
L1      SCREEN CREATED
=> SCR 119 AND 348
L2      SCREEN CREATED
=> SCR 41
L3      SCREEN CREATED
=> SCR 1832
L4      SCREEN CREATED
=> SCR 409 AND 271 AND 183 AND 193
L5      SCREEN CREATED
=> SCR 1918
L6      SCREEN CREATED
=> SCR 882 AND 895
L7      SCREEN CREATED
=> SCR 575 AND 576
L8      SCREEN CREATED
=> SCR 898 AND 828 AND 556 AND 576 AND 657
L9      SCREEN CREATED
=> SCR 712 OR 700
L10     SCREEN CREATED
=> SCR 576 OR 571
L11     SCREEN CREATED
=> QUERY
ENTER LOGIC EXPRESSION OR (END):L1 AND L7 AND (L2 OR L3) AND
      ((L4 AND L8) OR (L5 AND L9) OR L6) AND L10 AND L11
L12     QUE L1 AND L7 AND (L2 OR L3) AND ((L4 AND L8) OR (L5 AND
      L9) OR L6) AND L10 AND L11
```

The maximum retrieval for each set is as shown:

Set A	Set B	Set C	Set D	Set E	Set F
0.94%	5.24%	19.84%	6.53%	0.42%	14.84%
Set AA	Set DD	Set EE	Set GG	Set HH	
7.01%	15.42%	4.41%	7.78%	32.54%	

For the full search query, the limiting factor is the most specific intermediate screen set, still set A. The introduction of the new screen sets, though, nevertheless helps to decrease the actual search retrieval.

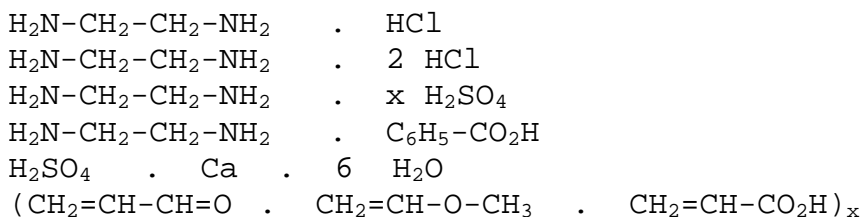
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## Searching for Multicomponent Substances

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### Multicomponent Substances

Multicomponent substances, in the STN databases, are substances such as addition compounds, alloys, copolymers, hydrates, mixtures, and salts. When structured according to CAS REGISTRY structuring conventions, each component is shown separately, with dots separating the individual structures. For example:



The number of components is one more than the number of dots used in the CAS “dot-disconnect” structuring convention and does not depend on any coefficients or multipliers that might be present. In the above examples, the first four are two-component substances and the last two are three-component substances.

---

### Single Atom Fragments

A component that contains only one non-hydrogen atom (to which hydrogen may be attached) is usually handled as a single atom fragment (SAF) by the CAS REGISTRY system. Exceptions are made for one-component substances that contain only one non-hydrogen atom (e.g., sodium and water), which are described by single-atom connection tables. As a consequence of screen number sharing, though, most elements do not have distinct screen numbers for the EC screen and the GM screen that specify an element's presence in the connection table (CT) graph and as an SAF, respectively. The distinction is made only for nine common elements (Br, Ca, Cl, H, I, K, N, Na, and O), which appear frequently enough as SAFs that distinct GM screens are beneficial. All of these elements except H also have the usual CT/SAF screen number that may be used to specify the element appearing in either CT or SAF.

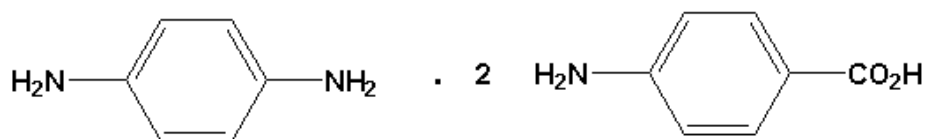
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**Multicomponent  
Screen  
Assignments**

In the STN structure search system, the search screens recorded for a multicomponent substance are obtained by generating the screens for each component. After performing a Boolean OR operation between them, add the appropriate GM multicomponent screen(s). For example, the substance



has element count screens EC 6 C,<sup>17</sup> EC 2 N, and EC 2 O. The screens EC 12 C, EC 3 N, EC 4 N, etc., are not set due to the OR'ing and ignoring of multipliers and coefficients.

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<sup>17</sup> Although seven C atoms are present, there is no EC 7 C screen, so EC 6 C is used instead.

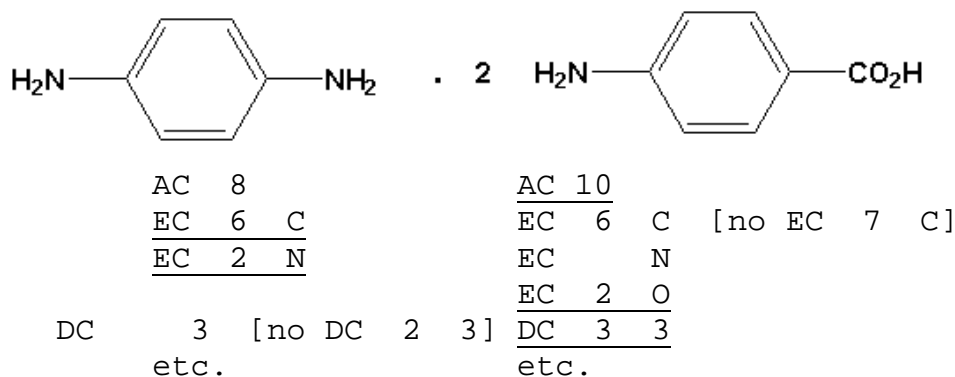
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## Search Query Encoding

This approach to search screens leads to the following considerations for search query encoding:

- When an ordinary query is encoded, no special action is needed to retrieve multicomponent substances that contain the desired substructure in one of the components.
- Special care should be taken with the use of NOT logic. If you are looking for acyclic structures, for example, you would miss multicomponent substances that contain an acyclic structure as one of the components if the search includes a NOT group to reject cyclic structures containing the RC 1 fragment.
- When a query is encoded for a multicomponent substance, you should follow the same procedure used for screen generation:
  - First, select the sets of screens for each component considered separately.
  - Second, combine these sets into a composite set by taking all screens that appeared in only one set and the screens with the highest numbers of occurrences that appeared in two or more sets.

For example, a search for:



would have a composite screen set including the screens shown underlined above, to which the GM screen for a multicomponent substance with two or more components (2127) can be added.

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## Appendix II: Tautomer and Alternating Bonds

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### Introduction

This appendix discusses tautomer and alternating bonds, their definitions, how they are handled in CAS REGISTRY, and how they must be considered when a search query is defined.

The first section of this appendix is a reprint of a paper by CAS staff that discusses tautomerism and alternating bonds in CAS REGISTRY and provides complete definitions of these bonds.

The second section discusses the formulation of search queries and provides some general guidelines for query encoding. A number of common tautomeric substructures are also presented, as a user aid.

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### Tautomeric Bonds

It is important to note that all normalized bonds are represented in CAS REGISTRY screens by the \*4 and -4 bond symbols:

- \*4 = alternating (aromatic or completely conjugated) or tautomeric or delocalized ring bond
  - 4 = tautomeric or delocalized chain bond
-

## The Chemical Abstracts Service Chemical Registry System. VII. Tautomerism and Alternating Bonds

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The Chemical Abstracts Service (CAS) Chemical Registry System is a computer-based information system that uniquely identifies chemical substances on the basis of their molecular structure. Substances that have several possible chemically equivalent representations are difficult to portray precisely by a single structure diagram or connection table. Among the major causes of this problem are aromatic rings, whose alternating single and double bonds can be represented in more than one way, and tautomerism, an equilibrium involving single/double bond shifts coupled with hydrogen migration. The CAS Chemical Registry System handles the problem by algorithmically recognizing tautomeric and alternating bond structures, replacing the explicit single and double bonds with special normalized bonds, and associating the migrating tautomeric hydrogen with groups of atoms rather than just single atoms. This article describes the normalization techniques used in handling alternating bonds and tautomeric bonds, as well as substructure search aspects involving these bond types, and denormalization procedures required for algorithmic structure display and name generation.

### INTRODUCTION

The Chemical Abstracts Service (CAS) Chemical Registry System is a computer-based system for the unique identification of chemical substances on the basis of structure.<sup>1</sup> The initial, experimental system, Registry I, began operation in 1964 and established the viability and validity of the registration concept for fully defined organic substances. In 1968, the scope of the system was increased as it began to handle additional classes of substances. The system, now known as Registry II, began to be integrated into the CAS indexing operation. In 1974, the most recent version, Registry III, made major adjustments in the Registry structure records to provide increased support to the process of generating names for the *Chemical Abstracts* (CA) Chemical Substance Index, and also to computer-based structure output operations through explicit identification of the ring systems present in a substance. As its use has expanded, the CAS Chemical Registry System has proven to be reliable and consistent as a structure identification

method and has become an essential CAS production tool supporting CA index input and compilation. It has also found widespread interest and support in the scientific and technical community.

The foundation of the CAS Chemical Registry System is an algorithm that generates a unique and unambiguous machine-readable description of the molecular structure of a substance. The principal component of the machine record is a connection table, a detailed description of the atoms and bonds that comprise the basic structure of the substance. Other components describe stereochemical characteristics, isotopic labeling, and derivatives (salts, hydrates, etc.).

The representation of a chemical substance by a unique structure diagram or connection table poses problems to both chemists and chemical information systems when the substance has several possible representations, chemically equivalent but structurally distinct. Resonant or aromatic bonds which have characteristics of both single and double bonds are one major

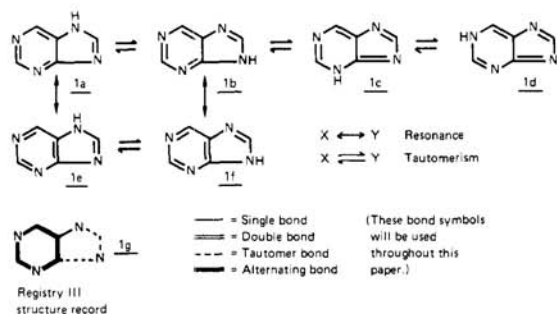


Figure 1. Purine representations.

cause of problems, and tautomerism, an equilibrium involving single/double bond shifts coupled with hydrogen migration, is the other (see Figure 1). These phenomena are quite common; about 70% of the structures in the CAS Registry Master File are aromatic, possessing rings containing alternating single and double bonds, and about 25% exhibit tautomerism.

To a chemist, the multiple representations of a substance resulting from tautomerism and alternating or aromatic bonds usually pose only minor problems. Their equivalence is recognized with little effort, as the result of chemical training and experience.

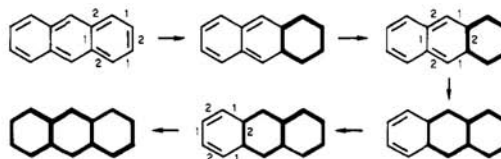
To a chemical information system based on structural diagrams (or their machine equivalents, connection tables), tautomerism and alternating bonds hinder the representation of a single chemical substance by a single diagram. The CAS Chemical Registry System handles the problem by normalizing (i.e., recognizing the equivalence of) tautomeric and alternating bond structures, replacing the explicit single and double bonds with special tautomer and alternating bonds, and associating the migrating hydrogen in a tautomer with a group of atoms rather than just a single atom. Since single/double bond patterns and specific migrating group locations have been replaced by normalized data, all forms of the tautomeric structure lead to the same Registry III structure record. Thus, the six possible representations of purine shown in Figure 1, each containing six single and four double bonds in differing arrangements, all lead to the same Registry III connection table containing one single bond, three tautomer bonds, and six alternating bonds (see structure 1g).

#### OVERVIEW OF ALTERNATING BONDS AND TAUTOMERISM

Alternating bonds are a compromise approach to the chemist's concept of aromatic bonds, bonds which have characteristics of both single and double bonds. The chemist represents such bonds with circles or dotted lines, or with alternating single and double bonds. In the latter case, it is implicitly understood that the actual arrangement of single and double bonds is not critical as long as they alternate. In the purine example (see Figure 1), structures 1a and 1e would be considered simply as different representations of an alternating bond situation, as would 1b and 1f.

Tautomerism is a state of equilibrium of two or more molecular structures that differ in the location of a mobile group, usually a hydrogen atom. Bonding changes occur at the same time as migration of the mobile group. In the purine example, the 1a-1b-1c-1d and 1e-1f equilibria are due to tautomerism. Tautomer and alternating bond situations may overlap, as shown by the purine example. The implications of this overlap will be discussed later.

The CAS Registry III System definition of tautomerism also allows migrating positive and negative charges, even though these would be considered more properly cases of resonance



The 1-2-1-2... indicates the alternating single and double bond path traced by the alternating bond identification procedure.

Figure 2. Identification of alternating bonds.

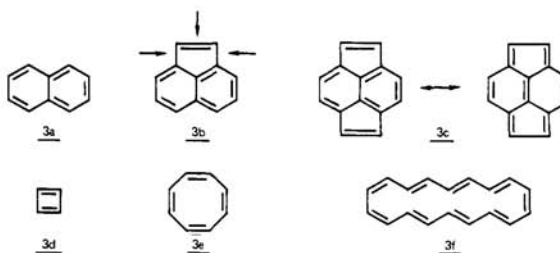


Figure 3. Alternating bond examples.

or charge delocalization. Only simple cases, such as the carboxylate or phosphate anions, are handled this way. More complex cases, such as the cycloheptatrienyl (tropylium) cation or the cyclopentadienyl anion, are handled with special delocalized charge procedures.

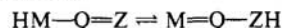
**Alternating Bonds.** The CAS Registry III System uses a path-tracing procedure to identify alternating bonds. It searches through a structure, backtracking when necessary, to find cyclic paths in which the bonds are alternately single and double, marking the bonds as alternating in such paths as they are found (see Figure 2). The search is exhaustive, tracing all possible paths.

The alternating bond procedure will accept a normalized bond in place of an explicit single or double bond on the assumption that the normalized bond could assume the required value. This approach is necessary for proper treatment of overlapping tautomers and alternating bonds, as will be discussed later. In addition, it speeds up the identification process by reducing the number and size of the paths that are traced.

At this point, it would be appropriate to consider the relationship between the chemist's aromatic bonds and the CAS Chemical Registry System's alternating bonds. Aromaticity is still an unsettled topic; for example, chemists would probably agree that the bonds in 3a-3c (see Figure 3) were aromatic and those in 3d and 3e were not, and would argue about 3f. The CAS Chemical Registry System procedures would find all bonds to be alternating except those emphasized in 3b, the sole criterion being the alternating single/double cyclic path.

These structures illustrate two key points. First, the substructure searcher must be concerned with the CAS Chemical Registry System's alternating bond concept and must look at a chemist's aromatic substructure from this viewpoint. Secondly, the searcher must always consider the environment of the substructure. For example, the three emphasized bonds in 3b are fixed single and double when the system is isolated, but are alternating bonds when the substructure is embedded in a larger system (3c).

**Tautomerism.** Tautomerism is a state of equilibrium in which a mobile group, typically a hydrogen, migrates between atoms with concurrent changes in bonding.<sup>2</sup> The basic generic tautomeric structure is



where M and Z are endpoints and Q is a centerpoint. In the

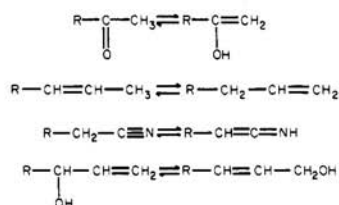


Figure 4. Tautomers not recognized by the CAS Registry III System.

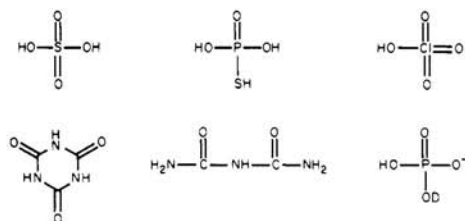


Figure 5. Tautomer examples.

CAS Registry III System, Q can be carbon or most any nonmetallic element, but M and Z are limited to nitrogen and chalcogen atoms. Olefinic and keto-enol tautomers are not recognized as such and are registered (and named by CAS) as distinct structures, as are other variations (see Figure 4).

This definition follows general chemical practice. The normalized tautomers are (1) substances whose names usually describe the structure as a whole, such as the trivial name Barbituric acid (cross-referred to the CA preferred name 2,4,6(1H,3H,5H)-Pyrimidinetrione); (2) structures where tautomerism affects only minor details of the name, such as substituent locants; or (3) functional groups where one form is invariably selected over the alternative, such as an amide over an imidic acid. Tautomers that are not normalized, such as keto-enol tautomers (the most common tautomeric system), are those whose alternative forms usually receive distinct names. Acetone, for example, is the trivial name of 2-Propanone but not its tautomer 1-Propen-2-ol,  $\text{CH}_2=\text{C}(\text{OH})\text{CH}_3$ .

Using the generic  $\text{HM}-\text{Q}=\text{Z}$  tautomeric structure, the CAS Registry III System requires that

- the centerpoint Q may be C, N, P, As, Sb, S, Se, Te, Cl, Br, or I, with any acceptable valence;
- the endpoints M and Z may be trivalent N or bivalent chalcogen (O, S, Se, or Te) in any combination;
- the centerpoint-endpoint tautomer bonds may be either cyclic or acyclic, or both types in combination;
- the mobile group H may be hydrogen (H or its isotopes D or T) or a -1 charge.

Tautomers handled by the CAS Registry III System are not limited to the basic three-atom  $\text{HM}-\text{Q}=\text{Z}$  substructure. Larger tautomers may be linear, as in  $\text{HM}-(\text{Q}=\text{N})_n-\text{Q}=\text{Z}$ , where "N" is trivalent nitrogen, or cyclic, or branched. A centerpoint may have more than two attached endpoints, as in  $\text{HM}-\text{Q}(=\text{Z})_n$  or  $\text{Z}=\text{Q}(\text{---MH})_n$ . Finally, the mobile groups in a tautomer may be all alike or may be different types in combination. (Examples are shown in Figure 5.) The description of a tautomer group in a Registry III structure record cites all of the endpoints in the group and the number of each type of mobile group that is associated with the endpoints. Centerpoints are not explicitly identified, but can be found readily by a check of the structure record connection table.

Tautomers are identified by a procedure that searches for potential endpoints, i.e., nitrogen or chalcogen atoms, that are doubly bonded to an atom acceptable as a centerpoint. When such a two-atom set is found, the remaining attachments of

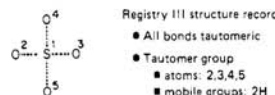
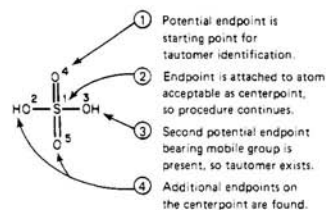


Figure 6. Tautomer identification.

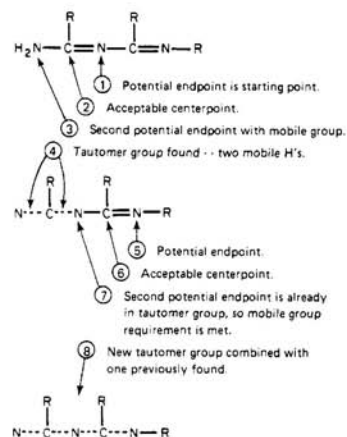


Figure 7. Example of endpoint reuse.

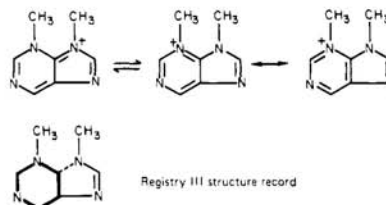
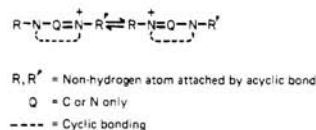


Figure 8. Tautomeric +1 charges.

the centerpoint are checked. If a potential endpoint bearing a mobile group is found, all qualifying endpoints and their mobile groups are included in the tautomer group, and the centerpoint-endpoint bonds are marked as tautomer bonds (see Figure 6). As with alternating bond identification, a previously normalized bond may be used wherever a single or double bond is required. In addition, previously identified nitrogen endpoints may be reused to expand a tautomer group by the addition of endpoints attached to a new centerpoint (see Figure 7).

The CAS Registry III System also recognizes a variety of tautomers in which the mobile group is a +1 charge (see Figure 8). This addition to the general tautomer definition was provided so that an "onium" substructure common in dyes could be normalized.

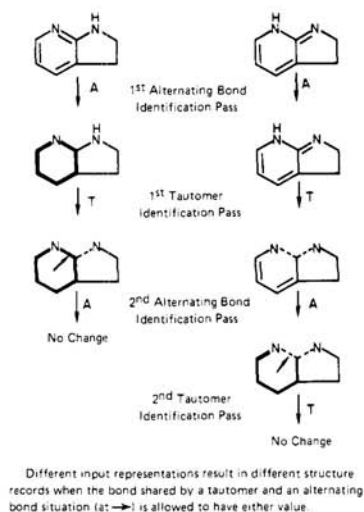


Figure 9. Multiple bond representations problem.

#### OVERLAP OF TAUTOMERS AND ALTERNATING BONDS

Tautomers and alternating bonds may overlap, as shown by the purine example (Figure 1). This possibility required careful consideration during the design of the CAS Registry III System so that multiple representations of a single structure would not be created by the normalization procedures.

Two distinct bond values for cyclic tautomer and alternating bonds are used in the connection table of the CAS Chemical Registry System structure record (in addition to the usual single, double, and triple bond values). Bonds that could be regarded as either tautomer or alternating bonds because of overlap (i.e., could be assigned either bond value) are arbitrarily classified as alternating bonds. If this were not done, the assigned bond values would depend on the bonding in the structure as input to the CAS Chemical Registry System (which could affect whether the bond was first recognized as tautomer or alternating), and this would lead to multiple representations of a single substance (see Figure 9).

Since tautomer and alternating bond situations may overlap, the two normalization procedures must be able to reuse previously normalized bonds of either type. The tautomer procedure, for example, must be able to use either tautomer or alternating bonds during its search for tautomers, not just tautomer bonds alone. If this were not done, the multiple representation problem would be quite severe.

Since tautomer bonds may be used in the identification of alternating bonds, and vice versa, the normalization procedures may need to be applied more than once to a given structure. After the identification of tautomers, for example, a new alternating bond path involving one of the just-normalized tautomer bonds might exist. If the normalization procedures were applied only once, some bonds might not get normalized, and multiple representations would result. In the CAS Registry III System, the alternating bond and tautomer procedures are applied alternately, in that order, until both procedures have been applied at least once and the last-used procedure has not found anything new to normalize (see Figure 10). (The alternating bond procedure is applied first simply because it is more likely to find bonds to be normalized.) Some structures require more than one or two passes. Structure 11a (in Figure 11) requires four passes before all the bonds are normalized, the process ending after the fourth tautomer pass. Larger systems, shown generically by 11b, would need still more.

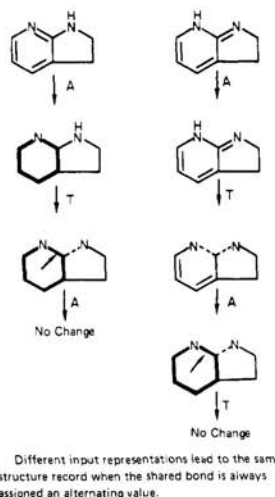


Figure 10. Alternating and tautomer bond identification.

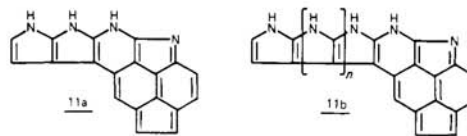


Figure 11. Structures requiring several normalization passes.

#### TAUTOMERS, ALTERNATING BONDS, AND SUBSTRUCTURE SEARCH

Tautomers and alternating bonds have always presented problems for substructure search systems, and this will most likely always be the case. This is true whether the system requires detailed encoding by the searcher or whether the searcher can input a query via a structure diagram. (In the latter case, the system's query input conventions must be designed carefully so that valid retrievals are not lost due to an incorrect treatment of tautomerism and alternating bonds thus causing an incorrect interpretation of a query. The key point, as has been mentioned earlier, is that the searcher must consider potentially tautomeric or alternating substructures with respect to their possible surroundings in full structures. This usually means searching for both fixed-bond and non-normalized-bond variations of such substructures.)

The searcher must keep in mind the CAS Registry III System definition of tautomerism while framing search questions. Thus, most bonds to nitrogen or chalcogen atoms must be regarded as potentially tautomeric. Only when there is clearly no possibility of a tautomer, as in an ether linkage ( $R-O-R'$ ), should the searcher look for fixed-bond substructures alone.

Similarly, many cyclic bonds which by themselves are not alternating bonds become alternating bonds when the substructure is embedded in a larger system. Fixed-bond substructures alone should be sought only when alternating-bond substructures are clearly impossible.

#### DENORMALIZATION OF TAUTOMERS AND ALTERNATING BONDS

Denormalization is an algorithmic procedure which regenerates single and double bonds from normalized tautomer and alternating bonds and fixes the positions of mobile groups (see Figure 12). Bond and mobile group placement follows input structuring conventions and nomenclature rules. Denormalization algorithms have been developed at CAS for use in



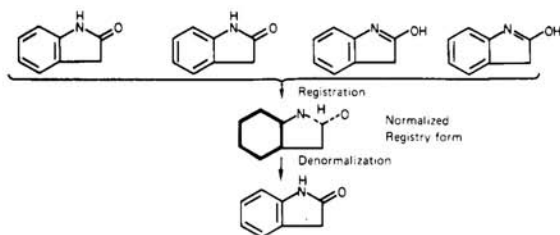


Figure 12. Example of denormalization.

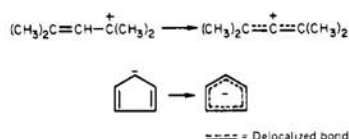


Figure 13. Examples of delocalized bonds.

algorithmic structure display and name generation.<sup>3,4</sup>

The denormalization algorithm used in name generation, which is the more recent and more accurate of the two, is incorporated in an algorithm which generates the systematic names of organic compounds for CA indexes from Registry III connection tables. It denormalizes the acyclic portions of tautomers prior to analysis for naming, since bond placement here primarily depends on structural considerations. Alternating bonds are also denormalized at this point, following input graphic standards for double bond placement. Cyclic tautomers and overlapping tautomer and alternating bond situations are denormalized during analysis for naming, when the preferred CA Index Name for the structure is being selected. Nomenclature rules such as "lowest locants for indicated hydrogen", "lowest locants for substituent prefixes", etc., determine double bond placement. The denormalization algorithm used in structure display operates similarly, although it must use a "best guess" approach to handle cyclic tautomers and overlapping tautomer-alternating situations since it does not have nomenclature rules to guide it.

#### OTHER ASPECTS

Delocalized bonds and charges are used to represent such species as allyl cations or cyclopentadienyl anions (see Figure 13). These bonds are identified by a chemist before the structure is input to the CAS Chemical Registry System, rather than by a machine procedure during registration.

Registry III includes a tautomer override feature that can be used to keep potential tautomers from being normalized. It is used only in those rare cases (only a few hundred to date)

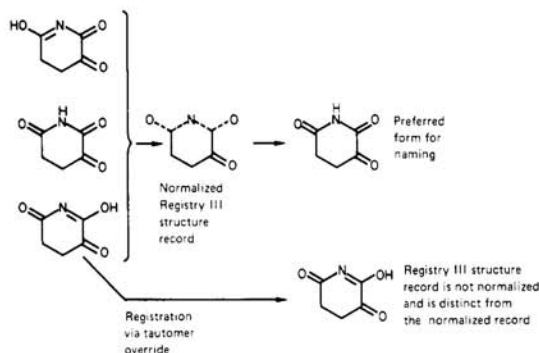


Figure 14. Application of the tautomer override feature.

when a specific tautomer which is not the CA preferred form for naming is emphasized (see Figure 14).

#### SUMMARY

Tautomerism and alternating (aromatic) bonds hinder the representation of a chemical substance by a single structural diagram or its machine equivalent, a connection table. The CAS Chemical Registry System handles the problem by normalizing such structures: replacing the explicit single and double bonds with special normalized bonds, so that all input representations lead to the same unique Registry III structure record. Denormalization procedures to regenerate the single and double bonds in accordance with input structuring conventions and nomenclature rules have been developed for use in the generation of structure diagrams and CA Index Names from CAS Registry III structure records.

#### ACKNOWLEDGMENT

The development of the CAS Chemical Registry System was substantially supported by the National Science Foundation. Chemical Abstracts Service, a division of the American Chemical Society, gratefully acknowledges this support.

#### REFERENCES AND NOTES

- (1) Dittmar, P. G.; Stobaugh, R. E.; Watson, C. E. "The Chemical Abstracts Service Chemical Registry System. I. General Design", *J. Chem. Inf. Comput. Sci.* **1976**, *16*, 111-121.
- (2) "Chemical Abstracts Index Guide", 1977, 1001-1031.
- (3) Dittmar, P. G.; Mockus, J.; Couvreur, K. M. "An Algorithmic Computer Graphics Program for Generating Chemical Structure Diagrams", *J. Chem. Inf. Comput. Sci.* **1977**, *17*, 186-192.
- (4) Mockus, J.; Isenberg, A. C.; Vander Stouw, G. G. "Algorithmic Generation of Chemical Abstracts Index Names. I. General Design", in preparation.



# Tautomers, Alternating Bonds, and Substructure Search

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## Introduction

Tautomers and alternating bonds present little or no problem to the substructure searcher if potentially tautomeric or alternating substructures are always considered with regard to their possible surroundings in full structures. This usually means searching for both fixed-bond and normalized-bond variations of such substructures or, alternatively, searching with less specific screens that specify only bond types and not bond values.

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## What to Consider

Keep in mind the CAS REGISTRY definition of tautomerism while framing search questions. Thus, most bonds to nitrogen or chalcogen (O, S, Se, or Te) atoms must be regarded as potentially tautomeric. Only when there is clearly no possibility of a tautomer, as in an R-O-R' ether linkage, for example, should you look for fixed-bond substructures alone.

Similarly, many cyclic bonds which by themselves are not alternating bonds become alternating bonds when the substructure is embedded in a larger ring system. Fixed-bond substructures alone should be sought only when alternating-bond substructures are clearly impossible.

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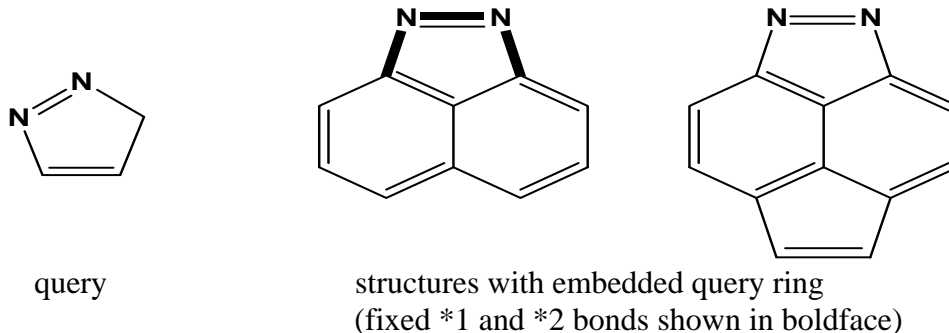
## Alternating Bonds

When a substructure search query contains a ring system, consider the possibility of alternating bonds when encoding the query. Many cyclic bonds which by themselves are not alternating bonds may become alternating when the query ring system is embedded in a larger ring system, as shown by the following example.

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### Example



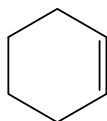
If a query were encoded with fixed single and double \*1 and \*2 bond values, structures containing the query ring embedded in a larger ring with alternating \*4 bonds would not be retrieved as answers to the search, and this would probably be undesirable. Better recall would be obtained if the query were encoded without the specification of bond values for the cyclic bonds.

---

### Three Cyclic Bond Cases

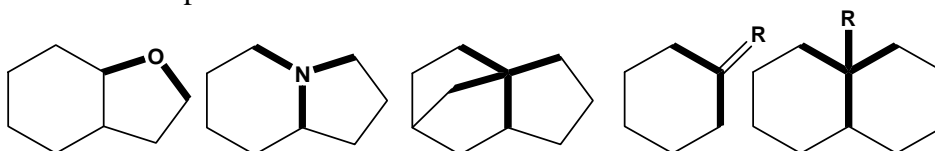
In general, there are only three cases where cyclic bond values may be included in a query without concern for a possible loss of recall:

- If the ring system contains \*4 alternating bonds, they can always be specified as \*4 bonds. Once the alternating single/double bond path exists in a ring system, it is there to stay, even if the sought ring system is embedded in a larger ring system.
- If the query specifies that the ring system should be “isolated” (i.e., that it is not permitted to be part of a larger ring system), then fixed \*1 and single and double bonds may be specified as desired. (This is not true for rings containing N atoms, as discussed in the tautomer section.)



“Isolated” cyclohexene ring with only one double bond


- If the ring system contains atoms that can have only \*1 single bonds due to structural restraints or substitution considerations, those bonds (shown boldface in the examples below) cannot participate in an alternating path and can be specified as \*1 bonds.

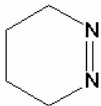
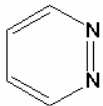



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
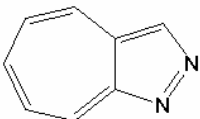
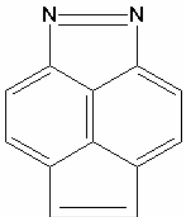
**Rings Having  
Alternative  
Element Values**

If the query ring system contains atoms having alternative element values specified, or “don’t care” atoms or bonds, then use caution when specifying fixed \*1 and \*2 single and double bonds. Specify these bond values only when no structure meeting the other query specifications can have \*4 alternating bonds. Otherwise, either bond values should not be specified at all or both fixed and alternating bond variations should be sought. As examples, consider the following queries:

Query:  N=N bond required with any values allowed for other bonds

Possible Answers:   first answer has a N \*2 N AA fragment but second has a N \*4 N AA fragment

Query:  N=N bond required, with any valence allowed for other bonds

Possible Answers:    First answer has N \*2 N, but second and third have N \*4 N AA fragment

---

**Fixed \*1 and \*2  
Bonds**

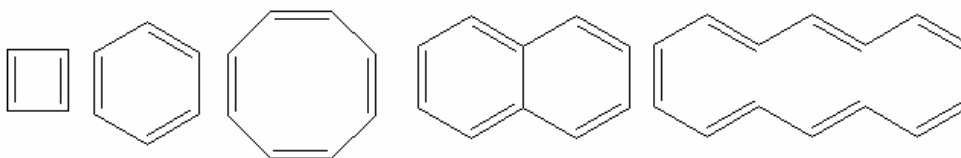
When all things are considered, it would be best to avoid specification of fixed \*1 and \*2 single and double bond values except when alternating bonds are clearly impossible. While this approach might affect the precision of the search by increasing the number of irrelevant structures that were retrieved, it provides total recall of structures that are possibly relevant.

---

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## Aromaticity

As a final point, you should remember that the CAS REGISTRY alternating bond concept is based simply upon the presence of paths containing alternating single and double bonds. The chemist's concept of aromaticity is another matter, as shown by these structures. All contain alternating bonds, but only some are generally considered to be aromatic.



---

## Tautomers

When you encode a substructure search query, consider many bonds to nitrogen or chalcogen (O, S, Se or Te) atoms as potentially tautomeric bonds, especially when the query substructure about these atoms is not fully defined. Only when there is clearly no possibility of a tautomer, when a chalcogen atom has two non-hydrogen substituents or a nitrogen atom has three, should you seek fixed-bond substructures alone.

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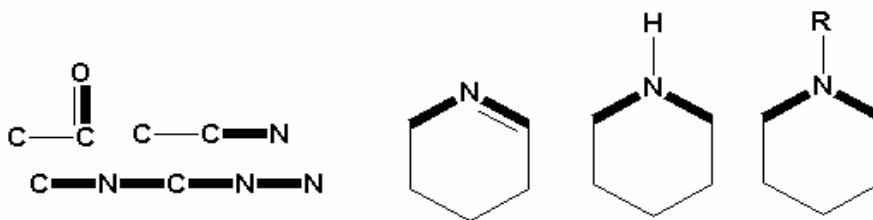
## Tautomer Rules

Given the basic tautomeric structures **HM-Q=Z** and **M=Q-ZH**, where the:

- Center point **Q** is C, N, P, As, Sb, S, Se, Te, Cl, Br, or I.
- End points **M** and **Z** are trivalent N or bivalent chalcogen in any combination.

It is easy to see how many bonds must be considered as potentially tautomeric.

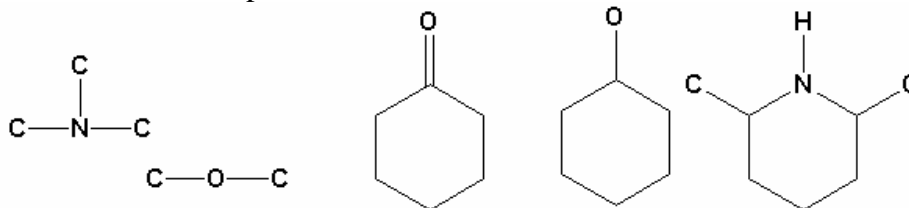
If the query contains an end point-center point pair **HM-Q** or **M=Q**, with the possibility of the second “Z” end point being found on the center point “Q”, then the **M-Q** or **M=Q** bond is potentially tautomeric. Consider both fixed- and tautomer-bond possibilities when the query profile is encoded. The examples below illustrate this, with the potentially tautomeric bonds shown in boldface.



---

### Nontautomeric Cases

Nontautomeric situations, where fixed-bond substructures can and should be sought, are those where a nitrogen or chalcogen atom is substituted so that it cannot participate in the single/double bond equilibrium, or where a HM-Q or M=Q end point-center point situation exists but a second end point cannot be present on the center point.



---

### Three Types of Substructures

The correct treatment of a substructure search query thus requires you to recognize and properly encode three types of substructures:

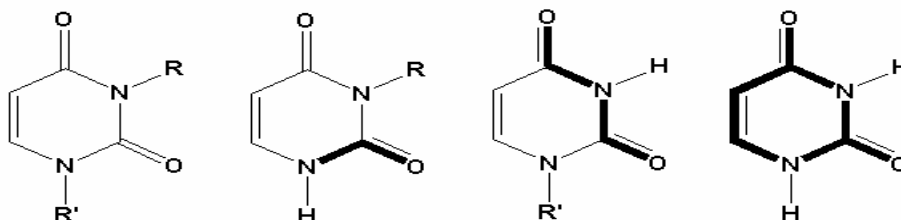
- Tautomeric situations: Encoded with -4 and \*4 tautomer bonds
- Nontautomeric situations: Encoded with fixed single and double bonds
- Potentially tautomeric situations: Encoded with both tautomeric- and fixed-bond alternatives specified, or with a more generic approach with only bond types but not bond values specified

As a user aid, some common tautomeric substructures are shown on page 95.

---

### Tautomers and Alternating Bonds

Note that you must also recognize the interaction between tautomeric situations and alternating bonds. The single/double bond shifts associated with alternating bonds can lead to a tautomeric situation, and vice-versa. For example, in the leftmost structure



Alternating and tautomer bonds shown in bold

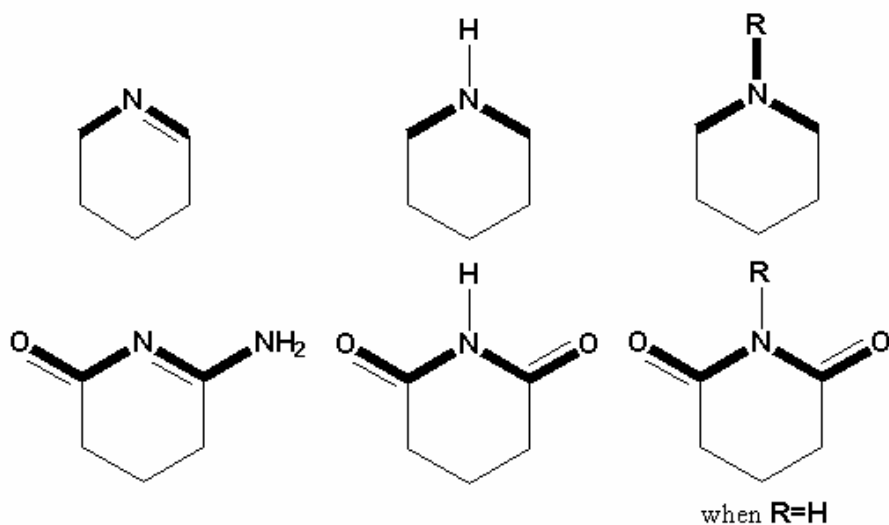
the possible bond values depend on whether or not the R and R' groups could be hydrogen. Any case where an -NH- was present would lead to \*4 bonds between the N atom and one or both of its neighbors and -4 bonds between those atoms and their attached oxygens, and if both R and R' were hydrogen, the ring would contain alternating bonds.

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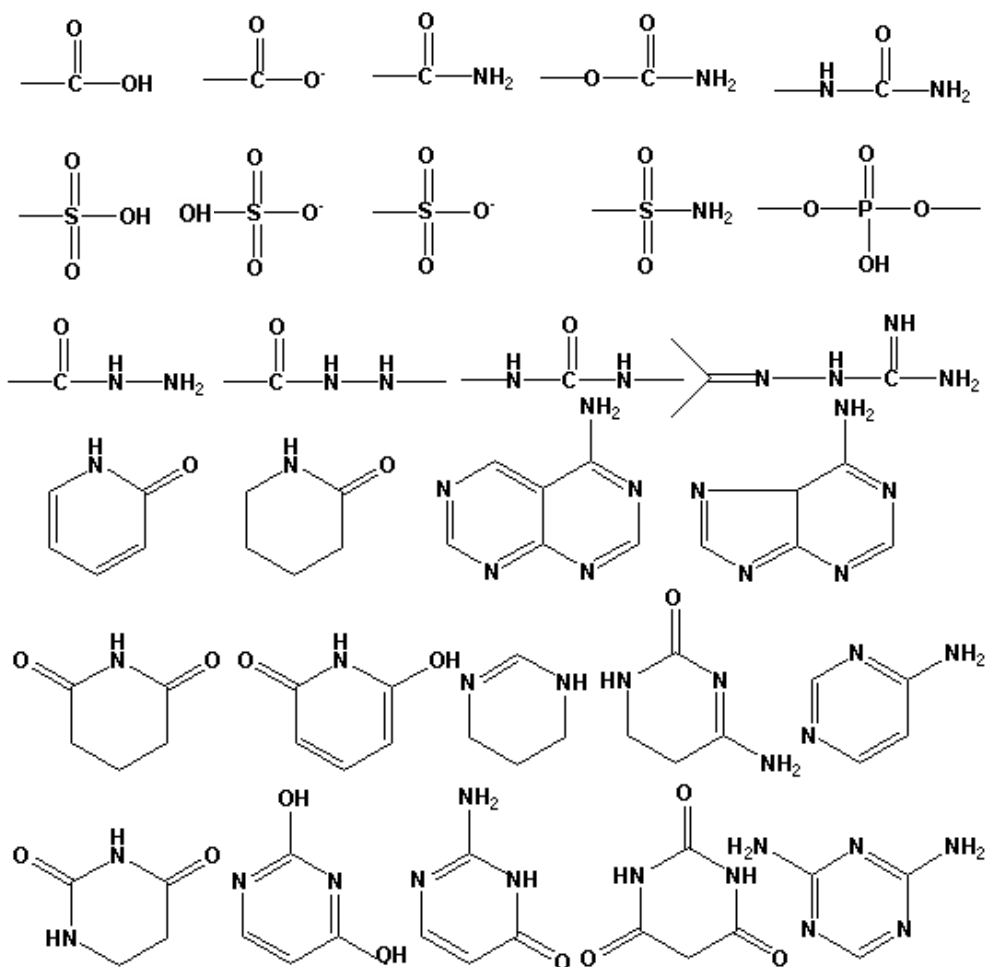
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**N-Atom in a Ring**

It was previously noted that bond values could safely be specified in a query describing an “isolated” ring system, but that this was not true for rings containing nitrogen atoms. This exception is due to the possibility of the ring bonds to the N atoms being tautomeric, which would depend on the substitution on the adjacent atoms. As examples, consider the three rings used earlier to illustrate potentially tautomeric bonds, shown here together with substituted rings where the potentially tautomeric bonds are in fact tautomeric.



**Common  
Tautomeric  
Substructures**



**Note**

Most bonds in the example substructures are tautomeric, but this may change if the hydrogen atoms in  $-OH$ ,  $-NH-$ , and  $-NH_2$  are replaced with non-hydrogen atoms.

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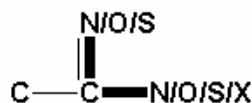
**AA Screens and  
Tautomer  
Combinations**

As a user aid, the screen dictionary contains a number of augmented atom screens that describe common potentially tautomeric groups. These screens group sets of related AA fragments having various combinations of fixed single and double bonds and tautomeric bonds, and some also include alternative element possibilities. One such set is shown below, and the most useful of the screens are given in the figure on the next page.

---

**Screen 1199  
Example**

1199	AA	C	-1C	-1N	-2N	43.86
	AA	C	-1C	-4N	-4N	
	AA	C	-1C	-1N	-2O	
	AA	C	-1C	-2N	-1O	
	AA	C	-1C	-4N	-4O	
	AA	C	-1C	-1N	-2S	
	AA	C	-1C	-2N	-1S	
	AA	C	-1C	-4N	-4S	
	AA	C	-1C	-2N	-1X	
	AA	C	-1C	-1O	-2O	
	AA	C	-1C	-4O	-4O	
	AA	C	-1C	-1O	-2S	
	AA	C	-1C	-2O	-1S	
	AA	C	-1C	-4O	-4S	
	AA	C	-1C	-2O	-1X	
	AA	C	-1C	-1S	-2S	
	AA	C	-1C	-4S	-4S	
	AA	C	-1C	-2S	-1X	



All combinations of end point  
element values are used.

C-C bond is -1, other bonds are  
either -1 and -2 or both -4 bonds

---

**Note**

No special effort is needed to make use of these special screens, since their screen numbers would be retrieved in the same manner as other screen numbers, by a check of the screen dictionary for a desired fragment.

---

**Final Point**

The final point to be noted about tautomers is that any structures having tautomeric D or T or tautomeric charges will be retrieved together with the structures with tautomeric H. No special coding is necessary. If the search is specifically for structures with tautomeric D, T, or charge, then the appropriate Graph Modifier (GM) screen should be used: 2040 GM “charge”, 2045 GM “deuterium”, or 2046 GM “tritium”. The 2076 GM “tautomer” screen may also prove to be useful for special cases.

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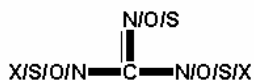
AA Screen Sets  
for Potentially  
Tautomeric  
Substructures

**1199**  
(43.86%)

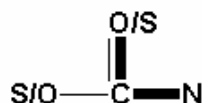


Generic  
“carboxy” group

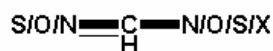
**1367**  
(9.76%)



**1503**  
(3.82%)

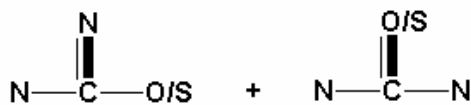


**1377**  
(0.47%)



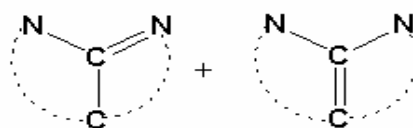
Note: HA screen  
not AA

**1451-1454**



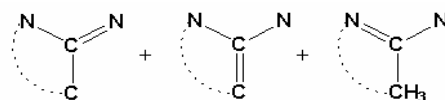
Four screen sets  
with various  
combinations of  
-1, -2, and -4  
bonds

**1252**  
(3.36%)



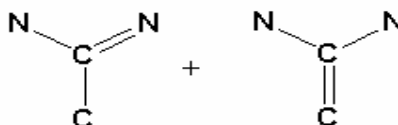
Various  
combinations of  
\*1/\*2/\*4 bonds

**1255**  
(4.33%)



Various bond  
combinations

**1261**  
(0.63%)



Various  
combinations of  
-1/-2/-4 bonds

---

**Notes**

- This list illustrates the major screen sets for potentially tautomeric substructures. It is not a complete list, since a number of screens for less common substructures have not been included.
  - The use of “N/O/S” as an element symbol, for example, indicates that the atom may have any of the cited values. The screen set includes all possible combinations of elements.
  - Boldface bonds or the phrase “various combinations...” indicates combinations of single and double bonds or tautomeric bonds.
  - The - lines in the drawings for screen sets 1252 and 1255 indicate rings implied by the use of cyclic bonds in the fragment descriptions.
-

# The Screen Dictionary

The sections of the Screen Dictionary follow in this order:

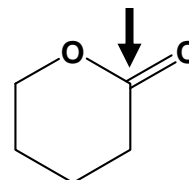
- Augmented Atoms
- Hydrogen Augmented Atoms
- Twin Augmented Atoms
- Atom Sequences
- Bond Sequences
- Connectivity Sequences
- Atom Count
- Degree of Connectivity
- Ring Count
- Type of Rings
- Element Count and Graph Modifier Fragments
- Screen Number Order

# Augmented Atoms

## AA Screens

The **augmented atom (AA) screen** describes an atom and its immediate non-hydrogen attachments, with the screen description citing the central atom first and then its attachments in element symbol order; bonds to the central atom are described in the most specific AA screens, while more generic screens use less specific bond descriptions. The indicated carbon atom, for example, could thus be described at three different levels of specificity:

AA	1	C	*1	C	*1	O	-2	O
AA	1	C	*	C	*	O	-	O
AA	1	C		C		O		O



where the AA indicates the screen type and the "1" that the screen occurs one or more times;<sup>1</sup> the bond symbols \*1 and -2 represent a single ring bond and a double chain bond, respectively, while \* and - represent simply ring and chain bonds of any value and a blank represents any bond.

## AA Screen Definitions

Bonds may be unspecified, specified just as ring or chain type, or completely specified using bond symbols. The level of bond specificity used for AA screens in the screen dictionary depends on the elements involved:

- screens for the frequently occurring C-N bond, for example, will usually completely specify bonds, as in AA C -1 N, AA C -2 N, etc.
- screens for the less common C-P bonds cite only bond types, as in AA C \* P and AA C - P
- the screen for the uncommon P-P bond is simply AA P P, with no bond specification at all

The central atom is cited first, followed by its attachments in element symbol order. If bonds are specified, a secondary ordering cites \* ring bonds before - chain bonds, and complete bond specifications in the order \*1 \*2 \*3 \*4 -1 -2 -3 -4.

<sup>1</sup> The counts of "1" are shown here for clarity; normally, only counts of 2 or higher are explicitly shown.

# Augmented Atoms

Screen Number	Fragment Definition							Frequency Percent
935	AA		A	* 2A				34.69
937	AA		A	* 3A				0.14
936	AA		A	* 4A				72.06
938	AA		A	- 2A				59.17
939	AA		A	- 4A				39.02
940	AA		A	* A	* A	* A		41.18
941	AA		A	* A	- A	- A		12.51
942	AA	2	A	* A	- A	- A		3.34
943	AA	3	A	* A	- A	- A		1.07
944	AA		A	- A	- A	- A		73.89
945	AA		A	* A	* A	* A	* A	7.17
946	AA	2	A	* A	* A	* A	* A	1.92
947	AA		A	* A	* A	* A	- A	7.64
948	AA	2	A	* A	* A	* A	- A	3.57
949	AA	3	A	* A	* A	* A	- A	1.36
1820	AA		As	As				# 0.35
1820	AA		As	B				# 0.35
1552	AA		As	* C				# 1.15
1558	AA		As	M				# 3.13
1391	AA		As	* M				# 6.30
1392	AA		As	- M				# 6.25
1667	AA		As	- 4N				# 2.86
1820	AA		As	P				# 0.35
1820	AA		As	Se				# 0.35
1820	AA		As	Si				# 0.35
1820	AA		As	Te				# 0.35
952	AA		As	X				# 0.53
1820	AA		B	As				# 0.35
1820	AA		B	B				# 0.35
1552	AA		B	* C				# 1.15
953	AA		B	- C				0.39
1558	AA		B	M				# 3.13
1391	AA		B	* M				# 6.30
1392	AA		B	- M				# 6.25
954	AA		B	N				0.22
1667	AA		B	- 4N				# 2.86
955	AA		B	* O				# 0.30
955	AA		B	- O				# 0.30
1820	AA		B	P				# 0.35
1820	AA		B	Se				# 0.35
1820	AA		B	Si				# 0.35
1820	AA		B	Te				# 0.35
952	AA		B	X				# 0.53
956	AA		Br	C				4.36
1552	AA		C	* As				# 1.15
1344	AA		C	- As	* C			# 2.97
1345	AA		C	- 1As	* 1C			# 0.47
1345	AA		C	- 1As	* 2C			# 0.47
1346	AA		C	- 1As	* 4C			# 2.63
1190	AA		C	- 1As	- 3C			# 0.20
1020	AA		C	- 2As	- 2C			# 0.14
1552	AA		C	* B				# 1.15
953	AA		C	- B				0.39
1344	AA		C	- B	* C			# 2.97
1345	AA		C	- 1B	* 1C			# 0.47

# Augmented Atoms

Screen Number	Fragment Definition					Frequency Percent
1345	AA		C	-1B	*2C	# 0.47
1346	AA		C	-1B	*4C	# 2.63
1190	AA		C	-1B	-3C	# 0.20
1020	AA		C	-2B	-2C	# 0.14
956	AA		C	Br		4.36
957	AA	2	C	Br		0.80
958	AA		C	Br	Br	0.09
959	AA		C	- Br	* C	3.55
960	AA	2	C	- Br	* C	0.64
961	AA		C	Br	Cl	# 0.16
961	AA		C	Br	F	# 0.16
961	AA		C	Br	I	# 0.16
962	AA		C	- Br	* N	0.11
968	AA		C	-2C		14.86
969	AA	4	C	-2C		3.19
971	AA	2	C	-3C		1.56
972	AA	4	C	-3C		0.28
974	AA		C	* C	* C	83.26
975	AA		C	* C	- C	70.68
976	AA	2	C	* C	- C	51.36
977	AA	3	C	* C	- C	30.91
978	AA	4	C	* C	- C	18.42
1367	AA		C	-4N	-4O -1X	# 9.76
979	AA	5	C	* C	- C	9.80
980	AA		C	*1C	*1C	38.78
981	AA	2	C	*1C	*1C	32.27
982	AA	3	C	*1C	*1C	24.82
983	AA	4	C	*1C	*1C	18.90
984	AA	5	C	*1C	*1C	15.08
985	AA	6	C	*1C	*1C	12.75
986	AA	7	C	*1C	*1C	8.38
987	AA	10	C	*1C	*1C	4.88
988	AA	14	C	*1C	*1C	2.59
992	AA		C	*1C	*2C	23.19
993	AA	2	C	*1C	*2C	16.26
994	AA	3	C	*1C	*2C	6.48
995	AA	4	C	*1C	*2C	4.73
998	AA		C	*4C	*4C	70.37
999	AA	4	C	*4C	*4C	68.05
1000	AA	7	C	*4C	*4C	46.29
1001	AA	9	C	*4C	*4C	44.62
1002	AA	12	C	*4C	*4C	41.35
1003	AA	15	C	*4C	*4C	18.54
1004	AA	18	C	*4C	*4C	16.22
1005	AA		C	- C	- C	59.87
1011	AA		C	-1C	-2C	14.27
1012	AA	2	C	-1C	-2C	8.12
1013	AA	3	C	-1C	-2C	2.10
1014	AA	6	C	-1C	-2C	0.42
1019	AA		C	-1C	-3C	1.58
1020	AA		C	-2C	-2C	# 0.14
1021	AA		C	* C	* C * C	29.30
1022	AA	2	C	* C	* C * C	19.00
1023	AA	3	C	* C	* C * C	9.59
1024	AA	5	C	* C	* C * C	4.24

# Augmented Atoms

Screen Number	Fragment Definition							Frequency Percent
1025	AA		C	*1C	*1C	*1C		7.74
1026	AA	2	C	*1C	*1C	*1C		5.66
1027	AA	3	C	*1C	*1C	*1C		3.23
1029	AA		C	*1C	*1C	*2C		3.99
1030	AA	2	C	*1C	*1C	*2C		0.98
1031	AA		C	*1C	*1C	-1C		16.17
1032	AA	2	C	*1C	*1C	-1C		6.87
1033	AA	3	C	*1C	*1C	-1C		2.67
1035	AA		C	*1C	*1C	-2C		1.98
1036	AA		C	*1C	*2C	-1C		10.48
1037	AA	2	C	*1C	*2C	-1C		2.50
1038	AA		C	*1C	*4C	*4C		16.87
1039	AA	2	C	*1C	*4C	*4C		8.65
1040	AA	3	C	*1C	*4C	*4C		3.02
1041	AA		C	*4C	*4C	*4C		6.96
1042	AA	2	C	*4C	*4C	*4C		4.96
1043	AA	3	C	*4C	*4C	*4C		1.64
1044	AA		C	*4C	*4C	-1C		53.13
1045	AA	2	C	*4C	*4C	-1C		29.03
1046	AA	3	C	*4C	*4C	-1C		12.69
1047	AA	5	C	*4C	*4C	-1C		2.69
1048	AA		C	- C	- C	- C		21.56
1049	AA		C	-1C	-1C	-1C		18.17
1050	AA	2	C	-1C	-1C	-1C		6.13
1054	AA		C	-1C	-1C	-2C		4.39
1055	AA	2	C	-1C	-1C	-2C		0.79
1056	AA		C	C	C	C	C	10.15
1057	AA	2	C	C	C	C	C	3.79
1058	AA	3	C	C	C	C	C	0.96
1059	AA	4	C	C	C	C	C	0.56
1060	AA	5	C	C	C	C	C	0.25
1061	AA		C	* C	* C	* C	* C	1.01
1062	AA		C	* C	* C	* C	- C	3.22
1063	AA		C	* C	* C	- C	- C	3.52
1064	AA		C	- C	- C	- C	- C	3.78
1068	AA		C	C	C	C	N	2.73
1069	AA	2	C	C	C	C	N	0.43
1066	AA		C	* C	* C	- C	- N	# 1.87
1070	AA		C	* C	- C	- C	* N	0.70
1071	AA		C	- C	- C	- C	- N	1.23
1072	AA		C	C	C	C	O	# 7.26
1073	AA	2	C	C	C	C	O	# 1.18
1074	AA	3	C	C	C	C	O	# 0.25
1066	AA		C	* C	* C	- C	- O	# 1.87
1075	AA		C	* C	- C	- C	* O	# 1.18
1076	AA		C	- C	- C	- C	- O	# 3.59
1072	AA		C	C	C	C	S	# 7.26
1073	AA	2	C	C	C	C	S	# 1.18
1074	AA	3	C	C	C	C	S	# 0.25
1066	AA		C	* C	* C	- C	- S	# 1.87
1075	AA		C	* C	- C	- C	* S	# 1.18
1076	AA		C	- C	- C	- C	- S	# 3.59
1065	AA		C	C	C	C	X	0.41
1066	AA		C	* C	* C	- C	- X	# 1.87
1067	AA		C	- C	- C	- C	- X	0.12

# Augmented Atoms

Screen Number	Fragment Definition						Frequency Percent
1092	AA		C	* C	* C	* N	18.01
1093	AA	2	C	* C	* C	* N	7.34
1094	AA	3	C	* C	* C	* N	2.48
1095	AA	4	C	* C	* C	* N	1.63
1096	AA	5	C	* C	* C	* N	0.82
1097	AA		C	* C	* C	- N	28.97
1098	AA	2	C	* C	* C	- N	10.75
1099	AA		C	* C	- C	* N	19.54
1100	AA	2	C	* C	- C	* N	6.42
1101	AA		C	*1C	*1C	*1N	2.52
1103	AA		C	*1C	*1C	*2N	0.63
1104	AA		C	*1C	*1C	-1N	5.62
1106	AA		C	*1C	*1C	-2N	0.85
1107	AA		C	*1C	*2C	*1N	1.97
1108	AA		C	*1C	*2C	-1N	1.18
1109	AA		C	*1C	*4C	*4N	1.45
1110	AA		C	*1C	-1C	*1N	7.36
1112	AA		C	*1C	-1C	*2N	3.47
1113	AA		C	*1C	-2C	*1N	0.48
1114	AA		C	*2C	-1C	*1N	6.96
1115	AA	2	C	*2C	-1C	*1N	1.52
1116	AA		C	*4C	*4C	*1N	10.82
1117	AA	2	C	*4C	*4C	*1N	3.71
1118	AA		C	*4C	*4C	*4N	3.24
1119	AA	2	C	*4C	*4C	*4N	1.15
1120	AA		C	*4C	*4C	-1N	23.48
1121	AA	2	C	*4C	*4C	-1N	8.53
1122	AA		C	*4C	-1C	*4N	3.89
1123	AA		C	- C	- C	- N	13.50
1124	AA	2	C	- C	- C	- N	5.13
1125	AA	3	C	- C	- C	- N	3.46
1087	AA		C	-1C	-1C	-2N	# 7.76
1128	AA		C	-1C	-1C	-2N	1.48
1129	AA		C	-1C	-2C	-1N	0.47
1130	AA		C	C	C	N N	0.19
1089	AA		C	* C	* C	- N - N	# 0.08
1090	AA		C	* C	- C	* N - N	# 0.12
1131	AA		C	- C	- C	* N * N	# 1.00
1087	AA		C	-1C	-1C	-1N -1N	# 7.76
1132	AA		C	C	C	N O	# 0.46
1089	AA		C	* C	* C	- N - O	# 0.08
1090	AA		C	* C	- C	* N - O	# 0.12
1091	AA		C	* C	- C	- N * O	# 0.12
1131	AA		C	- C	- C	* N * O	# 1.00
1087	AA		C	-1C	-1C	-1N -1O	# 7.76
1132	AA		C	C	C	N S	# 0.46
1089	AA		C	* C	* C	- N - S	# 0.08
1090	AA		C	* C	- C	* N - S	# 0.12
1091	AA		C	* C	- C	- N * S	# 0.12
1131	AA		C	- C	- C	* N * S	# 1.00
1087	AA		C	-1C	-1C	-1N -1S	# 7.76
1088	AA		C	C	C	N X	# 0.11
1089	AA		C	* C	* C	- N - X	# 0.08
1090	AA		C	* C	- C	* N - X	# 0.12
1087	AA		C	-1C	-1C	-1N -1X	# 7.76



# Augmented Atoms

Screen Number	Fragment Definition						Frequency Percent
1133	AA		C	* C	* C	* O	8.35
1134	AA	2	C	* C	* C	* O	4.34
1135	AA		C	* C	* C	- O	35.34
1136	AA	2	C	* C	* C	- O	17.07
1137	AA		C	*1C	*1C	*1O	3.06
1138	AA		C	*1C	*1C	-1O	8.84
1139	AA		C	*1C	*1C	-2O	5.34
1140	AA	2	C	*1C	*1C	-2O	1.31
1141	AA		C	*1C	*2C	*1O	0.47
1142	AA		C	*1C	*2C	-1O	1.32
1143	AA		C	*1C	-1C	*1O	7.20
1144	AA		C	*1C	-2C	*1O	0.14
1145	AA		C	*2C	-1C	*1O	2.75
1146	AA		C	- C	- C	- O	16.97
1147	AA	2	C	- C	- C	- O	3.76
1148	AA	3	C	- C	- C	- O	1.06
1087	AA		C	-1C	-1C	-2O	# 7.76
1151	AA		C	-1C	-1C	-2O	5.56
1152	AA	2	C	-1C	-1C	-2O	0.49
1153	AA		C	-1C	-2C	-1O	0.34
1168	AA		C	C	C	O O	#
1169	AA		C	* C	* C	- O - O	# 0.10
1091	AA		C	* C	- C	* O - O	# 0.12
1131	AA		C	- C	- C	* O * O	# 1.00
1087	AA		C	-1C	-1C	-1O -1O	# 7.76
1168	AA		C	C	C	O S	# 1.94
1169	AA		C	* C	* C	- O - S	# 0.10
1091	AA		C	* C	- C	* O - S	# 0.12
1091	AA		C	* C	- C	- O * S	# 0.12
1131	AA		C	- C	- C	* O * S	# 1.00
1087	AA		C	-1C	-1C	-1O -1S	# 7.76
1088	AA		C	C	C	O X	# 0.11
1089	AA		C	* C	* C	- O - X	# 0.08
1091	AA		C	* C	- C	* O - X	# 0.12
1087	AA		C	-1C	-1C	-1O -1X	# 7.76
1154	AA		C	C	C	P	2.04
1155	AA		C	- C	- C	- P	0.26
1156	AA		C	* C	* C	* S	3.07
1157	AA	2	C	* C	* C	* S	0.72
1158	AA		C	* C	* C	- S	7.91
1159	AA	2	C	* C	* C	- S	1.93
1160	AA		C	* C	- C	* S	3.95
1161	AA		C	*1C	*1C	-1S	0.51
1162	AA		C	*1C	*1C	-2S	# 0.44
1162	AA		C	*1C	*2C	-1S	# 0.44
1163	AA		C	-1C	-1C	-1S	0.85
1087	AA		C	-1C	-1C	-2S	# 7.76
1165	AA		C	-1C	-1C	-2S	# 0.15
1165	AA		C	-1C	-2C	-1S	# 0.15
1168	AA		C	C	C	S S	# 1.94
1169	AA		C	* C	* C	- S - S	# 0.10
1091	AA		C	* C	- C	* S - S	# 0.12
1131	AA		C	- C	- C	* S * S	# 1.00
1087	AA		C	-1C	-1C	-1S -1S	# 7.76
1088	AA		C	C	C	S X	# 0.11

# Augmented Atoms

Screen Number	Fragment Definition						Frequency Percent
1089	AA		C	* C	* C	- S - X	# 0.08
1091	AA		C	* C	- C	* S - X	# 0.12
1087	AA		C	-1C	-1C	-1S -1X	# 7.76
1077	AA		C	* C	* C	- X	18.59
1079	AA		C	- C	- C	- X	1.51
1080	AA	2	C	- C	- C	- X	0.55
1081	AA	3	C	- C	- C	- X	0.35
1082	AA		C	-1C	-1C	-1X	1.18
1084	AA		C	-1C	-2C	-1X	0.35
1085	AA		C	C	C	X X	0.86
1086	AA		C	* C	* C	- X - X	0.23
1087	AA		C	-1C	-1C	-1X -1X	# 7.76
1170	AA		C	* C	- Cl		11.60
1171	AA	2	C	* C	- Cl		3.88
1172	AA	3	C	* C	- Cl		0.86
1173	AA	4	C	* C	- Cl		0.39
1174	AA		C	* C	- F		5.23
1175	AA	2	C	* C	- F		1.54
1201	AA		C	* C	- I		0.76
1202	AA	2	C	* C	- I		0.16
2105	AA		C	C	M		# 31.14
2099	AA		C	C	N		69.37
2100	AA	2	C	C	N		62.62
1203	AA		C	* C	- N		32.73
1204	AA	2	C	* C	- N		13.07
1205	AA	3	C	* C	- N		4.45
1206	AA	5	C	* C	- N		0.92
1207	AA	7	C	* C	- N		0.38
1208	AA		C	*1C	*1N		27.22
1209	AA	2	C	*1C	*1N		20.48
1212	AA		C	*1C	*2N		6.60
1213	AA	2	C	*1C	*2N		1.69
1215	AA		C	*1C	*4N		4.72
1216	AA		C	*1C	-1N		8.08
1217	AA		C	*1C	-2N		1.15
1218	AA		C	*1C	-4N		0.66
1219	AA		C	*2C	*1N		14.18
1220	AA	2	C	*2C	*1N		5.96
1221	AA		C	*2C	-1N		2.66
1222	AA		C	*4C	*1N		11.39
1223	AA		C	*4C	*4N		13.12
1224	AA	3	C	*4C	*4N		3.41
1225	AA		C	*4C	-1N		24.08
1226	AA		C	*4C	-4N		1.99
1227	AA		C	- C	* N		24.24
1228	AA	2	C	- C	* N		9.01
1229	AA	3	C	- C	* N		2.39
1230	AA		C	-1C	*1N		16.13
1231	AA		C	-1C	*2N		7.86
1232	AA		C	-1C	*4N		5.34
1233	AA		C	-1C	-1N		35.46
1234	AA	2	C	-1C	-1N		18.10
1240	AA		C	-1C	-2N		4.59
1243	AA		C	-1C	-3N		4.12
1242	AA		C	-1C	-4N		20.28

# Augmented Atoms

Screen Number	Fragment Definition						Frequency Percent
1244	AA	C	-2C	*1N			0.78
1245	AA	C	-2C	-1N			1.05
1020	AA	C	-2C	-2N		#	0.14
1190	AA	C	-3C	-1N		#	0.20
1247	AA	C	* C	* N	* N		3.51
1248	AA	2	C	* C	* N	* N	0.68
1249	AA		C	* C	* N	- N	4.43
1250	AA		C	*1C	*1N	*1N	0.15
1252	AA		C	*1C	*1N	*2N	# 3.36
1253	AA		C	*1C	*1N	-1N	# 0.45
1255	AA		C	*1C	*1N	-2N	# 4.33
1255	AA		C	*1C	*2N	-1N	# 4.33
1252	AA		C	*1C	*4N	*4N	# 3.36
1255	AA		C	*1C	*4N	-4N	# 4.33
1252	AA		C	*2C	*1N	*1N	# 3.36
1255	AA		C	*2C	*1N	-1N	# 4.33
1252	AA		C	*4C	*1N	*4N	# 3.36
1252	AA		C	*4C	*4N	*4N	# 3.36
1255	AA		C	*4C	*4N	-1N	# 4.33
1255	AA		C	*4C	*4N	-4N	# 4.33
1256	AA		C	- C	* N	* N	4.52
1257	AA		C	- C	- N	- N	0.76
1258	AA		C	-1C	*1N	*1N	0.25
1199	AA		C	-1C	-1N	-2N	# 43.86
1261	AA		C	-1C	-1N	-2N	# 0.63
1199	AA		C	-1C	-4N	-4N	# 43.86
1261	AA		C	-1C	-4N	-4N	# 0.63
1261	AA		C	-2C	-1N	-1N	# 0.63
1195	AA		C	C	N	N N	# 0.40
1090	AA		C	* C	* N	- N - N	# 0.12
1200	AA		C	- C	* N	* N - N	# 0.05
1196	AA		C	-1C	-1N	-1N -1N	# 0.97
1195	AA		C	C	N	N O	# 0.40
1090	AA		C	* C	* N	- N - O	# 0.12
1091	AA		C	* C	- N	- N * O	# 0.12
1200	AA		C	- C	* N	* N - O	# 0.05
1200	AA		C	- C	* N	- N * O	# 0.05
1196	AA		C	-1C	-1N	-1N -1O	# 0.97
1195	AA		C	C	N	N S	# 0.40
1090	AA		C	* C	* N	- N - S	# 0.12
1091	AA		C	* C	- N	- N * S	# 0.12
1200	AA		C	- C	* N	* N - S	# 0.05
1200	AA		C	- C	* N	- N * S	# 0.05
1196	AA		C	-1C	-1N	-1N -1S	# 0.97
1195	AA		C	C	N	N X	# 0.40
1090	AA		C	* C	* N	- N - X	# 0.12
1200	AA		C	- C	* N	* N - X	# 0.05
1196	AA		C	-1C	-1N	-1N -1X	# 0.97
1262	AA		C	* C	* N	* O	0.53
1263	AA		C	* C	* N	- O	12.82
1264	AA	2	C	* C	* N	- O	3.42
1265	AA		C	* C	- N	* O	1.51
1253	AA		C	*1C	*1N	-1O	# 0.45
1266	AA		C	- C	* N	* O	1.53
1267	AA		C	- C	- N	- O	24.08

# Augmented Atoms

Screen Number	Fragment Definition							Frequency Percent
1268	AA	2	C	- C	- N	- O		8.22
1199	AA		C	-1C	-1N	-2O	#	43.86
1199	AA		C	-1C	-2N	-1O	#	43.86
1199	AA		C	-1C	-4N	-4O	#	43.86
1195	AA		C	C	N	O	O	# 0.40
1090	AA		C	* C	* N	- O	- O	# 0.12
1091	AA		C	* C	- N	* O	- O	# 0.12
1200	AA		C	- C	* N	* O	- O	# 0.05
1200	AA		C	- C	- N	* O	* O	# 0.05
1196	AA		C	-1C	-1N	-1O	-1O	# 0.97
1195	AA		C	C	N	O	S	# 0.40
1090	AA		C	* C	* N	- O	- S	# 0.12
1091	AA		C	* C	- N	* O	- S	# 0.12
1091	AA		C	* C	- N	- O	* S	# 0.12
1200	AA		C	- C	* N	* O	- S	# 0.05
1200	AA		C	- C	* N	- O	* S	# 0.05
1200	AA		C	- C	- N	* O	* S	# 0.05
1196	AA		C	-1C	-1N	-1O	-1S	# 0.97
1195	AA		C	C	N	O	X	# 0.40
1090	AA		C	* C	* N	- O	- X	# 0.12
1091	AA		C	* C	- N	* O	- X	# 0.12
1200	AA		C	- C	* N	* O	- X	# 0.05
1196	AA		C	-1C	-1N	-1O	-1X	# 0.97
1269	AA		C	* C	* N	* S		1.27
1270	AA		C	* C	* N	- S		0.84
1271	AA		C	* C	- N	* S		0.68
1253	AA		C	*1C	*1N	-1S	#	0.45
1272	AA		C	- C	* N	* S		1.39
1273	AA		C	- C	- N	- S		0.29
1199	AA		C	-1C	-1N	-2S	#	43.86
1199	AA		C	-1C	-2N	-1S	#	43.86
1199	AA		C	-1C	-4N	-4S	#	43.86
1195	AA		C	C	N	S	S	# 0.40
1090	AA		C	* C	* N	- S	- S	# 0.12
1091	AA		C	* C	- N	* S	- S	# 0.12
1200	AA		C	- C	* N	* S	- S	# 0.05
1200	AA		C	- C	- N	* S	* S	# 0.05
1196	AA		C	-1C	-1N	-1S	-1S	# 0.97
1195	AA		C	C	N	S	X	# 0.40
1090	AA		C	* C	* N	- S	- X	# 0.12
1091	AA		C	* C	- N	* S	- X	# 0.12
1200	AA		C	- C	* N	* S	- X	# 0.05
1196	AA		C	-1C	-1N	-1S	-1X	# 0.97
1197	AA		C	* C	* N	- X		0.81
1199	AA		C	-1C	-2N	-1X	#	43.86
1193	AA		C	-2C	-1N	-1X	#	0.25
1195	AA		C	C	N	X	X	# 0.40
1090	AA		C	* C	* N	- X	- X	# 0.12
1196	AA		C	-1C	-1N	-1X	-1X	# 0.97
2101	AA		C	C	O			75.88
2102	AA	2	C	C	O			60.80
1275	AA		C	* C	- O			45.33
1276	AA	2	C	* C	- O			23.50
1277	AA		C	*1C	*1O			14.92
1278	AA	2	C	*1C	*1O			11.83

# Augmented Atoms

Screen Number	Fragment Definition						Frequency Percent
1279	AA		C	*1C	-10		10.84
1280	AA	2	C	*1C	-10		4.74
1281	AA	3	C	*1C	-10		2.71
1282	AA	4	C	*1C	-10		1.93
1283	AA		C	*1C	-20		16.45
1284	AA		C	*1C	-40		2.70
1285	AA		C	*2C	*10		3.96
1286	AA		C	*2C	-10		1.67
1287	AA		C	*4C	*10		5.34
1288	AA	2	C	*4C	*10		2.39
1289	AA	3	C	*4C	*10		0.48
1290	AA		C	*4C	-10		25.19
1291	AA	2	C	*4C	-10		10.71
1292	AA	3	C	*4C	-10		3.45
1293	AA	4	C	*4C	-10		1.58
1294	AA		C	*4C	-40		1.10
1295	AA		C	-1C	*10		11.58
1296	AA		C	-1C	-10		40.88
1302	AA		C	-1C	-20		28.91
1303	AA	2	C	-1C	-20		8.29
1306	AA		C	-1C	-40		26.47
1307	AA		C	-2C	*10		0.20
1308	AA		C	-2C	-10		0.80
1020	AA		C	-2C	-20	#	0.14
1190	AA		C	-3C	-10	#	0.20
1309	AA		C	* C	* O	* O	0.90
1310	AA		C	* C	* O	- O	5.39
1311	AA		C	- C	* O	* O	1.47
1312	AA		C	- C	- O	- O	28.04
1313	AA	2	C	- C	- O	- O	8.84
1199	AA		C	-1C	-10	-20	# 43.86
1199	AA		C	-1C	-40	-40	# 43.86
1195	AA		C	C	O	O O	# 0.40
1091	AA		C	* C	- O	- O - O	# 0.12
1200	AA		C	- C	* O	* O - O	# 0.05
1196	AA		C	-1C	-10	-10 -10	# 0.97
1195	AA		C	C	O	O S	# 0.40
1091	AA		C	* C	- O	- O - S	# 0.12
1200	AA		C	- C	* O	* O - S	# 0.05
1200	AA		C	- C	* O	- O * S	# 0.05
1196	AA		C	-1C	-10	-10 -1S	# 0.97
1195	AA		C	C	O	O X	# 0.40
1091	AA		C	* C	* O	- O - X	# 0.12
1200	AA		C	- C	* O	* O - X	# 0.05
1196	AA		C	-1C	-10	-10 -1X	# 0.97
1314	AA		C	C	O	S	0.64
1199	AA		C	-1C	-10	-2S	# 43.86
1199	AA		C	-1C	-20	-1S	# 43.86
1199	AA		C	-1C	-40	-4S	# 43.86
1195	AA		C	C	O	S S	# 0.40
1091	AA		C	* C	- O	- S - S	# 0.12
1200	AA		C	- C	* O	* S - S	# 0.05
1200	AA		C	- C	- O	* S * S	# 0.05
1196	AA		C	-1C	-10	-1S -1S	# 0.97
1195	AA		C	C	O	S X	# 0.40

# Augmented Atoms

Screen Number	Fragment Definition							Frequency Percent
1091	AA	C	* C	* O	- S	- X	#	0.12
1091	AA	C	* C	- O	* S	- X	#	0.12
1200	AA	C	- C	* O	* S	- X	#	0.05
1196	AA	C	-1C	-1O	-1S	-1X	#	0.97
1199	AA	C	-1C	-2O	-1X		#	43.86
1193	AA	C	-2C	-1O	-1X		#	0.25
1195	AA	C	C	O	X	X	#	0.40
1091	AA	C	* C	* O	- X	- X	#	0.12
1196	AA	C	-1C	-1O	-1X	-1X	#	0.97
2106	AA	C	C	P			#	36.37
1344	AA	C	* C	- P			#	2.97
1345	AA	C	*1C	-1P			#	0.47
1345	AA	C	*2C	-1P			#	0.47
1346	AA	C	*4C	-1P			#	2.63
1315	AA	C	- C	- P				1.30
1316	AA	C	-2C	-1P				0.11
1020	AA	C	-2C	-2P			#	0.14
1190	AA	C	-3C	-1P			#	0.20
2105	AA	C	C	S			#	31.14
1317	AA	C	* C	- S				8.93
1318	AA	2	C	* C	- S			2.23
1319	AA	3	C	* C	- S			0.54
1320	AA		C	*1C	*1S			4.10
1321	AA	2	C	*1C	*1S			1.72
1322	AA		C	*1C	-1S			1.16
1323	AA		C	*1C	-2S		#	1.03
1323	AA		C	*1C	-4S		#	1.03
1324	AA		C	*2C	*1S			5.45
1323	AA		C	*2C	-1S		#	1.03
1325	AA		C	*4C	*1S			2.38
1326	AA	2	C	*4C	*1S			0.58
1327	AA		C	*4C	-1S			7.63
1323	AA		C	*4C	-4S		#	1.03
1328	AA		C	-1C	*1S			4.50
1329	AA		C	-1C	-1S			7.34
1330	AA	2	C	-1C	-1S			1.98
1331	AA	3	C	-1C	-1S			0.43
1333	AA		C	-1C	-2S		#	0.25
1333	AA		C	-1C	-4S		#	0.25
1335	AA		C	-2C	*1S			0.91
1336	AA		C	-2C	-1S			0.40
1020	AA		C	-2C	-2S		#	0.14
1190	AA		C	-3C	-1S		#	0.20
1337	AA		C	C	S	S		0.74
1199	AA		C	-1C	-1S	-2S	#	43.86
1199	AA		C	-1C	-4S	-4S	#	43.86
1195	AA		C	C	S	S	S	0.40
1091	AA		C	* C	- S	- S	- S	0.12
1200	AA		C	- C	* S	* S	- S	0.05
1196	AA		C	-1C	-1S	-1S	-1S	0.97
1195	AA		C	C	S	S	X	0.40
1091	AA		C	* C	* S	- S	- X	0.12
1200	AA		C	- C	* S	* S	- X	0.05
1196	AA		C	-1C	-1S	-1S	-1X	0.97
1199	AA		C	-1C	-2S	-1X		43.86

# Augmented Atoms

Screen Number	Fragment Definition						Frequency Percent
1193	AA	C	-2C	-1S	-1X		# 0.25
1195	AA	C	C	S	X	X	# 0.40
1091	AA	C	* C	* S	- X	- X	# 0.12
1196	AA	C	-1C	-1S	-1X	-1X	# 0.97
1344	AA	C	* C	- Se			# 2.97
1345	AA	C	*1C	-1Se			# 0.47
1345	AA	C	*2C	-1Se			# 0.47
1346	AA	C	*4C	-1Se			# 2.63
1020	AA	C	-2C	-2Se			# 0.14
1190	AA	C	-3C	-1Se			# 0.20
1344	AA	C	* C	- Si			# 2.97
1345	AA	C	*1C	-1Si			# 0.47
1345	AA	C	*2C	-1Si			# 0.47
1346	AA	C	*4C	-1Si			# 2.63
1020	AA	C	-2C	-2Si			# 0.14
1190	AA	C	-3C	-1Si			# 0.20
1344	AA	C	* C	- Te			# 2.97
1345	AA	C	*1C	-1Te			# 0.47
1345	AA	C	*2C	-1Te			# 0.47
1346	AA	C	*4C	-1Te			# 2.63
1020	AA	C	-2C	-2Te			# 0.14
1190	AA	C	-3C	-1Te			# 0.20
2109	AA	C	C	X			# 33.25
1176	AA	C	* C	- X			19.40
1177	AA	2	C	* C	- X		7.30
1178	AA	3	C	* C	- X		2.13
1179	AA		C	*1C	-1X		1.94
1180	AA		C	*2C	-1X		1.34
1181	AA		C	*4C	-1X		17.48
1182	AA		C	- C	- X		7.92
1183	AA	2	C	- C	- X		2.18
1184	AA	3	C	- C	- X		0.81
1185	AA		C	-1C	-1X		7.60
1188	AA		C	-2C	-1X		0.69
1190	AA		C	-3C	-1X		# 0.20
1191	AA		C	-1C	-1X	-1X	4.83
1193	AA		C	-2C	-1X	-1X	# 0.25
1194	AA		C	C	X	X	X 4.37
1347	AA		C	Cl			14.11
1348	AA	2	C	Cl			4.63
1349	AA	3	C	Cl			1.04
1350	AA		C	Cl	Cl		0.77
1351	AA		C	Cl	Cl	Cl	0.35
961	AA		C	Cl	F		# 0.16
961	AA		C	Cl	I		# 0.16
1352	AA		C	- Cl	* N		0.85
1353	AA		C	F			10.12
1354	AA	2	C	F			3.32
1355	AA	3	C	F			1.39
1356	AA		C	F	F		5.18
1357	AA		C	F	F	F	4.49
1358	AA	2	C	F	F	F	0.88
961	AA		C	F	I		# 0.16
1359	AA		C	- F	* N		0.11
1386	AA		C	I			1.01

# Augmented Atoms

Screen Number	Fragment Definition						Frequency Percent
1387	AA	2	C	I			0.19
1388	AA		C	I	I		0.01
1389	AA		C	- I	* N		0.02
1390	AA		C	M			3.55
1391	AA		C	* M			# 6.30
1392	AA		C	- M			# 6.25
1393	AA		C	* N			49.27
1394	AA		C	*1N			40.50
1395	AA		C	*2N			14.45
1396	AA		C	*4N			20.41
1397	AA		C	-1N			58.10
1402	AA		C	-2N			6.98
1404	AA		C	-3N			4.65
1405	AA	2	C	-3N			0.94
1403	AA		C	-4N			27.74
2106	AA		C	N	N		# 36.37
1406	AA		C	* N	* N		15.53
1407	AA	2	C	* N	* N		5.53
1408	AA	3	C	* N	* N		2.43
1409	AA		C	* N	- N		8.70
1410	AA	2	C	* N	- N		1.83
1411	AA	3	C	* N	- N		0.54
1412	AA		C	*1N	*1N		2.53
1414	AA		C	*1N	*2N		6.52
1416	AA		C	*1N	*4N		3.07
1417	AA		C	*1N	-1N		1.07
1418	AA		C	*1N	-2N		0.86
1419	AA		C	*1N	-4N		0.32
1420	AA		C	*2N	-1N		0.82
1421	AA		C	*4N	*4N		6.90
1422	AA		C	*4N	-1N		1.30
1423	AA		C	*4N	-4N		5.40
1424	AA		C	- N	- N		6.63
1425	AA	2	C	- N	- N		1.16
1426	AA	3	C	- N	- N		0.31
1427	AA		C	-1N	-1N		0.60
1428	AA		C	-1N	-2N		0.29
1430	AA		C	-1N	-3N		0.14
1429	AA		C	-1N	-4N		1.22
1431	AA		C	-2N	-2N		0.02
1432	AA		C	-4N	-4N		4.68
1433	AA		C	N	N	N	5.10
1434	AA	2	C	N	N	N	1.41
1435	AA	3	C	N	N	N	0.56
1436	AA		C	* N	* N	* N	# 0.88
1437	AA		C	* N	* N	- N	2.57
1438	AA		C	- N	- N	- N	2.24
1439	AA		C	-1N	-1N	-1N	# 0.04
1367	AA		C	-1N	-1N	-2N	# 9.76
1367	AA		C	-1N	-4N	-4N	# 9.76
1367	AA		C	-4N	-4N	-4N	# 9.76
1365	AA		C	N	N	N	# 0.59
1200	AA		C	* N	* N	- N	# 0.05
1196	AA		C	-1N	-1N	-1N	# 0.97
1365	AA		C	N	N	N	# 0.59



# Augmented Atoms

Screen Number			Fragment Definition					Frequency Percent
1200	AA		C	* N	* N	- N	- O	# 0.05
1200	AA		C	* N	- N	- N	* O	# 0.05
1196	AA		C	-1N	-1N	-1N	-1O	# 0.97
1365	AA		C	N	N	N	S	# 0.59
1200	AA		C	* N	* N	- N	- S	# 0.05
1200	AA		C	* N	- N	- N	* S	# 0.05
1196	AA		C	-1N	-1N	-1N	-1S	# 0.97
1365	AA		C	N	N	N	X	# 0.59
1200	AA		C	* N	* N	- N	- X	# 0.05
1196	AA		C	-1N	-1N	-1N	-1X	# 0.97
1436	AA		C	* N	* N	* O		# 0.88
1440	AA		C	* N	* N	- O		2.77
1441	AA	2	C	* N	* N	- O		0.47
1442	AA		C	* N	- N	* O		0.15
1443	AA		C	- N	- N	- O		2.24
1444	AA	2	C	- N	- N	- O		0.14
1439	AA		C	-1N	-1N	-1O		# 0.04
1451	AA		C	-1N	-1N	-2O		# 0.21
1367	AA		C	-1N	-2N	-1O		# 9.76
1452	AA		C	-1N	-2N	-1O		# 0.18
1367	AA		C	-1N	-4N	-4O		# 9.76
1453	AA		C	-1N	-4N	-4O		# 1.09
1367	AA		C	-4N	-4N	-1O		# 9.76
1452	AA		C	-4N	-4N	-1O		# 0.18
1367	AA		C	-4N	-4N	-4O		# 9.76
1454	AA		C	-4N	-4N	-4O		# 1.91
1365	AA		C	N	N	O	O	# 0.59
1200	AA		C	* N	* N	- O	- O	# 0.05
1200	AA		C	* N	- N	* O	- O	# 0.05
1200	AA		C	- N	- N	* O	* O	# 0.05
1196	AA		C	-1N	-1N	-1O	-1O	# 0.97
1200	AA		C	* N	* N	- O	- S	# 0.05
1200	AA		C	* N	- N	* O	- S	# 0.05
1200	AA		C	* N	- N	- O	* S	# 0.05
1200	AA		C	- N	- N	* O	* S	# 0.05
1196	AA		C	-1N	-1N	-1O	-1S	# 0.97
1365	AA		C	N	N	O	X	# 0.59
1200	AA		C	* N	* N	- O	- X	# 0.05
1200	AA		C	* N	- N	* O	- X	# 0.05
1196	AA		C	-1N	-1N	-1O	-1X	# 0.97
1436	AA		C	* N	* N	* S		# 0.88
1445	AA		C	* N	* N	- S		1.97
1446	AA	2	C	* N	* N	- S		0.07
1447	AA		C	* N	- N	* S		2.29
1448	AA	2	C	* N	- N	* S		0.12
1449	AA		C	- N	- N	- S		1.12
1450	AA	2	C	- N	- N	- S		0.08
1439	AA		C	-1N	-1N	-1S		# 0.04
1367	AA		C	-1N	-1N	-2S		# 9.76
1451	AA		C	-1N	-1N	-2S		# 0.21
1367	AA		C	-1N	-2N	-1S		# 9.76
1452	AA		C	-1N	-2N	-1S		# 0.18
1367	AA		C	-1N	-4N	-4S		# 9.76
1453	AA		C	-1N	-4N	-4S		# 1.09
1367	AA		C	-4N	-4N	-1S		# 9.76

# Augmented Atoms

Screen Number	Fragment Definition						Frequency Percent
1452	AA	C	-4N	-4N	-1S		# 0.18
1367	AA	C	-4N	-4N	-4S		# 9.76
1454	AA	C	-4N	-4N	-4S		# 1.91
1365	AA	C	N	N	S	S	# 0.59
1200	AA	C	* N	* N	- S	- S	# 0.05
1200	AA	C	* N	- N	* S	- S	# 0.05
1200	AA	C	- N	- N	* S	* S	# 0.05
1196	AA	C	-1N	-1N	-1S	-1S	# 0.97
1365	AA	C	N	N	S	X	# 0.59
1200	AA	C	* N	* N	- S	- X	# 0.05
1200	AA	C	* N	- N	* S	- X	# 0.05
1196	AA	C	-1N	-1N	-1S	-1X	# 0.97
1378	AA	C	N	N	X		# 0.40
1379	AA	C	* N	* N	- X		0.29
1367	AA	C	-1N	-2N	-1X		# 9.76
1367	AA	C	-4N	-4N	-1X		# 9.76
1365	AA	C	N	N	X	X	# 0.59
1200	AA	C	* N	* N	- X	- X	# 0.05
1196	AA	C	-1N	-1N	-1X	-1X	# 0.97
2108	AA	C	N	O			# 44.41
1455	AA	C	* N	* O			2.73
1456	AA	2	C	* N	* O		0.63
1457	AA	C	* N	- O			14.41
1458	AA	2	C	* N	- O		5.00
1459	AA	3	C	* N	- O		1.38
1460	AA	C	*1N	*1O			0.99
1461	AA	C	*1N	-1O			0.63
1462	AA	C	*1N	-2O			9.29
1463	AA	C	*1N	-4O			1.16
1464	AA	C	*2N	*1O			1.38
1465	AA	C	*2N	-1O			0.30
1466	AA	C	*4N	*1O			0.25
1467	AA	C	*4N	-1O			0.95
1468	AA	C	*4N	-4O			4.42
1469	AA	C	- N	* O			1.68
1470	AA	C	- N	- O			28.84
1471	AA	2	C	- N	- O		10.44
1472	AA	3	C	- N	- O		4.87
1473	AA	4	C	- N	- O		3.68
1500	AA	C	-1N	*1O			# 2.47
1474	AA	C	-1N	-1O			1.75
1475	AA	C	-1N	-2O			8.11
1501	AA	C	-2N	*1O			# 1.94
1476	AA	C	-2N	-1O			0.13
1367	AA	C	-1N	-1N	-2O		# 9.76
1477	AA	C	-2N	-2O			0.39
1502	AA	C	-3N	-1O			# 0.12
1501	AA	C	-4N	*1O			# 1.94
1478	AA	C	-4N	-4O			23.05
1479	AA	C	N	O	O		4.22
1480	AA	2	C	N	O	O	0.55
1436	AA	C	* N	* O	* O		# 0.88
1481	AA	C	* N	* O	- O		0.46
1482	AA	C	- N	- O	- O		3.78
1439	AA	C	-1N	-1O	-1O		# 0.04

# Augmented Atoms

Screen Number			Fragment Definition				Frequency Percent
1367	AA	C	-1N	-1O	-2O		# 9.76
1503	AA	C	-1N	-1O	-2O		# 3.82
1367	AA	C	-1N	-4O	-4O		# 9.76
1367	AA	C	-2N	-1O	-1O		# 9.76
1367	AA	C	-4N	-1O	-4O		# 9.76
1365	AA	C	N	N	O	S	# 0.59
1503	AA	C	-4N	-1O	-4O		# 3.82
1367	AA	C	-4N	-4O	-4O		# 9.76
1365	AA	C	N	O	O	O	# 0.59
1200	AA	C	* N	* O	- O	- O	# 0.05
1504	AA	C	- N	* O	* O	- O	# 0.00
1196	AA	C	-1N	-1O	-1O	-1O	# 0.97
1365	AA	C	N	O	O	S	# 0.59
1200	AA	C	* N	* O	- O	- S	# 0.05
1200	AA	C	* N	- O	- O	* S	# 0.05
1504	AA	C	- N	* O	* O	- S	# 0.00
1504	AA	C	- N	* O	- O	* S	# 0.00
1196	AA	C	-1N	-1O	-1O	-1S	# 0.97
1365	AA	C	N	O	O	X	# 0.59
1200	AA	C	* N	* O	- O	- X	# 0.05
1200	AA	C	- N	* O	* O	- X	# 0.05
1196	AA	C	-1N	-1O	-1O	-1X	# 0.97
1483	AA	C	N	O	S		# 0.54
1436	AA	C	* N	* O	* S		# 0.88
1439	AA	C	-1N	-1O	-1S		# 0.04
1367	AA	C	-1N	-1O	-2S		# 9.76
1503	AA	C	-1N	-1O	-2S		# 3.82
1367	AA	C	-1N	-2O	-1S		# 9.76
1503	AA	C	-1N	-2O	-1S		# 3.82
1367	AA	C	-1N	-4O	-4S		# 9.76
1367	AA	C	-2N	-1O	-1S		# 9.76
1367	AA	C	-4N	-1O	-4S		# 9.76
1503	AA	C	-4N	-1O	-4S		# 3.82
1367	AA	C	-4N	-4O	-1S		# 9.76
1503	AA	C	-4N	-4O	-1S		# 3.82
1367	AA	C	-4N	-4O	-4S		# 9.76
1365	AA	C	N	O	S	S	# 0.59
1200	AA	C	* N	* O	- S	- S	# 0.05
1200	AA	C	* N	- O	* S	- S	# 0.05
1504	AA	C	- N	* O	* S	- S	# 0.00
1504	AA	C	- N	- O	* S	* S	# 0.00
1196	AA	C	-1N	-1O	-1S	-1S	# 0.97
1365	AA	C	N	O	S	X	# 0.59
1200	AA	C	* N	* O	- S	- X	# 0.05
1200	AA	C	* N	- O	* S	- X	# 0.05
1200	AA	C	- N	* O	* S	- X	# 0.05
1196	AA	C	-1N	-1O	-1S	-1X	# 0.97
1378	AA	C	N	O	X		# 0.40
1367	AA	C	-1N	-2O	-1X		# 9.76
1367	AA	C	-2N	-1O	-1X		# 9.76
1365	AA	C	N	O	X	X	# 0.59
1200	AA	C	* N	* O	- X	- X	# 0.05
1196	AA	C	-1N	-1O	-1X	-1X	# 0.97
1484	AA	C	N	P			# 0.29
2107	AA	C	N	S			# 42.77

# Augmented Atoms

Screen Number	Fragment Definition						Frequency Percent
1485	AA		C	* N	* S		5.70
1486	AA	2	C	* N	* S		1.19
1487	AA		C	* N	- S		3.57
1488	AA	2	C	* N	- S		0.25
1489	AA		C	*1N	*1S		2.72
1490	AA		C	*2N	*1S		2.26
1491	AA		C	*4N	*1S		1.62
1492	AA		C	- N	- S		2.05
1493	AA	2	C	- N	- S		0.27
1500	AA		C	-1N	*1S	#	2.47
1494	AA		C	-1N	-1S		0.29
1495	AA		C	-1N	-2S		0.18
1501	AA		C	-2N	*1S	#	1.94
1496	AA		C	-2N	-1S		0.11
1497	AA		C	-2N	-2S		0.16
1502	AA		C	-3N	-1S	#	0.12
1501	AA		C	-4N	*1S	#	1.94
1498	AA		C	-4N	-4S		1.15
1499	AA		C	N	S	S	0.92
1436	AA		C	* N	* S	* S	# 0.88
1439	AA		C	-1N	-1S	-1S	# 0.04
1367	AA		C	-1N	-1S	-2S	# 9.76
1503	AA		C	-1N	-1S	-2S	# 3.82
1367	AA		C	-1N	-4S	-4S	# 9.76
1367	AA		C	-2N	-1S	-1S	# 9.76
1367	AA		C	-4N	-1S	-4S	# 9.76
1503	AA		C	-4N	-1S	-4S	# 3.82
1367	AA		C	-4N	-4S	-4S	# 9.76
1365	AA		C	N	S	S S	# 0.59
1200	AA		C	* N	* S	- S - S	# 0.05
1504	AA		C	- N	* S	* S - S	# 0.00
1196	AA		C	-1N	-1S	-1S -1S	# 0.97
1365	AA		C	N	S	S X	# 0.59
1200	AA		C	* N	* S	- S - X	# 0.05
1200	AA		C	- N	* S	* S - X	# 0.05
1196	AA		C	-1N	-1S	-1S -1X	# 0.97
1378	AA		C	N	S	X	# 0.40
1367	AA		C	-1N	-2S	-1X	# 9.76
1367	AA		C	-2N	-1S	-1X	# 9.76
1367	AA		C	-4N	-4S	-1X	# 9.76
1365	AA		C	N	S	X X	# 0.59
1200	AA		C	* N	* S	- X - X	# 0.05
1196	AA		C	-1N	-1S	-1X -1X	# 0.97
1368	AA		C	N	X		1.28
1369	AA		C	* N	- X		1.09
1370	AA	2	C	* N	- X		0.18
1371	AA	3	C	* N	- X		0.02
1372	AA		C	*1N	-1X		0.25
1373	AA		C	*2N	-1X		0.14
1374	AA		C	*4N	-1X		0.75
1375	AA		C	-1N	-1X		0.14
1366	AA		C	N	X	X	# 0.99
1367	AA		C	-2N	-1X	-1X	# 9.76
1365	AA		C	N	X	X X	# 0.59
1196	AA		C	-1N	-1X	-1X -1X	# 0.97

# Augmented Atoms

Screen Number	Fragment Definition						Frequency Percent
1505	AA	C	* O				20.22
1510	AA	C	-2O				41.18
1511	AA	C	-4O				31.52
2107	AA	C	O	O			# 42.77
1376	AA	C	-2N	-1X			0.06
1512	AA	C	* O	* O			2.94
1513	AA	2	C	* O	* O		0.67
1514	AA		C	* O	- O		5.68
1515	AA	2	C	* O	- O		1.92
1516	AA		C	*1O	-1O		2.36
1517	AA		C	*1O	-2O		3.54
1518	AA		C	- O	- O		29.91
1519	AA	2	C	- O	- O		10.19
1520	AA	3	C	- O	- O		3.17
1521	AA	4	C	- O	- O		1.56
1522	AA		C	-1O	-1O		1.52
1523	AA		C	-1O	-2O		18.25
1524	AA	2	C	-1O	-2O		4.97
1525	AA		C	-1O	-4O		2.49
1526	AA		C	-4O	-4O		11.09
1527	AA	2	C	-4O	-4O		3.39
1551	AA		C	O	O	O	# 0.63
1436	AA		C	* O	* O	* O	# 0.88
1439	AA		C	-1O	-1O	-1O	# 0.04
1367	AA		C	-1O	-1O	-2O	# 9.76
1367	AA		C	-1O	-4O	-4O	# 9.76
1367	AA		C	-4O	-4O	-4O	# 9.76
1365	AA		C	O	O	O	# 0.59
1200	AA		C	* O	* O	- O	# 0.05
1196	AA		C	-1O	-1O	-1O	# 0.97
1365	AA		C	O	O	O	# 0.59
1200	AA		C	* O	* O	- O	# 0.05
1200	AA		C	* O	- O	- O	# 0.05
1196	AA		C	-1O	-1O	-1O	# 0.97
1365	AA		C	O	O	O	# 0.59
1200	AA		C	* O	* O	- O	# 0.05
1196	AA		C	-1O	-1O	-1O	# 0.97
1551	AA		C	O	O	S	# 0.63
1436	AA		C	* O	* O	* S	# 0.88
1439	AA		C	-1O	-1O	-1S	# 0.04
1367	AA		C	-1O	-1O	-2S	# 9.76
1367	AA		C	-1O	-2O	-1S	# 9.76
1367	AA		C	-1O	-4O	-4S	# 9.76
1367	AA		C	-4O	-4O	-1S	# 9.76
1367	AA		C	-4O	-4O	-4S	# 9.76
1365	AA		C	O	O	S	# 0.59
1200	AA		C	* O	* O	- S	# 0.05
1200	AA		C	* O	- O	* S	# 0.05
1200	AA		C	- O	- O	* S	# 0.05
1196	AA		C	-1O	-1O	-1S	# 0.97
1365	AA		C	O	O	S	# 0.59
1200	AA		C	* O	* O	- S	# 0.05
1200	AA		C	* O	- O	* S	# 0.05
1196	AA		C	-1O	-1O	-1S	# 0.97
1365	AA		C	O	O	S	# 0.59
1200	AA		C	* O	* O	- S	# 0.05
1200	AA		C	* O	- O	* S	# 0.05
1196	AA		C	-1O	-1O	-1S	# 0.97
1378	AA		C	O	O	X	# 0.40

# Augmented Atoms

Screen Number			Fragment Definition				Frequency Percent
1367	AA	C	-1O	-2O	-1X		# 9.76
1367	AA	C	-4O	-4O	-1X		# 9.76
1365	AA	C	O	O	X	X	# 0.59
1200	AA	C	* O	* O	- X	- X	# 0.05
1196	AA	C	-1O	-1O	-1X	-1X	# 0.97
1528	AA	C	O	P			0.20
2106	AA	C	O	S			# 36.37
1529	AA	C	* O	* S			0.08
1530	AA	C	* O	- S			0.29
1531	AA	C	- O	* S			0.37
1532	AA	C	- O	- S			0.55
1551	AA	C	O	S	S		# 0.63
1436	AA	C	* O	* S	* S		# 0.88
1439	AA	C	-1O	-1S	-1S		# 0.04
1367	AA	C	-1O	-1S	-2S		# 9.76
1367	AA	C	-1O	-4S	-4S		# 9.76
1367	AA	C	-2O	-1S	-1S		# 9.76
1367	AA	C	-4O	-1S	-4S		# 9.76
1367	AA	C	-4O	-4S	-4S		# 9.76
1365	AA	C	O	S	S	S	# 0.59
1200	AA	C	* O	* S	- S	- S	# 0.05
1200	AA	C	- O	* S	* S	- S	# 0.05
1196	AA	C	-1O	-1S	-1S	-1S	# 0.97
1365	AA	C	O	S	S	X	# 0.59
1200	AA	C	* O	* S	- S	- X	# 0.05
1200	AA	C	- O	* S	* S	- X	# 0.05
1196	AA	C	-1O	-1S	-1S	-1X	# 0.97
1378	AA	C	O	S	X		# 0.40
1367	AA	C	-1O	-2S	-1X		# 9.76
1367	AA	C	-2O	-1S	-1X		# 9.76
1367	AA	C	-4O	-4S	-1X		# 9.76
1365	AA	C	O	S	X	X	# 0.59
1200	AA	C	* O	* S	- X	- X	# 0.05
1196	AA	C	-1O	-1S	-1X	-1X	# 0.97
1380	AA	C	O	X			1.00
1383	AA	C	* O	- X			# 0.37
1384	AA	C	-1O	-1X			# 1.03
1385	AA	C	-2O	-1X			# 0.34
1366	AA	C	O	X	X		# 0.99
1367	AA	C	-2O	-1X	-1X		# 9.76
1365	AA	C	O	X	X	X	# 0.59
1196	AA	C	-1O	-1X	-1X	-1X	# 0.97
1552	AA	C	* P				# 1.15
1533	AA	C	- P				2.98
1534	AA	C	-2P				# 0.07
1534	AA	C	-3P				# 0.07
1534	AA	C	-4P				# 0.07
1535	AA	C	P	P			0.19
1536	AA	C	P	S			0.04
1381	AA	C	P	X			0.08
1537	AA	C	* S				10.23
1538	AA	C	- S				17.07
1539	AA	C	-1S				14.89
1542	AA	C	-2S				# 2.60
1542	AA	C	-4S				# 2.60

# Augmented Atoms

Screen Number	Fragment Definition						Frequency Percent
2106	AA	C	S	S			# 36.37
1543	AA	C	* S	* S			0.47
1544	AA	C	* S	- S			0.96
1545	AA	C	- S	- S			0.38
1551	AA	C	S	S	S		# 0.63
1436	AA	C	* S	* S	* S		# 0.88
1439	AA	C	-1S	-1S	-1S		# 0.04
1367	AA	C	-1S	-1S	-2S		# 9.76
1367	AA	C	-1S	-4S	-4S		# 9.76
1367	AA	C	-4S	-4S	-4S		# 9.76
1365	AA	C	S	S	S	S	# 0.59
1200	AA	C	* S	* S	- S	- S	# 0.05
1196	AA	C	-1S	-1S	-1S	-1S	# 0.97
1365	AA	C	S	S	S	X	# 0.59
1200	AA	C	* S	* S	- S	- X	# 0.05
1196	AA	C	-1S	-1S	-1S	-1X	# 0.97
1378	AA	C	S	S	X		# 0.40
1367	AA	C	-1S	-2S	-1X		# 9.76
1367	AA	C	-4S	-4S	-1X		# 9.76
1365	AA	C	S	S	X	X	# 0.59
1200	AA	C	* S	* S	- X	- X	# 0.05
1196	AA	C	-1S	-1S	-1X	-1X	# 0.97
1382	AA	C	S	X			0.74
1383	AA	C	* S	- X			# 0.37
1384	AA	C	-1S	-1X			# 1.03
1385	AA	C	-2S	-1X			# 0.34
1366	AA	C	S	X	X		# 0.99
1367	AA	C	-2S	-1X	-1X		# 9.76
1365	AA	C	S	X	X	X	# 0.59
1196	AA	C	-1S	-1X	-1X	-1X	# 0.97
1552	AA	C	* Se				# 1.15
1546	AA	2 C	Si				2.69
1547	AA	3 C	Si				2.51
1548	AA	4 C	Si				1.43
1552	AA	C	* Si				# 1.15
1549	AA	C	- Si				2.84
1552	AA	C	* Te				# 1.15
1360	AA	C	X				26.42
1361	AA	C	X	X			6.02
1362	AA	2 C	X	X			1.63
1364	AA	C	X	X	X		4.93
1365	AA	C	X	X	X	X	# 0.59
1347	AA	Cl	C				14.11
1553	AA	Cl	P				0.13
1554	AA	Cl	S				0.08
1353	AA	F	C				10.12
1555	AA	F	P				0.27
1556	AA	F	S				0.06
1386	AA	I	C				1.01
1558	AA	M	As				# 3.13
1391	AA	M	* As				# 6.30
1392	AA	M	- As				# 6.25
1558	AA	M	B				# 3.13
1391	AA	M	* B				# 6.30
1392	AA	M	- B				# 6.25

# Augmented Atoms

Screen Number	Fragment Definition				Frequency Percent
1390	AA	M	C		3.55
1391	AA	M	* C		# 6.30
1392	AA	M	- C		# 6.25
1563	AA	M	N		4.05
1391	AA	M	* N		# 6.30
1392	AA	M	- N		# 6.25
1564	AA	M	O		# 4.03
1391	AA	M	* O		# 6.30
1392	AA	M	- O		# 6.25
1558	AA	M	P		# 3.13
1391	AA	M	* P		# 6.30
1392	AA	M	- P		# 6.25
1564	AA	M	S		# 4.03
1391	AA	M	* S		# 6.30
1392	AA	M	- S		# 6.25
1558	AA	M	Se		# 3.13
1391	AA	M	* Se		# 6.30
1392	AA	M	- Se		# 6.25
1558	AA	M	Si		# 3.13
1391	AA	M	* Si		# 6.30
1392	AA	M	- Si		# 6.25
1558	AA	M	Te		# 3.13
1391	AA	M	* Te		# 6.30
1392	AA	M	- Te		# 6.25
1558	AA	M	X		# 3.13
1391	AA	M	* X		# 6.30
1392	AA	M	- X		# 6.25
1667	AA	N	-4As		# 2.86
1653	AA	N	- As	* N	# 0.13
1654	AA	N	As	P	# 0.20
954	AA	N	B		0.22
1667	AA	N	-4B		# 2.86
1653	AA	N	- B	* N	# 0.13
1654	AA	N	B	P	# 0.20
1393	AA	N	* C		49.27
1565	AA	4	N	* C	8.42
1566	AA	5	N	* C	3.53
1567	AA	6	N	* C	2.31
1394	AA		N	*1C	40.50
1395	AA		N	*2C	14.45
1396	AA		N	*4C	20.41
1397	AA		N	-1C	58.10
1402	AA		N	-2C	6.98
1404	AA		N	-3C	4.65
1403	AA		N	-4C	27.74
2103	AA		N	C C	61.82
1573	AA		N	* C * C	43.08
1574	AA	2	N	* C * C	23.90
1575	AA	3	N	* C * C	10.35
1576	AA	4	N	* C * C	5.64
1577	AA		N	* C - C	26.04
1578	AA	2	N	* C - C	7.82
1579	AA	3	N	* C - C	1.99
1580	AA		N	*1C *1C	30.13
1581	AA	2	N	*1C *1C	10.29



# Augmented Atoms

Screen Number	Fragment Definition							Frequency Percent
1582	AA	3	N	*1C	*1C			2.86
1585	AA		N	*1C	*2C			8.37
1586	AA	2	N	*1C	*2C			1.31
1587	AA		N	*2C	-1C			0.65
1588	AA		N	*4C	*4C			14.32
1589	AA	2	N	*4C	*4C			6.63
1590	AA	3	N	*4C	*4C			2.11
1591	AA		N	*4C	-1C			0.87
1592	AA		N	- C	- C			35.21
1593	AA	2	N	- C	- C			13.94
1594	AA	3	N	- C	- C			5.73
1595	AA		N	-1C	-1C			14.72
1596	AA	2	N	-1C	-1C			2.46
1599	AA		N	-1C	-2C			2.33
1600	AA		N	-1C	-4C			21.05
1601	AA		N	-4C	-4C			1.92
1602	AA		N	C	C	C		31.96
1603	AA	2	N	C	C	C		10.54
1604	AA	3	N	C	C	C		2.71
1605	AA		N	* C	* C	* C		3.71
1606	AA	2	N	* C	* C	* C		0.51
1607	AA		N	* C	* C	- C		22.55
1608	AA		N	*1C	*1C	-1C		21.59
1609	AA		N	- C	- C	- C		8.91
1610	AA	2	N	- C	- C	- C		1.24
1611	AA		N	C	C	C	C	1.17
1612	AA	2	N	C	C	C	C	0.16
1613	AA		N	* C	* C	* C	* C	# 0.35
1613	AA		N	* C	* C	* C	- C	# 0.35
1613	AA		N	* C	* C	- C	- C	# 0.35
1614	AA		N	- C	- C	- C	- C	0.83
1615	AA		N	C	C	C	N	# 0.08
1615	AA		N	C	C	C	O	# 0.08
1615	AA		N	C	C	C	S	# 0.08
1616	AA		N	C	C	N		5.31
1617	AA		N	* C	* C	* N		# 0.97
1618	AA		N	- C	- C	- N		0.41
1619	AA		N	C	C	O		0.98
1617	AA		N	* C	* C	* O		# 0.97
1620	AA		N	* C	* C	- O		0.53
1621	AA		N	- C	- C	- O		0.27
1622	AA		N	C	C	P		0.32
1623	AA		N	C	C	S		2.00
1617	AA		N	* C	* C	* S		# 0.97
1624	AA		N	- C	- C	- S		0.90
2108	AA		N	C	N			# 44.41
1625	AA		N	* C	- N			0.76
1626	AA		N	*1C	*1N			5.00
1628	AA		N	*2C	*1N			5.47
1629	AA	2	N	*2C	*1N			1.61
1630	AA		N	- C	* N			3.78
1631	AA	2	N	- C	* N			0.54
1632	AA		N	-1C	-1N			1.19
1634	AA		N	-2C	-1N			2.84
1635	AA		N	-4C	-1N			2.74

# Augmented Atoms

Screen Number	Fragment Definition				Frequency Percent
2109	AA	N	C	O	# 33.25
1636	AA	N	* C	* O	1.22
1637	AA	N	* C	- O	0.71
1638	AA	N	*4C	-2O	0.19
1639	AA	N	- C	* O	0.15
1640	AA	N	- C	- O	6.80
1641	AA	N	-1C	-1O	0.30
1642	AA	N	-1C	-2O	5.21
1643	AA	N	-2C	-1O	1.03
1644	AA	N	C	P	0.62
1645	AA	N	C	S	4.46
1646	AA	N	* C	- S	0.98
1647	AA	N	- C	* S	0.19
1648	AA	N	- C	- S	3.03
1649	AA	N	-1C	-1S	0.97
1650	AA	N	-1C	-4S	1.46
1651	AA	N	-4C	-4S	0.57
2105	AA	N	C	X	# 31.14
1563	AA	N	M		4.05
1391	AA	N	* M		# 6.30
1392	AA	N	- M		# 6.25
1655	AA	N	N		13.07
1656	AA	3	N	N	3.57
1657	AA	5	N	N	0.66
1658	AA	7	N	N	0.24
1659	AA	N	*1N		6.78
1660	AA	N	*2N		0.99
1661	AA	N	*4N		0.64
1662	AA	N	- N		6.18
1663	AA	N	-1N		4.36
1665	AA	N	-2N		1.77
1666	AA	3	N	-2N	0.78
1668	AA	N	-3N		0.08
1667	AA	N	-4N		# 2.86
2106	AA	N	N	N	# 36.37
1669	AA	N	* N	* N	1.06
1653	AA	N	* N	- N	# 0.13
1670	AA	N	- N	- N	0.43
1671	AA	N	N	O	0.28
1653	AA	N	* N	- O	# 0.13
1654	AA	N	N	P	# 0.20
1653	AA	N	* N	- P	# 0.13
1672	AA	N	N	S	0.22
1653	AA	N	* N	- S	# 0.13
1653	AA	N	* N	- Se	# 0.13
1653	AA	N	* N	- Si	# 0.13
1653	AA	N	* N	- Te	# 0.13
1653	AA	N	* N	- X	# 0.13
1673	AA	2	N	O	1.99
1674	AA	3	N	O	0.63
1675	AA	5	N	O	0.07
1676	AA	N	* O		1.31
1677	AA	N	- O		8.04
1678	AA	N	-1O		2.25
1679	AA	N	-2O		5.78

# Augmented Atoms

Screen Number	Fragment Definition					Frequency Percent
1667	AA	N	-4O			# 2.86
1680	AA	N	O	O		5.54
1681	AA	2	N	O	O	1.28
1682	AA	3	N	O	O	0.42
1683	AA	5	N	O	O	0.03
1684	AA		N	O	O O	0.29
1654	AA		N	O	P	# 0.20
1694	AA		N	O	S	# 0.10
1685	AA		N	* P		0.20
1686	AA		N	- P		0.60
1687	AA		N	-1P		0.36
1688	AA		N	-2P		0.09
1667	AA		N	-4P		# 2.86
1689	AA		N	-4P		0.21
1654	AA		N	P	P	# 0.20
1654	AA		N	P	S	# 0.20
1654	AA		N	P	Se	# 0.20
1654	AA		N	P	Si	# 0.20
1654	AA		N	P	Te	# 0.20
1654	AA		N	P	X	# 0.20
1690	AA	2	N	S		0.62
1691	AA		N	* S		0.62
1692	AA		N	*2S		# 2.59
1692	AA		N	*4S		# 2.59
1693	AA		N	- S		4.40
1692	AA		N	-2S		# 2.59
1667	AA		N	-4S		# 2.86
1692	AA		N	-4S		# 2.59
1694	AA		N	S	S	# 0.10
1667	AA		N	-4Se		# 2.86
1695	AA		N	Si		0.24
1667	AA		N	-4Si		# 2.86
1667	AA		N	-4Te		# 2.86
1559	AA		N	X		0.06
1718	AA		O	As	As	# 0.63
1718	AA		O	As	B	# 0.63
1718	AA		O	As	N	# 0.63
1718	AA		O	As	O	# 0.63
1718	AA		O	As	P	# 0.63
1718	AA		O	As	S	# 0.63
1718	AA		O	As	Se	# 0.63
1718	AA		O	As	Si	# 0.63
1718	AA		O	As	Te	# 0.63
1718	AA		O	As	X	# 0.63
955	AA		O	* B		# 0.30
955	AA		O	- B		# 0.30
1718	AA		O	B	B	# 0.63
1718	AA		O	B	N	# 0.63
1718	AA		O	B	O	# 0.63
1718	AA		O	B	P	# 0.63
1718	AA		O	B	S	# 0.63
1718	AA		O	B	Se	# 0.63
1718	AA		O	B	Si	# 0.63
1718	AA		O	B	Te	# 0.63
1718	AA		O	B	X	# 0.63

# Augmented Atoms

Screen Number	Fragment Definition					Frequency Percent
1505	AA		O	* C		20.22
1697	AA	2	O	* C		8.15
1698	AA	3	O	* C		3.30
1699	AA	4	O	* C		2.15
1510	AA		O	-2C		41.18
1511	AA		O	-4C		31.52
2104	AA		O	C	C	47.10
1706	AA		O	* C	* C	17.14
1818	AA		O	* C	- C	# 0.15
1707	AA		O	- C	- C	38.39
1708	AA	2	O	- C	- C	17.09
1709	AA	3	O	- C	- C	6.63
1710	AA	4	O	- C	- C	3.26
1819	AA		O	C	C C	# 0.46
2105	AA		O	C	M	# 31.14
2105	AA		O	C	N	# 31.14
1711	AA		O	* C	* N	1.07
1712	AA		O	- C	- N	1.20
2105	AA		O	C	O	# 31.14
1713	AA		O	C	P	2.32
2105	AA		O	C	P	# 31.14
1714	AA	2	O	C	P	1.72
1715	AA	3	O	C	P	0.73
1716	AA		O	C	S	0.97
1717	AA	2	O	C	S	0.15
1564	AA		O	M		# 4.03
1391	AA		O	* M		# 6.30
1392	AA		O	- M		# 6.25
1676	AA		O	* N		1.31
1677	AA		O	- N		8.04
1678	AA		O	-1N		2.25
1679	AA		O	-2N		5.78
1667	AA		O	-4N		# 2.86
1718	AA		O	N	N	# 0.63
1718	AA		O	N	O	# 0.63
1718	AA		O	N	P	# 0.63
1718	AA		O	N	S	# 0.63
1718	AA		O	N	Se	# 0.63
1718	AA		O	N	Si	# 0.63
1718	AA		O	N	Te	# 0.63
1718	AA		O	N	X	# 0.63
1720	AA		O	O		0.23
1718	AA		O	O	O	# 0.63
1718	AA		O	O	P	# 0.63
1718	AA		O	O	S	# 0.63
1718	AA		O	O	Se	# 0.63
1718	AA		O	O	Si	# 0.63
1718	AA		O	O	Te	# 0.63
1718	AA		O	O	X	# 0.63
1721	AA		O	* P		0.36
1722	AA		O	-1P		2.22
1723	AA		O	-2P		1.11
1724	AA		O	-4P		1.35
1725	AA	2	O	-4P		1.20
1726	AA	3	O	-4P		0.83

# Augmented Atoms

Screen Number	Fragment Definition						Frequency Percent
1729	AA		O	-2S			4.78
1718	AA		O	P	P		# 0.63
1718	AA		O	P	S		# 0.63
1718	AA		O	P	Se		# 0.63
1718	AA		O	P	Si		# 0.63
1718	AA		O	P	Te		# 0.63
1718	AA		O	P	X		# 0.63
1727	AA		O	* S			0.09
1728	AA		O	-1S			1.03
1730	AA		O	-4S			4.43
1731	AA	2	O	-4S			4.41
1732	AA	3	O	-4S			2.17
1718	AA		O	S	S		# 0.63
1718	AA		O	S	Se		# 0.63
1718	AA		O	S	Si		# 0.63
1718	AA		O	S	Te		# 0.63
1718	AA		O	S	X		# 0.63
1718	AA		O	Se	Se		# 0.63
1718	AA		O	Se	Si		# 0.63
1718	AA		O	Se	Te		# 0.63
1718	AA		O	Se	X		# 0.63
1733	AA	2	O	Si			0.86
1734	AA		O	* Si			0.15
1735	AA		O	- Si			1.82
1718	AA		O	Si	Si		# 0.63
1718	AA		O	Si	Te		# 0.63
1718	AA		O	Si	X		# 0.63
1718	AA		O	Te	Te		# 0.63
1718	AA		O	Te	X		# 0.63
1560	AA		O	X			0.51
1718	AA		O	X	X		# 0.63
1820	AA		P	As			# 0.35
1820	AA		P	B			# 0.35
1738	AA	2	P	C			1.26
1552	AA		P	* C			# 1.15
1533	AA		P	- C			2.98
1534	AA		P	-2C			# 0.07
1534	AA		P	-3C			# 0.07
1534	AA		P	-4C			# 0.07
1739	AA		P	C	C		2.11
2105	AA		P	C	C		# 31.14
1740	AA		P	- C	- C		1.95
1741	AA		P	C	C	C	1.75
1742	AA		P	C	C	O	0.37
1743	AA		P	C	N		0.29
1744	AA		P	C	O		1.25
1745	AA		P	C	O	O	0.94
1746	AA		P	C	O	O	O 0.69
1748	AA		P	C	O	O	O # 0.75
1748	AA		P	C	O	O	S # 0.75
1748	AA		P	C	O	S	S # 0.75
1747	AA		P	C	S		0.17
1748	AA		P	C	S	S	S # 0.75
1553	AA		P	Cl			0.13
1555	AA		P	F			0.27

# Augmented Atoms

Screen Number	Fragment Definition						Frequency Percent
1558	AA	P	M				# 3.13
1391	AA	P	* M				# 6.30
1392	AA	P	- M				# 6.25
1750	AA	2	P	N			0.18
1685	AA	P	* N				0.20
1686	AA	P	- N				0.60
1687	AA	P	-1N				0.36
1688	AA	P	-2N				0.09
1667	AA	P	-4N				# 2.86
1689	AA	P	-4N				0.21
1751	AA	P	N	N			0.27
1752	AA	P	N	O			0.49
1753	AA	P	N	O	O		0.33
1755	AA	P	N	O	O	O	# 0.19
1755	AA	P	N	O	O	S	# 0.19
1755	AA	P	N	O	S	S	# 0.19
1754	AA	P	N	S			0.13
1755	AA	P	N	S	S	S	# 0.19
1756	AA	2	P	O			0.77
1721	AA	P	* O				0.36
1722	AA	P	-1O				2.22
1723	AA	P	-2O				1.11
1724	AA	P	-4O				1.35
1767	AA	2	P	-4O			# 0.41
1768	AA	3	P	-4O			# 0.23
1757	AA	P	O	O			2.69
1758	AA	P	O	O	O		2.16
1759	AA	P	O	O	O	O	1.06
1762	AA	P	* S				0.06
1769	AA	P	O	O	O	O	# 1.29
1769	AA	P	O	O	O	S	# 1.29
1769	AA	P	O	O	S	S	# 1.29
1760	AA	P	O	S			0.41
1769	AA	P	O	S	S	S	# 1.29
1820	AA	P	P				# 0.35
1761	AA	P	S				0.53
1763	AA	P	-1S				0.22
1764	AA	P	-2S				0.25
1765	AA	P	-4S				0.11
1767	AA	2	P	-4S			# 0.41
1768	AA	3	P	-4S			# 0.23
1766	AA	P	S	S			0.18
1769	AA	P	S	S	S	S	# 1.29
1820	AA	P	Se				# 0.35
1820	AA	P	Si				# 0.35
1820	AA	P	Te				# 0.35
1561	AA	P	X				0.42
1749	AA	P	X	X			0.32
1537	AA	S	* C				10.23
1538	AA	S	- C				17.07
1770	AA	2	S	- C			3.55
1539	AA	S	-1C				14.89
1542	AA	S	-2C				# 2.60
1542	AA	S	-4C				# 2.60
2106	AA	S	C	C			# 36.37

# Augmented Atoms

Screen Number	Fragment Definition						Frequency Percent
1772	AA		S	* C	* C		9.14
1773	AA	2	S	* C	* C		1.52
1818	AA		S	* C	- C		# 0.15
1774	AA		S	- C	- C		7.80
1775	AA	2	S	- C	- C		0.91
1819	AA		S	C	C	C	# 0.46
1776	AA		S	C	C	N	0.05
1777	AA		S	C	C	O	1.96
1778	AA	2	S	C	C	O	0.18
1779	AA		S	* C	* C	- O	0.35
1780	AA		S	- C	- C	- O	1.61
1781	AA		S	* C	* C	- O - O	0.25
1782	AA		S	- C	- C	- O - O	1.23
2109	AA		S	C	N		# 33.25
1783	AA		S	* C	* N		0.48
1784	AA		S	- C	- N		4.15
1785	AA	2	S	- C	- N		0.34
1786	AA		S	C	N	O O	4.19
1787	AA		S	* C	* N	- O - O	0.19
1788	AA		S	- C	- N	- O - O	4.02
1789	AA		S	* C	* O		0.04
1790	AA		S	* C	- O		0.59
1791	AA		S	- C	- O		7.61
1792	AA	2	S	- C	- O		1.22
1793	AA	3	S	- C	- O		0.38
1794	AA		S	* C	- O	- O	0.47
1795	AA		S	- C	- O	- O	7.20
1796	AA		S	C	O	O O	2.09
1797	AA	2	S	C	O	O O	0.65
1798	AA		S	C	P		0.21
1799	AA	2	S	C	P		0.04
2105	AA		S	C	S		# 31.14
1554	AA		S	Cl			0.08
1556	AA		S	F			0.06
1564	AA		S	M			# 4.03
1391	AA		S	* M			# 6.30
1392	AA		S	- M			# 6.25
1801	AA	2	S	N			0.47
1691	AA		S	* N			0.62
1692	AA		S	* 2N			# 2.59
1692	AA		S	* 4N			# 2.59
1693	AA		S	- N			4.40
1692	AA		S	- 2N			# 2.59
1667	AA		S	- 4N			# 2.86
1692	AA		S	- 4N			# 2.59
1802	AA		S	N	N		0.25
1803	AA		S	N	O		4.51
1804	AA	2	S	N	O		0.39
1805	AA	3	S	N	O		0.04
1806	AA		S	* N	- O		0.26
1807	AA		S	N	O	O O	0.09
1808	AA		S	N	P		0.00
1809	AA	2	S	O			1.44
1810	AA	3	S	O			0.45
1727	AA		S	* O			0.09

# Augmented Atoms

Screen Number	Fragment Definition						Frequency Percent
1728	AA	S	-1O				1.03
1729	AA	S	-2O				4.78
1730	AA	S	-4O				4.43
1811	AA	S	O	O			8.41
1812	AA	S	O	O	O		2.72
1813	AA	S	O	O	O	O	0.47
1814	AA	S	O	P			0.00
1761	AA	S	P				0.53
1762	AA	S	* P				0.06
1763	AA	S	-1P				0.22
1764	AA	S	-2P				0.25
1765	AA	S	-4P				0.11
1815	AA	S	* S				0.21
1816	AA	S	- S				0.24
1562	AA	S	X				0.14
1800	AA	S	X	X			0.02
1820	AA	Se	As			#	0.35
1820	AA	Se	B			#	0.35
1552	AA	Se	* C			#	1.15
1558	AA	Se	M			#	3.13
1391	AA	Se	* M			#	6.30
1392	AA	Se	- M			#	6.25
1667	AA	Se	-4N			#	2.86
1820	AA	Se	P			#	0.35
1820	AA	Se	Se			#	0.35
1820	AA	Se	Si			#	0.35
1820	AA	Se	Te			#	0.35
952	AA	Se	X			#	0.53
1820	AA	Si	As			#	0.35
1820	AA	Si	B			#	0.35
1552	AA	Si	* C			#	1.15
1549	AA	Si	- C				2.84
1558	AA	Si	M			#	3.13
1391	AA	Si	* M			#	6.30
1392	AA	Si	- M			#	6.25
1695	AA	Si	N				0.24
1667	AA	Si	-4N			#	2.86
1734	AA	Si	* O				0.15
1735	AA	Si	- O				1.82
1820	AA	Si	P			#	0.35
1820	AA	Si	Se			#	0.35
1820	AA	Si	Si			#	0.35
1820	AA	Si	Te			#	0.35
952	AA	Si	X			#	0.53
1817	AA	Si	X				0.15
1820	AA	Te	As			#	0.35
1820	AA	Te	B			#	0.35
1552	AA	Te	* C			#	1.15
1558	AA	Te	M			#	3.13
1391	AA	Te	* M			#	6.30
1392	AA	Te	- M			#	6.25
1667	AA	Te	-4N			#	2.86
1820	AA	Te	P			#	0.35
1820	AA	Te	Se			#	0.35
1820	AA	Te	Si			#	0.35



# Augmented Atoms

Screen Number		Fragment Definition		Frequency Percent	
1820	AA	Te	Te	#	0.35
952	AA	Te	X	#	0.53
952	AA	X	As	#	0.53
952	AA	X	B	#	0.53
1360	AA	X	C		26.42
1558	AA	X	M	#	3.13
1391	AA	X	* M	#	6.30
1392	AA	X	- M	#	6.25
1559	AA	X	N		0.06
1560	AA	X	O		0.51
1561	AA	X	P		0.42
1562	AA	X	S		0.14
952	AA	X	Se	#	0.53
952	AA	X	Si	#	0.53
1817	AA	X	Si		0.15
952	AA	X	Te	#	0.53
1557	AA	X	X		0.06

## Hydrogen Augmented Atoms

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### HA Screens

**Hydrogen augmented atom (HA)** add hydrogen count specifications to the basic AA description. HA screens give the hydrogen count for the central atom.

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### HA Screen Definitions

These screens are augmented atoms whose definitions include a specification of the hydrogen attached to the central atom. The HA fragments used as screens are only those that occur relatively frequently, most having carbon, nitrogen or oxygen central atoms.

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# Hydrogen Augmented Atoms

Screen Number			Fragment Definition	Frequency Percent
951	HA		AlH2-1C	# 0.07
951	HA		AlH -1C -1C	# 0.07
951	HA		AsH2-1C	# 0.07
951	HA		AsH -1C -1C	# 0.07
951	HA		B H2-1C	# 0.07
951	HA		B H -1C -1C	# 0.07
963	HA		C H3-1C	57.28
964	HA	2	C H3-1C	37.58
965	HA	3	C H3-1C	22.43
966	HA	4	C H3-1C	14.08
967	HA	6	C H3-1C	6.24
970	HA		C H2-2C	5.09
973	HA		C H -3C	0.52
989	HA		C H2*1C *1C	27.77
990	HA	2	C H2*1C *1C	22.12
991	HA	3	C H2*1C *1C	14.50
996	HA		C H *1C *2C	12.78
997	HA	2	C H *1C *2C	6.93
1006	HA		C H2-1C -1C	35.14
1007	HA	2	C H2-1C -1C	22.54
1008	HA	3	C H2-1C -1C	15.40
1009	HA	5	C H2-1C -1C	9.31
1010	HA	8	C H2-1C -1C	6.05
1015	HA		C H -1C -2C	12.02
1016	HA	2	C H -1C -2C	5.64
1017	HA	3	C H -1C -2C	1.54
1018	HA	4	C H -1C -2C	0.99
1028	HA		C H *1C *1C *1C	6.09
1034	HA		C H *1C *1C -1C	10.75
1051	HA		C H -1C -1C -1C	10.06
1052	HA	2	C H -1C -1C -1C	3.43
1053	HA	3	C H -1C -1C -1C	1.59
1102	HA		C H *1C *1C *1N	# 3.90
1105	HA		C H *1C *1C -1N	5.12
1111	HA		C H *1C -1C *1N	6.44
1126	HA		C H -1C -1C -1N	10.60
1127	HA	2	C H -1C -1C -1N	4.59
1102	HA		C H *1C *1C *1O	# 3.90
1166	HA		C H *1C *1C -1O	# 7.88
1167	HA		C H *1C -1C *1O	# 6.41
1149	HA		C H -1C -1C -1O	8.63
1150	HA	2	C H -1C -1C -1O	2.01
1102	HA		C H *1C *1C *1S	# 3.90
1166	HA		C H *1C *1C -1S	# 7.88
1167	HA		C H *1C -1C *1S	# 6.41
1164	HA		C H -1C -1C -1S	0.62
1078	HA		C H *1C *1C -1X	0.47
1083	HA		C H -1C -1C -1X	0.44
1210	HA		C H2*1C *1N	16.15
1211	HA	2	C H2*1C *1N	11.14
1214	HA		C H *1C *2N	# 14.42
1214	HA		C H *2C *1N	# 14.42
1214	HA		C H *4C *4N	# 14.42
1235	HA		C H2-1C -1N	26.67
1236	HA	2	C H2-1C -1N	11.86

# Hydrogen Augmented Atoms

Screen Number			Fragment Definition			Frequency Percent
1237	HA	3	C H2-1C	-1N		4.79
1238	HA	4	C H2-1C	-1N		2.51
1239	HA	5	C H2-1C	-1N		1.08
1192	HA		C H -1C	-2N		# 5.19
1241	HA		C H -1C	-2N		2.80
1246	HA		C H -2C	-1N		0.53
1251	HA		C H *1C	*1N	*1N	# 1.12
1254	HA		C H *1C	*1N	-1N	# 1.20
1259	HA		C H -1C	*1N	*1N	# 0.85
1192	HA		C H -1C	-1N	-1N	# 5.19
1260	HA		C H -1C	-1N	-1N	# 0.96
1251	HA		C H *1C	*1N	*1O	# 1.12
1274	HA		C H *1C	*1N	-1O	# 2.43
1254	HA		C H *1C	-1N	*1O	# 1.20
1259	HA		C H -1C	*1N	*1O	# 0.85
1192	HA		C H -1C	-1N	-1O	# 5.19
1260	HA		C H -1C	-1N	-1O	# 0.96
1251	HA		C H *1C	*1N	*1S	# 1.12
1274	HA		C H *1C	*1N	-1S	# 2.43
1254	HA		C H *1C	-1N	*1S	# 1.20
1259	HA		C H -1C	*1N	*1S	# 0.85
1192	HA		C H -1C	-1N	-1S	# 5.19
1260	HA		C H -1C	-1N	-1S	# 0.96
1198	HA		C H *1C	*1N	-1X	# 0.05
1192	HA		C H -1C	-1N	-1X	# 5.19
1338	HA		C H2*1C	*1O		# 8.20
1339	HA	2	C H2*1C	*1O		# 3.90
1340	HA		C H *2C	*1O		# 4.19
1341	HA	2	C H *2C	*1O		# 0.63
1297	HA		C H2-1C	-1O		28.13
1298	HA	2	C H2-1C	-1O		10.61
1299	HA	3	C H2-1C	-1O		4.00
1300	HA	4	C H2-1C	-1O		2.34
1301	HA	5	C H2-1C	-1O		1.26
1192	HA		C H -1C	-2O		# 5.19
1304	HA		C H -1C	-2O		1.12
1305	HA	2	C H -1C	-2O		0.08
1342	HA		C H -2C	-1O		# 0.59
1251	HA		C H *1C	*1O	*1O	# 1.12
1343	HA		C H *1C	*1O	*1O	# 0.36
1274	HA		C H *1C	*1O	-1O	# 2.43
1259	HA		C H -1C	*1O	*1O	# 0.85
1192	HA		C H -1C	-1O	-1O	# 5.19
1260	HA		C H -1C	-1O	-1O	# 0.96
1251	HA		C H *1C	*1O	*1S	# 1.12
1343	HA		C H *1C	*1O	*1S	# 0.36
1274	HA		C H *1C	*1O	-1S	# 2.43
1274	HA		C H *1C	-1O	*1S	# 2.43
1259	HA		C H -1C	*1O	*1S	# 0.85
1192	HA		C H -1C	-1O	-1S	# 5.19
1260	HA		C H -1C	-1O	-1S	# 0.96
1198	HA		C H *1C	*1O	-1X	# 0.05
1192	HA		C H -1C	-1O	-1X	# 5.19
1338	HA		C H2*1C	*1S		# 8.20
1339	HA	2	C H2*1C	*1S		# 3.90

# Hydrogen Augmented Atoms

Screen Number			Fragment Definition			Frequency Percent
1340	HA		C H *2C	*1S	#	4.19
1341	HA	2	C H *2C	*1S	#	0.63
1332	HA		C H2-1C	-1S		6.20
1192	HA		C H -1C	-2S	#	5.19
1334	HA		C H -1C	-2S		0.00
1342	HA		C H -2C	-1S	#	0.59
1251	HA		C H *1C	*1S *1S	#	1.12
1343	HA		C H *1C	*1S *1S	#	0.36
1274	HA		C H *1C	*1S -1S	#	2.43
1259	HA		C H -1C	*1S *1S	#	0.85
1192	HA		C H -1C	-1S -1S	#	5.19
1260	HA		C H -1C	-1S -1S	#	0.96
1198	HA		C H *1C	*1S -1X	#	0.05
1192	HA		C H -1C	-1S -1X	#	5.19
1186	HA		C H2-1C	-1X		1.70
1187	HA	2	C H2-1C	-1X		0.26
1189	HA		C H -2C	-1X		0.15
1192	HA		C H -1C	-1X -1X	#	5.19
1398	HA		C H3-1N			10.55
1399	HA	2	C H3-1N			4.78
1400	HA	3	C H3-1N			1.35
1401	HA	4	C H3-1N			0.74
1363	HA		C H2-2N		#	1.18
1413	HA		C H2*1N	*1N	#	0.31
1415	HA		C H *1N	*2N	#	3.87
1415	HA		C H *4N	*4N	#	3.87
1363	HA		C H2-1N	-1N	#	1.18
1377	HA		C H -1N	-2N	#	0.47
1377	HA		C H -4N	-4N	#	0.47
1251	HA		C H *1N	*1N *1N	#	1.12
1254	HA		C H *1N	*1N -1N	#	1.20
1196	HA		C H -1N	-1N -1N	#	0.97
1251	HA		C H *1N	*1N *1O	#	1.12
1274	HA		C H *1N	*1N -1O	#	2.43
1254	HA		C H *1N	-1N *1O	#	1.20
1196	HA		C H -1N	-1N -1O	#	0.97
1251	HA		C H *1N	*1N *1S	#	1.12
1274	HA		C H *1N	*1N -1S	#	2.43
1254	HA		C H *1N	-1N *1S	#	1.20
1196	HA		C H -1N	-1N -1S	#	0.97
1198	HA		C H *1N	*1N -1X	#	0.05
1196	HA		C H -1N	-1N -1X	#	0.97
1413	HA		C H2*1N	*1O	#	0.31
1415	HA		C H *2N	*1O	#	3.87
1363	HA		C H2-1N	-1O	#	1.18
1377	HA		C H -1N	-2O	#	0.47
1377	HA		C H -2N	-1O	#	0.47
1377	HA		C H -4N	-4O	#	0.47
1251	HA		C H *1N	*1O *1O	#	1.12
1274	HA		C H *1N	*1O -1O	#	2.43
1254	HA		C H -1N	*1O *1O	#	1.20
1196	HA		C H -1N	-1O -1O	#	0.97
1251	HA		C H *1N	*1O *1S	#	1.12
1274	HA		C H *1N	*1O -1S	#	2.43
1274	HA		C H *1N	-1O *1S	#	2.43

# Hydrogen Augmented Atoms

Screen Number			Fragment Definition			Frequency Percent
1254	HA		C H -1N	*1O	*1S	# 1.20
1196	HA		C H -1N	-1O	-1S	# 0.97
1198	HA		C H *1N	*1O	-1X	# 0.05
1196	HA		C H -1N	-1O	-1X	# 0.97
1413	HA		C H2*1N	*1S		# 0.31
1415	HA		C H *2N	*1S		# 3.87
1363	HA		C H2-1N	-1S		# 1.18
1377	HA		C H -1N	-2S		# 0.47
1377	HA		C H -2N	-1S		# 0.47
1377	HA		C H -4N	-4S		# 0.47
1251	HA		C H *1N	*1S	*1S	# 1.12
1274	HA		C H *1N	*1S	-1S	# 2.43
1254	HA		C H -1N	*1S	*1S	# 1.20
1196	HA		C H -1N	-1S	-1S	# 0.97
1198	HA		C H *1N	*1S	-1X	# 0.05
1196	HA		C H -1N	-1S	-1X	# 0.97
1363	HA		C H2-1N	-1X		# 1.18
1377	HA		C H -2N	-1X		# 0.47
1196	HA		C H -1N	-1X	-1X	# 0.97
1506	HA		C H3-1O			17.33
1507	HA	2	C H3-1O			5.70
1508	HA	3	C H3-1O			1.69
1509	HA	4	C H3-1O			0.67
1363	HA		C H2-2O			# 1.18
1550	HA		C H2*1O	*1O		# 0.80
1363	HA		C H2-1O	-1O		# 1.18
1377	HA		C H -1O	-2O		# 0.47
1377	HA		C H -4O	-4O		# 0.47
1251	HA		C H *1O	*1O	*1O	# 1.12
1274	HA		C H *1O	*1O	-1O	# 2.43
1196	HA		C H -1O	-1O	-1O	# 0.97
1251	HA		C H *1O	*1O	*1S	# 1.12
1274	HA		C H *1O	*1O	-1S	# 2.43
1274	HA		C H *1O	-1O	*1S	# 2.43
1196	HA		C H -1O	-1O	-1S	# 0.97
1198	HA		C H *1O	*1O	-1X	# 0.05
1196	HA		C H -1O	-1O	-1X	# 0.97
1550	HA		C H2*1O	*1S		# 0.80
1363	HA		C H2-1O	-1S		# 1.18
1377	HA		C H -1O	-2S		# 0.47
1377	HA		C H -2O	-1S		# 0.47
1377	HA		C H -4O	-4S		# 0.47
1251	HA		C H *1O	*1S	*1S	# 1.12
1274	HA		C H *1O	*1S	-1S	# 2.43
1274	HA		C H -1O	*1S	*1S	# 2.43
1196	HA		C H -1O	-1S	-1S	# 0.97
1198	HA		C H *1O	*1S	-1X	# 0.05
1196	HA		C H -1O	-1S	-1X	# 0.97
1363	HA		C H2-1O	-1X		# 1.18
1377	HA		C H -2O	-1X		# 0.47
1196	HA		C H -1O	-1X	-1X	# 0.97
1540	HA		C H3-1S			2.72
1541	HA	2	C H3-1S			0.39
1363	HA		C H2-2S			# 1.18
1550	HA		C H2*1S	*1S		# 0.80

# Hydrogen Augmented Atoms

Screen Number			Fragment Definition	Frequency Percent
1363	HA		C H2-1S -1S	# 1.18
1377	HA		C H -1S -2S	# 0.47
1377	HA		C H -4S -4S	# 0.47
1251	HA		C H *1S *1S *1S	# 1.12
1274	HA		C H *1S *1S -1S	# 2.43
1196	HA		C H -1S -1S -1S	# 0.97
1198	HA		C H *1S *1S -1X	# 0.05
1196	HA		C H -1S -1S -1X	# 0.97
1363	HA		C H2-1S -1X	# 1.18
1377	HA		C H -2S -1X	# 0.47
1196	HA		C H -1S -1X -1X	# 0.97
1363	HA		C H2-1X -1X	# 1.18
951	HA		GeH3-1C	# 0.07
951	HA		GeH2-1C -1C	# 0.07
951	HA		GeH -1C -1C -1C	# 0.07
1696	HA		N H2-1As	# 0.03
1572	HA		N H -2As	# 0.36
1696	HA		N H2-1B	# 0.03
1572	HA		N H -2B	# 0.36
1568	HA		N H2-1C	7.57
1569	HA	2	N H2-1C	2.12
1570	HA	3	N H2-1C	0.62
1571	HA		N H -2C	0.34
1572	HA		N H -2C	# 0.36
1583	HA		N H *1C *1C	4.55
1584	HA	2	N H *1C *1C	0.72
1597	HA		N H -1C -1C	4.20
1598	HA	2	N H -1C -1C	0.48
1627	HA		N H *1C *1N	# 0.67
1633	HA		N H -1C -1N	0.77
1627	HA		N H *1C *1O	# 0.67
1652	HA		N H -1C -1O	# 0.08
1627	HA		N H *1C *1S	# 0.67
1652	HA		N H -1C -1S	# 0.08
1664	HA		N H2-1N	0.41
1572	HA		N H -2N	# 0.36
1696	HA		N H2-1O	# 0.03
1572	HA		N H -2O	# 0.36
1696	HA		N H2-1P	# 0.03
1572	HA		N H -2P	# 0.36
1696	HA		N H2-1S	# 0.03
1572	HA		N H -2S	# 0.36
1696	HA		N H2-1Se	# 0.03
1572	HA		N H -2Se	# 0.36
1696	HA		N H2-1Si	# 0.03
1572	HA		N H -2Si	# 0.36
1696	HA		N H2-1Te	# 0.03
1572	HA		N H -2Te	# 0.36
1737	HA		O H -1As	# 0.16
1737	HA		O H -1B	# 0.16
1700	HA		O H -1C	20.14
1701	HA	2	O H -1C	7.80
1702	HA	3	O H -1C	3.33
1703	HA	4	O H -1C	1.93
1704	HA	5	O H -1C	1.15

# Hydrogen Augmented Atoms

Screen Number			Fragment Definition	Frequency Percent
1705	HA	6	O H -1C	0.81
1719	HA		O H -1N	0.80
1736	HA		O H -1O	# 0.06
1737	HA		O H -1P	# 0.16
1736	HA		O H -1S	# 0.06
1737	HA		O H -1Se	# 0.16
1737	HA		O H -1Si	# 0.16
1737	HA		O H -1Te	# 0.16
951	HA		P H2-1C	# 0.07
951	HA		P H -1C -1C	# 0.07
1771	HA		S H -1C	0.85
951	HA		SbH2-1C	# 0.07
951	HA		SbH -1C -1C	# 0.07
951	HA		SeH -1C	# 0.07
951	HA		SiH3-1C	# 0.07
951	HA		SiH2-1C -1C	# 0.07
951	HA		SiH -1C -1C -1C	# 0.07
951	HA		SnH3-1C	# 0.07
951	HA		SnH2-1C -1C	# 0.07
951	HA		SnH -1C -1C -1C	# 0.07
951	HA		TeH -1C	# 0.07



## Twin Augmented Atoms

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**TW Screens**      **Twin augmented atom (TW)** are for the central atom and one attached atom.

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**TW Screen Definitions**      These screens are augmented atoms whose definitions include the specification of the hydrogen attached to the central atom and to one of its attached atoms. Only a few TW screens are present in the screen dictionary, to describe common occurrences of  $-\text{CH}_3$ ,  $-\text{NH}_2$ ,  $-\text{OH}$ , and  $-\text{SH}$  groups.

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### Twin Augmented Atoms

Screen Number				Fragment Definition	Frequency Percent
1821	TW		C *1C	*1C -1C H3	5.04
1822	TW		C H *1C	*1C -1C H3	2.13
1823	TW		C *1C	*2C -1C H3	2.48
1824	TW		C *4C	*4C -1C H3	9.55
1825	TW	2	C *4C	*4C -1C H3	3.33
1826	TW		C -1C	-1C -1C -1O H	# 0.83
1826	TW		C -1C	-1C -1C -1S H	# 0.83
1827	TW		C *1C	*1C -1N H2	# 0.63
1827	TW		C H *1C	*1C -1N H2	# 0.63
1827	TW		C *1C	*2C -1N H2	# 0.63
1828	TW		C *4C	*4C -1N H2	1.65
1829	TW	2	C *4C	*4C -1N H2	0.46
1830	TW		C H -1C	-1C -1N H2	3.13
1831	TW		C *1C	*1C -1O H	# 5.45
1831	TW		C H *1C	*1C -1O H	# 5.45
1831	TW		C *1C	*2C -1O H	# 5.45
1832	TW		C *4C	*4C -1O H	# 6.53
1833	TW	2	C *4C	*4C -1O H	# 1.82
1834	TW		C H -1C	-1C -1O H	# 5.02
1831	TW		C *1C	*1C -1S H	# 5.45
1831	TW		C H *1C	*1C -1S H	# 5.45
1831	TW		C *1C	*2C -1S H	# 5.45
1832	TW		C *4C	*4C -1S H	# 6.53
1833	TW	2	C *4C	*4C -1S H	# 1.82
1834	TW		C H -1C	-1C -1S H	# 5.02
1835	TW		C H2-1C	-1N H2	2.72
1836	TW		C H2-1C	-1O H	# 6.73
1837	TW	2	C H2-1C	-1O H	# 2.13
1836	TW		C H2-1C	-1S H	# 6.73
1837	TW	2	C H2-1C	-1S H	# 2.13

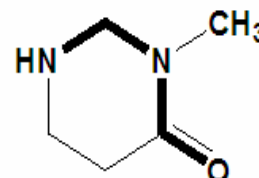
## Atom Sequences

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### AS Screens

**AS screens** describe linear 4- to 6-atom strings. The example screen shown below describes the 5-atom string (NCNCO) indicated in the structure given here. The strings are linear, so that an atom cannot appear twice in any given sequence.

An atom sequence (AS) screen specifies the element values of the atoms in the string and the types of bonds between them (i.e., whether these bonds are ring or chain), as in:



**AS 1 N \* C \* N \* C - O**

AS screens are the largest type of screen in the dictionary.

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### AS Screen Definitions

These screens are descriptions of linear sequences of 4, 5, or 6 atoms. Bond types may be specified for the more common AS fragments, but bond values are not used.

As an aid to the searcher, screen dictionary entries for AS screens, are "double posted" -- if the screen definition is not symmetrical, both the "forward" and "reverse" definitions are entries; both definitions for the AS example given here would appear in the dictionary.

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# Atom Sequences

Screen Number	Fragment Definition							Frequency Percent
331	AS	As	C	C	As			# 1.39
331	AS	As	C	C	B			# 1.39
331	AS	As	C	C	Br			# 1.39
134	AS	As	C	C	C			# 4.57
311	AS	As	C	C	C	As		# 1.14
311	AS	As	C	C	C	B		# 1.14
311	AS	As	C	C	C	Br		# 1.14
291	AS	As	C	C	C	C	As	# 0.79
291	AS	As	C	C	C	C	B	# 0.79
291	AS	As	C	C	C	C	Br	# 0.79
47	AS	As	C	C	C	C	C	# 3.83
291	AS	As	C	C	C	C	Cl	# 0.79
291	AS	As	C	C	C	C	F	# 0.79
291	AS	As	C	C	C	C	I	# 0.79
291	AS	As	C	C	C	C	N	# 0.79
291	AS	As	C	C	C	C	O	# 0.79
291	AS	As	C	C	C	C	P	# 0.79
291	AS	As	C	C	C	C	S	# 0.79
291	AS	As	C	C	C	C	Se	# 0.79
291	AS	As	C	C	C	C	Si	# 0.79
291	AS	As	C	C	C	C	Te	# 0.79
311	AS	As	C	C	C	C	Cl	# 1.14
311	AS	As	C	C	C	C	F	# 1.14
311	AS	As	C	C	C	C	I	# 1.14
311	AS	As	C	C	C	C	N	# 1.14
302	AS	As	C	C	C	N	As	# 0.44
302	AS	As	C	C	C	N	B	# 0.44
302	AS	As	C	C	C	N	P	# 0.44
302	AS	As	C	C	C	N	Se	# 0.44
302	AS	As	C	C	C	N	Si	# 0.44
302	AS	As	C	C	C	N	Te	# 0.44
311	AS	As	C	C	C	O		# 1.14
310	AS	As	C	C	C	O	As	# 2.38
310	AS	As	C	C	C	O	B	# 2.38
310	AS	As	C	C	C	O	P	# 2.38
310	AS	As	C	C	C	O	Se	# 2.38
310	AS	As	C	C	C	O	Si	# 2.38
310	AS	As	C	C	C	O	Te	# 2.38
311	AS	As	C	C	C	P		# 1.14
311	AS	As	C	C	C	S		# 1.14
310	AS	As	C	C	C	S	As	# 2.38
310	AS	As	C	C	C	S	B	# 2.38
310	AS	As	C	C	C	S	P	# 2.38
310	AS	As	C	C	C	S	Se	# 2.38
310	AS	As	C	C	C	S	Si	# 2.38
310	AS	As	C	C	C	S	Te	# 2.38
311	AS	As	C	C	C	Se		# 1.14
311	AS	As	C	C	C	Si		# 1.14
311	AS	As	C	C	C	Te		# 1.14
331	AS	As	C	C	Cl			# 1.39
331	AS	As	C	C	F			# 1.39
331	AS	As	C	C	I			# 1.39
331	AS	As	C	C	N			# 1.39
302	AS	As	C	C	N	As		# 0.44
302	AS	As	C	C	N	B		# 0.44

# Atom Sequences

Screen Number	Fragment Definition							Frequency Percent	
302	AS	As	C	C	N	P	#	0.44	
302	AS	As	C	C	N	Se	#	0.44	
302	AS	As	C	C	N	Si	#	0.44	
302	AS	As	C	C	N	Te	#	0.44	
331	AS	As	C	C	O		#	1.39	
310	AS	As	C	C	O	As	#	2.38	
310	AS	As	C	C	O	B	#	2.38	
310	AS	As	C	C	O	P	#	2.38	
310	AS	As	C	C	O	Se	#	2.38	
310	AS	As	C	C	O	Si	#	2.38	
310	AS	As	C	C	O	Te	#	2.38	
331	AS	As	C	C	P		#	1.39	
331	AS	As	C	C	S		#	1.39	
310	AS	As	C	C	S	As	#	2.38	
310	AS	As	C	C	S	B	#	2.38	
310	AS	As	C	C	S	P	#	2.38	
310	AS	As	C	C	S	Se	#	2.38	
310	AS	As	C	C	S	Si	#	2.38	
310	AS	As	C	C	S	Te	#	2.38	
331	AS	As	C	C	Se		#	1.39	
331	AS	As	C	C	Si		#	1.39	
331	AS	As	C	C	Te		#	1.39	
302	AS	As	N	C	C	As	#	0.44	
302	AS	As	N	C	C	B	#	0.44	
302	AS	As	N	C	C	Br	#	0.44	
302	AS	As	N	C	C	C	As	#	0.44
302	AS	As	N	C	C	C	B	#	0.44
302	AS	As	N	C	C	C	Br	#	0.44
302	AS	As	N	C	C	C	Cl	#	0.44
302	AS	As	N	C	C	C	F	#	0.44
302	AS	As	N	C	C	C	I	#	0.44
302	AS	As	N	C	C	C	N	#	0.44
302	AS	As	N	C	C	C	O	#	0.44
302	AS	As	N	C	C	C	P	#	0.44
302	AS	As	N	C	C	C	S	#	0.44
302	AS	As	N	C	C	C	Se	#	0.44
302	AS	As	N	C	C	C	Si	#	0.44
302	AS	As	N	C	C	C	Te	#	0.44
302	AS	As	N	C	C	C	Cl	#	0.44
302	AS	As	N	C	C	F		#	0.44
302	AS	As	N	C	C	I		#	0.44
302	AS	As	N	C	C	N		#	0.44
302	AS	As	N	C	C	O		#	0.44
302	AS	As	N	C	C	P		#	0.44
302	AS	As	N	C	C	S		#	0.44
302	AS	As	N	C	C	Se		#	0.44
302	AS	As	N	C	C	Si		#	0.44
302	AS	As	N	C	C	Te		#	0.44
310	AS	As	O	C	C	As		#	2.38
310	AS	As	O	C	C	B		#	2.38
310	AS	As	O	C	C	Br		#	2.38
310	AS	As	O	C	C	C	As	#	2.38
310	AS	As	O	C	C	C	B	#	2.38
310	AS	As	O	C	C	C	Br	#	2.38
310	AS	As	O	C	C	C	Cl	#	2.38

# Atom Sequences

Screen Number	Fragment Definition							Frequency Percent
310	AS	As	O	C	C	C	F	# 2.38
310	AS	As	O	C	C	C	I	# 2.38
310	AS	As	O	C	C	C	N	# 2.38
310	AS	As	O	C	C	C	O	# 2.38
310	AS	As	O	C	C	C	P	# 2.38
310	AS	As	O	C	C	C	S	# 2.38
310	AS	As	O	C	C	C	Se	# 2.38
310	AS	As	O	C	C	C	Si	# 2.38
310	AS	As	O	C	C	C	Te	# 2.38
310	AS	As	O	C	C	Cl		# 2.38
310	AS	As	O	C	C	F		# 2.38
310	AS	As	O	C	C	I		# 2.38
310	AS	As	O	C	C	N		# 2.38
310	AS	As	O	C	C	O		# 2.38
310	AS	As	O	C	C	P		# 2.38
310	AS	As	O	C	C	S		# 2.38
310	AS	As	O	C	C	Se		# 2.38
310	AS	As	O	C	C	Si		# 2.38
310	AS	As	O	C	C	Te		# 2.38
310	AS	As	S	C	C	As		# 2.38
310	AS	As	S	C	C	B		# 2.38
310	AS	As	S	C	C	Br		# 2.38
310	AS	As	S	C	C	C	As	# 2.38
310	AS	As	S	C	C	C	B	# 2.38
310	AS	As	S	C	C	C	Br	# 2.38
310	AS	As	S	C	C	C	Cl	# 2.38
310	AS	As	S	C	C	C	F	# 2.38
310	AS	As	S	C	C	C	I	# 2.38
310	AS	As	S	C	C	C	N	# 2.38
310	AS	As	S	C	C	C	O	# 2.38
310	AS	As	S	C	C	C	P	# 2.38
310	AS	As	S	C	C	C	S	# 2.38
310	AS	As	S	C	C	C	Se	# 2.38
310	AS	As	S	C	C	C	Si	# 2.38
310	AS	As	S	C	C	C	Te	# 2.38
310	AS	As	S	C	C	Cl		# 2.38
310	AS	As	S	C	C	F		# 2.38
310	AS	As	S	C	C	I		# 2.38
310	AS	As	S	C	C	N		# 2.38
310	AS	As	S	C	C	O		# 2.38
310	AS	As	S	C	C	P		# 2.38
310	AS	As	S	C	C	S		# 2.38
310	AS	As	S	C	C	Se		# 2.38
310	AS	As	S	C	C	Si		# 2.38
310	AS	As	S	C	C	Te		# 2.38
331	AS	B	C	C	As			# 1.39
331	AS	B	C	C	B			# 1.39
331	AS	B	C	C	Br			# 1.39
134	AS	B	C	C	C			# 4.57
311	AS	B	C	C	C	As		# 1.14
311	AS	B	C	C	C	B		# 1.14
311	AS	B	C	C	C	Br		# 1.14
291	AS	B	C	C	C	C	As	# 0.79
291	AS	B	C	C	C	C	B	# 0.79
291	AS	B	C	C	C	C	Br	# 0.79

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
47	AS B C C C C C C	# 3.83
291	AS B C C C C C Cl	# 0.79
291	AS B C C C C C F	# 0.79
291	AS B C C C C C I	# 0.79
291	AS B C C C C C N	# 0.79
291	AS B C C C C C O	# 0.79
291	AS B C C C C C P	# 0.79
291	AS B C C C C C S	# 0.79
291	AS B C C C C C Se	# 0.79
291	AS B C C C C C Si	# 0.79
291	AS B C C C C C Te	# 0.79
311	AS B C C C C Cl	# 1.14
311	AS B C C C C F	# 1.14
311	AS B C C C C I	# 1.14
311	AS B C C C C N	# 1.14
302	AS B C C C N As	# 0.44
302	AS B C C C N B	# 0.44
302	AS B C C C N P	# 0.44
302	AS B C C C N Se	# 0.44
302	AS B C C C N Si	# 0.44
302	AS B C C C N Te	# 0.44
311	AS B C C C O	# 1.14
310	AS B C C C O As	# 2.38
310	AS B C C C O B	# 2.38
310	AS B C C C O P	# 2.38
310	AS B C C C O Se	# 2.38
310	AS B C C C O Si	# 2.38
310	AS B C C C O Te	# 2.38
311	AS B C C C P	# 1.14
311	AS B C C C S	# 1.14
310	AS B C C C S As	# 2.38
310	AS B C C C S B	# 2.38
310	AS B C C C S P	# 2.38
310	AS B C C C S Se	# 2.38
310	AS B C C C S Si	# 2.38
310	AS B C C C S Te	# 2.38
311	AS B C C C Se	# 1.14
311	AS B C C C Si	# 1.14
311	AS B C C C Te	# 1.14
331	AS B C C Cl	# 1.39
331	AS B C C F	# 1.39
331	AS B C C I	# 1.39
331	AS B C C N	# 1.39
302	AS B C C N As	# 0.44
302	AS B C C N B	# 0.44
302	AS B C C N P	# 0.44
302	AS B C C N Se	# 0.44
302	AS B C C N Si	# 0.44
302	AS B C C N Te	# 0.44
331	AS B C C O	# 1.39
310	AS B C C O As	# 2.38
310	AS B C C O B	# 2.38
310	AS B C C O P	# 2.38
310	AS B C C O Se	# 2.38
310	AS B C C O Si	# 2.38

# Atom Sequences

Screen Number	Fragment Definition						Frequency Percent
310	AS	B	C	C	O	Te	# 2.38
331	AS	B	C	C	P		# 1.39
331	AS	B	C	C	S		# 1.39
310	AS	B	C	C	S	As	# 2.38
310	AS	B	C	C	S	B	# 2.38
310	AS	B	C	C	S	P	# 2.38
310	AS	B	C	C	S	Se	# 2.38
310	AS	B	C	C	S	Si	# 2.38
310	AS	B	C	C	S	Te	# 2.38
331	AS	B	C	C	Se		# 1.39
331	AS	B	C	C	Si		# 1.39
331	AS	B	C	C	Te		# 1.39
302	AS	B	N	C	C	As	# 0.44
302	AS	B	N	C	C	B	# 0.44
302	AS	B	N	C	C	Br	# 0.44
302	AS	B	N	C	C	C	As
302	AS	B	N	C	C	C	B
302	AS	B	N	C	C	C	Br
302	AS	B	N	C	C	C	Cl
302	AS	B	N	C	C	C	F
302	AS	B	N	C	C	C	I
302	AS	B	N	C	C	C	N
302	AS	B	N	C	C	C	O
302	AS	B	N	C	C	C	P
302	AS	B	N	C	C	C	S
302	AS	B	N	C	C	C	Se
302	AS	B	N	C	C	C	Si
302	AS	B	N	C	C	C	Te
310	AS	B	O	C	C	As	# 2.38
310	AS	B	O	C	C	B	# 2.38
310	AS	B	O	C	C	Br	# 2.38
310	AS	B	O	C	C	Cl	# 2.38
310	AS	B	O	C	C	C	F
310	AS	B	O	C	C	C	I
310	AS	B	O	C	C	C	N
310	AS	B	O	C	C	C	O
310	AS	B	O	C	C	C	P
310	AS	B	O	C	C	C	S
310	AS	B	O	C	C	C	Se
310	AS	B	O	C	C	C	Si
310	AS	B	O	C	C	C	Te
310	AS	B	O	C	C	Cl	# 2.38

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
310	AS B O C C F	# 2.38
310	AS B O C C I	# 2.38
310	AS B O C C N	# 2.38
310	AS B O C C O	# 2.38
310	AS B O C C P	# 2.38
310	AS B O C C S	# 2.38
310	AS B O C C Se	# 2.38
310	AS B O C C Si	# 2.38
310	AS B O C C Te	# 2.38
310	AS B S C C As	# 2.38
310	AS B S C C B	# 2.38
310	AS B S C C Br	# 2.38
310	AS B S C C C As	# 2.38
310	AS B S C C C B	# 2.38
310	AS B S C C C Br	# 2.38
310	AS B S C C C Cl	# 2.38
310	AS B S C C C F	# 2.38
310	AS B S C C C I	# 2.38
310	AS B S C C C N	# 2.38
310	AS B S C C C O	# 2.38
310	AS B S C C C P	# 2.38
310	AS B S C C C S	# 2.38
310	AS B S C C C Se	# 2.38
310	AS B S C C C Si	# 2.38
310	AS B S C C C Te	# 2.38
310	AS B S C C Cl	# 2.38
310	AS B S C C F	# 2.38
310	AS B S C C I	# 2.38
310	AS B S C C N	# 2.38
310	AS B S C C O	# 2.38
310	AS B S C C P	# 2.38
310	AS B S C C S	# 2.38
310	AS B S C C Se	# 2.38
310	AS B S C C Si	# 2.38
310	AS B S C C Te	# 2.38
331	AS Br C C As	# 1.39
331	AS Br C C B	# 1.39
312	AS Br- C * C - Br	# 2.00
313	AS Br- C - C - Br	# 0.90
88	AS Br- C * C - C	# 4.80
87	AS Br- C - C * C	# 3.30
89	AS Br- C - C - C	# 2.86
311	AS Br C C C As	# 1.14
311	AS Br C C C B	# 1.14
292	AS Br- C * C * C - Br	# 3.37
293	AS Br- C * C - C - Br	# 0.20
293	AS Br- C - C * C - Br	# 0.20
294	AS Br- C - C - C - Br	# 0.74
49	AS Br- C * C * C - C	# 4.52
6	AS Br- C * C - C * C	# 7.08
21	AS Br- C * C - C * C	# 1.70
50	AS Br- C * C - C - C	# 1.14
48	AS Br- C - C - C * C	# 0.77
51	AS Br- C - C - C - C	# 1.49
291	AS Br C C C C As	# 0.79



# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
291 AS	Br C C C C B	# 0.79
283 AS	Br- C * C * C * C - Br	# 1.11
284 AS	Br- C - C - C - C - Br	# 0.36
22 AS	Br- C * C * C * C - C	# 5.91
14 AS	Br- C * C - C - C * C	# 3.46
21 AS	Br- C * C - C - C * C	# 1.70
23 AS	Br- C - C - C - C - C	# 0.96
283 AS	Br- C * C * C * C - Cl	# 1.11
284 AS	Br- C - C - C - C - Cl	# 0.36
283 AS	Br- C * C * C * C - F	# 1.11
284 AS	Br- C - C - C - C - F	# 0.36
283 AS	Br- C * C * C * C - I	# 1.11
284 AS	Br- C - C - C - C - I	# 0.36
285 AS	Br C C C C N	# 7.02
286 AS	Br- C * C * C * C - N	# 2.55
287 AS	Br- C * C * C - C - N	# 1.22
288 AS	Br C C C C O	# 6.39
289 AS	Br- C * C * C * C - O	# 3.00
290 AS	Br- C * C * C - C - O	# 1.30
291 AS	Br C C C C P	# 0.79
288 AS	Br C C C C S	# 6.39
289 AS	Br- C * C * C * C - S	# 3.00
290 AS	Br- C * C * C - C - S	# 1.30
291 AS	Br C C C C Se	# 0.79
291 AS	Br C C C C Si	# 0.79
291 AS	Br C C C C Te	# 0.79
292 AS	Br- C * C * C - Cl	# 3.37
293 AS	Br- C * C - C - Cl	# 0.20
293 AS	Br- C - C * C - Cl	# 0.20
294 AS	Br- C - C - C - Cl	# 0.74
292 AS	Br- C * C * C - F	# 3.37
293 AS	Br- C * C - C - F	# 0.20
293 AS	Br- C - C * C - F	# 0.20
294 AS	Br- C - C - C - F	# 0.74
292 AS	Br- C * C * C - I	# 3.37
293 AS	Br- C * C - C - I	# 0.20
293 AS	Br- C - C * C - I	# 0.20
294 AS	Br- C - C - C - I	# 0.74
295 AS	Br C C C C N	# 5.58
296 AS	Br- C * C * C * C - N	# 1.36
297 AS	Br- C * C * C - N	# 1.96
298 AS	Br- C * C - C - N	# 1.26
299 AS	Br- C - C - C - N	# 0.37
302 AS	Br C C C N As	# 0.44
302 AS	Br C C C N B	# 0.44
300 AS	Br C C C N N	# 0.84
301 AS	Br C C C N O	# 0.55
302 AS	Br C C C N P	# 0.44
301 AS	Br C C C N S	# 0.55
302 AS	Br C C C N Se	# 0.44
302 AS	Br C C C N Si	# 0.44
302 AS	Br C C C N Te	# 0.44
303 AS	Br C C C O	# 5.10
304 AS	Br- C * C * C * O	# 0.64
305 AS	Br- C * C * C - O	# 1.72

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
306	AS	Br- C * C - C - O	# 1.61
307	AS	Br- C - C - C - O	# 0.86
310	AS	Br C C C O As	# 2.38
310	AS	Br C C C O B	# 2.38
256	AS	Br C C C O C	# 3.02
308	AS	Br C C C O N	# 0.26
309	AS	Br C C C O O	# 0.37
310	AS	Br C C C O P	# 2.38
309	AS	Br C C C O S	# 0.37
310	AS	Br C C C O Se	# 2.38
310	AS	Br C C C O Si	# 2.38
310	AS	Br C C C O Te	# 2.38
311	AS	Br C C C P	# 1.14
303	AS	Br C C C S	# 5.10
304	AS	Br- C * C * C * S	# 0.64
305	AS	Br- C * C * C - S	# 1.72
306	AS	Br- C * C - C - S	# 1.61
307	AS	Br- C - C - C - S	# 0.86
310	AS	Br C C C S As	# 2.38
310	AS	Br C C C S B	# 2.38
256	AS	Br C C C S C	# 3.02
308	AS	Br C C C S N	# 0.26
309	AS	Br C C C S O	# 0.37
310	AS	Br C C C S P	# 2.38
309	AS	Br C C C S S	# 0.37
310	AS	Br C C C S Se	# 2.38
310	AS	Br C C C S Si	# 2.38
310	AS	Br C C C S Te	# 2.38
311	AS	Br C C C Se	# 1.14
311	AS	Br C C C Si	# 1.14
311	AS	Br C C C Te	# 1.14
312	AS	Br- C * C - Cl	# 2.00
313	AS	Br- C - C - Cl	# 0.90
312	AS	Br- C * C - F	# 2.00
313	AS	Br- C - C - F	# 0.90
312	AS	Br- C * C - I	# 2.00
313	AS	Br- C - C - I	# 0.90
314	AS	Br- C * C * N	# 1.48
315	AS	Br- C * C - N	# 2.34
316	AS	Br- C - C * N	# 0.64
317	AS	Br- C - C - N	# 1.12
302	AS	Br C C N As	# 0.44
302	AS	Br C C N B	# 0.44
212	AS	Br C C N C	# 4.26
21	AS	Br- C * C - N - C * C	# 1.70
102	AS	Br- C * C - N - C * C	# 0.92
318	AS	Br C C N C N	# 1.48
319	AS	Br C C N C O	# 1.84
320	AS	Br- C * C - N - C - O	# 0.72
319	AS	Br C C N C S	# 1.84
320	AS	Br- C * C - N - C - S	# 0.72
321	AS	Br C C N N	# 0.82
322	AS	Br C C N O	# 0.39
302	AS	Br C C N P	# 0.44
322	AS	Br C C N S	# 0.39

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
302	AS Br C C N Se	# 0.44
302	AS Br C C N Si	# 0.44
302	AS Br C C N Te	# 0.44
323	AS Br- C * C * O	# 0.61
324	AS Br- C * C - O	# 2.95
325	AS Br- C - C * O	# 0.45
326	AS Br- C - C - O	# 2.53
310	AS Br C C O As	# 2.38
310	AS Br C C O B	# 2.38
265	AS Br- C * C - O - C	# 1.77
186	AS Br C C O C C	# 2.66
21	AS Br- C * C - O - C * C	# 1.70
126	AS Br- C * C - O - C * C	# 2.20
327	AS Br C C O C N	# 0.27
328	AS Br C C O C O	# 0.64
328	AS Br C C O C S	# 0.64
329	AS Br C C O N	# 0.30
330	AS Br C C O O	# 0.43
310	AS Br C C O P	# 2.38
330	AS Br C C O S	# 0.43
310	AS Br C C O Se	# 2.38
310	AS Br C C O Si	# 2.38
310	AS Br C C O Te	# 2.38
331	AS Br C C P	# 1.39
323	AS Br- C * C * S	# 0.61
324	AS Br- C * C - S	# 2.95
325	AS Br- C - C * S	# 0.45
326	AS Br- C - C - S	# 2.53
310	AS Br C C S As	# 2.38
310	AS Br C C S B	# 2.38
265	AS Br- C * C - S - C	# 1.77
186	AS Br C C S C C	# 2.66
21	AS Br- C * C - S - C * C	# 1.70
126	AS Br- C * C - S - C * C	# 2.20
327	AS Br C C S C N	# 0.27
328	AS Br C C S C O	# 0.64
328	AS Br C C S C S	# 0.64
329	AS Br C C S N	# 0.30
330	AS Br C C S O	# 0.43
310	AS Br C C S P	# 2.38
330	AS Br C C S S	# 0.43
310	AS Br C C S Se	# 2.38
310	AS Br C C S Si	# 2.38
310	AS Br C C S Te	# 2.38
331	AS Br C C Se	# 1.39
331	AS Br C C Si	# 1.39
331	AS Br C C Te	# 1.39
332	AS Br C N C Br	# 0.12
332	AS Br C N C Cl	# 0.12
332	AS Br C N C F	# 0.12
332	AS Br C N C I	# 0.12
333	AS Br C N C N	# 0.53
334	AS Br C N C O	# 0.18
334	AS Br C N C S	# 0.18
335	AS Br C N O	# 0.09

# Atom Sequences

Screen Number		Fragment Definition				Frequency Percent	
335	AS	Br	C	N	S	#	0.09
336	AS	Br	C	O	O	#	0.37
336	AS	Br	C	O	S	#	0.37
336	AS	Br	C	S	O	#	0.37
336	AS	Br	C	S	S	#	0.37
196	AS	Br	O	C	C	#	0.10
196	AS	Br	S	C	C	#	0.10
134	AS	C	C	C	As	#	4.57
134	AS	C	C	C	B	#	4.57
87	AS	C	*	C	- C - Br	#	3.30
88	AS	C	- C	*	C - Br	#	4.80
89	AS	C	- C	- C	- Br	#	2.86
1	AS	C	*	C	- C * C		13.51
2	AS	C	*	C	- C - C		34.96
3	AS	C	- C	*	C - C		14.19
2	AS	C	- C	- C	* C		34.96
4	AS	C	- C	- C	- C		32.65
6	AS	C	*	C	- C * C - Br	#	7.08
21	AS	C	*	C	- C * C - Br	#	1.70
48	AS	C	*	C	- C - C - Br	#	0.77
49	AS	C	- C	* C	* C - Br	#	4.52
50	AS	C	- C	- C	* C - Br	#	1.14
51	AS	C	- C	- C	- C - Br	#	1.49
5	AS	C	*	C	* C * C * C		78.62
6	AS	C	*	C	- C * C - C	#	7.08
7	AS	C	*	C	- C * C - C	#	6.85
8	AS	C	*	C	- C - C * C		6.91
9	AS	C	*	C	- C - C - C		17.57
10	AS	C	- C	* C	* C - C		12.64
6	AS	C	- C	* C	- C * C	#	7.08
7	AS	C	- C	* C	- C * C	#	6.85
11	AS	C	- C	* C	- C - C		6.14
11	AS	C	- C	- C	* C - C		6.14
9	AS	C	- C	- C	- C * C		17.57
12	AS	C	- C	- C	- C - C		19.16
47	AS	C	C	C	C C As	#	3.83
47	AS	C	C	C	C C B	#	3.83
14	AS	C	*	C	- C - C * C - Br	#	3.46
21	AS	C	*	C	- C - C * C - Br	#	1.70
22	AS	C	- C	* C	* C * C - Br	#	5.91
23	AS	C	- C	- C	- C - C - Br	#	0.96
13	AS	C	*	C	* C * C * C * C		74.51
7	AS	C	*	C	- C - C * C - C	#	6.85
14	AS	C	*	C	- C - C * C - C	#	3.46
15	AS	C	*	C	- C - C - C * C		1.98
16	AS	C	*	C	- C - C - C - C		6.81
17	AS	C	- C	* C	* C * C - C		11.88
18	AS	C	- C	* C	* C - C - C		4.49
7	AS	C	- C	* C	- C - C * C	#	6.85
14	AS	C	- C	* C	- C - C * C	#	3.46
18	AS	C	- C	- C	* C * C - C		4.49
19	AS	C	- C	- C	* C - C - C		1.06
16	AS	C	- C	- C	- C - C * C		6.81
20	AS	C	- C	- C	- C - C - C		12.15
14	AS	C	*	C	- C - C * C - Cl	#	3.46

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
21	AS	C * C - C - C * C - Cl	# 1.70
22	AS	C - C * C * C * C - Cl	# 5.91
23	AS	C - C - C - C - C - Cl	# 0.96
14	AS	C * C - C - C * C - F	# 3.46
21	AS	C * C - C - C * C - F	# 1.70
22	AS	C - C * C * C * C - F	# 5.91
23	AS	C - C - C - C - C - F	# 0.96
14	AS	C * C - C - C * C - I	# 3.46
21	AS	C * C - C - C * C - I	# 1.70
22	AS	C - C * C * C * C - I	# 5.91
23	AS	C - C - C - C - C - I	# 0.96
24	AS	C * C * C * C * C * N	27.22
25	AS	C * C - C * C * C * N	4.17
14	AS	C * C - C - C * C - N	# 3.46
26	AS	C * C - C - C * C - N	# 1.63
27	AS	C * C - C - C - C - N	5.29
28	AS	C - C * C * C * C * N	11.69
29	AS	C - C * C * C * C - N	8.40
30	AS	C - C * C * C - C - N	2.36
31	AS	C - C * C - C - C - N	0.41
32	AS	C - C - C * C * C - N	0.92
33	AS	C - C - C * C - C - N	0.34
34	AS	C - C - C - C - C - N	7.98
35	AS	C * C * C * C * C * O	# 14.10
36	AS	C * C - C * C * C * O	# 1.56
37	AS	C * C - C * C * C - O	# 2.60
14	AS	C * C - C - C * C - O	# 3.46
38	AS	C * C - C - C * C - O	# 5.99
39	AS	C * C - C - C - C - O	# 7.78
40	AS	C - C * C * C * C * O	# 9.53
41	AS	C - C * C * C * C - O	# 19.86
42	AS	C - C * C * C - C - O	# 4.15
43	AS	C - C * C - C - C - O	# 1.01
44	AS	C - C - C * C * C - O	# 4.16
45	AS	C - C - C * C - C - O	# 1.26
46	AS	C - C - C - C - C - O	# 12.64
47	AS	C C C C C P	# 3.83
35	AS	C * C * C * C * C * S	# 14.10
36	AS	C * C - C * C * C * S	# 1.56
37	AS	C * C - C * C * C - S	# 2.60
14	AS	C * C - C - C * C - S	# 3.46
38	AS	C * C - C - C * C - S	# 5.99
39	AS	C * C - C - C - C - S	# 7.78
40	AS	C - C * C * C * C * S	# 9.53
41	AS	C - C * C * C * C - S	# 19.86
42	AS	C - C * C * C - C - S	# 4.15
43	AS	C - C * C - C - C - S	# 1.01
44	AS	C - C - C * C * C - S	# 4.16
45	AS	C - C - C * C - C - S	# 1.26
46	AS	C - C - C - C - C - S	# 12.64
47	AS	C C C C C Se	# 3.83
47	AS	C C C C C Si	# 3.83
47	AS	C C C C C Te	# 3.83
6	AS	C * C - C * C - Cl	# 7.08
21	AS	C * C - C * C - Cl	# 1.70

# Atom Sequences

Screen Number		Fragment Definition		Frequency Percent	
48	AS	C * C - C - C - Cl	#	0.77	
49	AS	C - C * C * C - Cl	#	4.52	
50	AS	C - C - C - C * C - Cl	#	1.14	
51	AS	C - C - C - C - C - Cl	#	1.49	
6	AS	C * C - C * C - F	#	7.08	
21	AS	C * C - C * C - F	#	1.70	
48	AS	C * C - C - C - F	#	0.77	
49	AS	C - C * C * C - F	#	4.52	
50	AS	C - C - C * C - F	#	1.14	
51	AS	C - C - C - C - F	#	1.49	
6	AS	C * C - C * C - I	#	7.08	
21	AS	C * C - C * C - I	#	1.70	
48	AS	C * C - C - C - I	#	0.77	
49	AS	C - C * C * C - I	#	4.52	
50	AS	C - C - C * C - I	#	1.14	
51	AS	C - C - C - C - I	#	1.49	
52	AS	C * C * C * C * N		31.81	
53	AS	C * C - C * C * N		2.97	
6	AS	C * C - C * C - N	#	7.08	
26	AS	C * C - C * C - N	#	1.63	
54	AS	C * C - C - C * N		1.62	
55	AS	C * C - C - C - N		8.56	
56	AS	C - C * C * C * N		13.91	
57	AS	C - C * C * C - N		6.09	
58	AS	C - C * C - C - N		2.87	
59	AS	C - C - C * C * N		7.01	
60	AS	C - C - C * C - N		1.24	
61	AS	C - C - C - C - N		14.08	
62	AS	C * C - C - C - N * C		1.14	
63	AS	C * C - C - C - N - C		5.95	
64	AS	C - C * C * C * N - C		5.71	
65	AS	C - C * C * C - N - C		2.97	
66	AS	C - C * C - C - N - C		1.27	
67	AS	C * C * C * C * N * N		2.26	
68	AS	C * C - C - C - N - N		0.23	
69	AS	C - C * C * C - N - N		0.49	
70	AS	C * C - C - C - N - O	#	0.32	
71	AS	C - C * C * C - N - O	#	1.36	
70	AS	C * C - C - C - N - S	#	0.32	
71	AS	C - C * C * C - N - S	#	1.36	
72	AS	C * C * C * C * O	#	19.48	
73	AS	C * C - C * C * O	#	2.01	
6	AS	C * C - C * C - O	#	7.08	
38	AS	C * C - C * C - O	#	5.99	
74	AS	C * C - C - C * O	#	1.34	
75	AS	C * C - C - C - O	#	6.25	
76	AS	C - C * C * C * O	#	7.10	
77	AS	C - C * C * C - O	#	14.59	
78	AS	C - C * C - C - O	#	6.22	
79	AS	C - C - C * C - O	#	6.96	
80	AS	C - C - C - C - O	#	21.57	
81	AS	C * C - C - C - O - C	#	2.56	
82	AS	C - C * C * C - O - C	#	7.34	
83	AS	C - C * C - C - O - C	#	2.79	
84	AS	C - C - C * C - O - C	#	1.91	

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
85	AS	C - C * C * C - O - N	# 0.42
86	AS	C - C * C * C - O - O	# 0.75
86	AS	C - C * C * C - O - S	# 0.75
72	AS	C * C * C * C * S	# 19.48
73	AS	C * C - C * C * S	# 2.01
6	AS	C * C - C * C - S	# 7.08
38	AS	C * C - C * C - S	# 5.99
74	AS	C * C - C - C * S	# 1.34
75	AS	C * C - C - C - S	# 6.25
76	AS	C - C * C * C * S	# 7.10
77	AS	C - C * C * C - S	# 14.59
78	AS	C - C * C - C - S	# 6.22
79	AS	C - C - C * C - S	# 6.96
80	AS	C - C - C - C - S	# 21.57
81	AS	C * C - C - C - S - C	# 2.56
82	AS	C - C * C * C - S - C	# 7.34
83	AS	C - C * C - C - S - C	# 2.79
84	AS	C - C - C * C - S - C	# 1.91
85	AS	C - C * C * C - S - N	# 0.42
86	AS	C - C * C * C - S - O	# 0.75
86	AS	C - C * C * C - S - S	# 0.75
87	AS	C * C - C - Cl	# 3.30
88	AS	C - C * C - Cl	# 4.80
89	AS	C - C - C - Cl	# 2.86
87	AS	C * C - C - F	# 3.30
88	AS	C - C * C - F	# 4.80
89	AS	C - C - C - F	# 2.86
87	AS	C * C - C - I	# 3.30
88	AS	C - C * C - I	# 4.80
89	AS	C - C - C - I	# 2.86
2080	AS	C C C N	67.06
90	AS	C * C - C * N	8.61
91	AS	C * C - C - N	22.25
92	AS	C - C * C * N	16.85
93	AS	C - C * C - N	6.37
94	AS	C - C - C * N	6.85
95	AS	C - C - C - N	24.66
96	AS	C * C - C - N * C	4.61
97	AS	C * C - C - N - C	12.91
98	AS	C - C * C * N - C	5.92
99	AS	C - C * C - N - C	1.84
100	AS	C - C - C - N * C	7.00
101	AS	C * C - C - N - C * C	4.57
7	AS	C - C * C - N - C * C	# 6.85
102	AS	C - C * C - N - C * C	# 0.92
103	AS	C * C * C * N * C * N	9.30
104	AS	C * C - C - N - C - N	0.88
105	AS	C - C * C - N - C - N	0.37
106	AS	C * C * C * N * C * O	# 2.79
107	AS	C * C - C - N * C - O	# 1.02
108	AS	C * C - C - N - C - O	# 3.00
109	AS	C - C * C - N - C - O	# 2.05
106	AS	C * C * C * N * C * S	# 2.79
107	AS	C * C - C - N * C - S	# 1.02
108	AS	C * C - C - N - C - S	# 3.00

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
109	AS	C - C * C - N - C - S	# 2.05
110	AS	C * C * C * N * N	4.61
111	AS	C * C - C - N - N	2.65
112	AS	C - C * C - N - N	0.55
113	AS	C - C - C - N - N	1.14
114	AS	C * C - C - N - O	# 1.22
115	AS	C - C * C - N - O	# 0.94
114	AS	C * C - C - N - S	# 1.22
115	AS	C - C * C - N - S	# 0.94
2081	AS	C C C O	# 76.51
116	AS	C * C - C * O	# 4.30
117	AS	C * C - C - O	# 33.04
118	AS	C - C * C * O	# 9.42
119	AS	C - C * C - O	# 18.18
120	AS	C - C - C * O	# 5.21
121	AS	C - C - C - O	# 32.90
122	AS	C * C - C - O - C	# 13.92
123	AS	C - C * C - O - C	# 6.93
124	AS	C - C - C - O - C	# 16.58
125	AS	C * C - C - O - C * C	# 4.07
7	AS	C - C * C - O - C * C	# 6.85
126	AS	C - C * C - O - C * C	# 2.20
127	AS	C - C - C - O - C * C	# 5.20
128	AS	C * C - C - O - C - O	# 3.28
128	AS	C * C - C - O - C - S	# 3.28
129	AS	C * C - C - O - N	# 0.35
130	AS	C - C * C - O - N	# 0.32
131	AS	C * C - C - O - O	# 0.48
132	AS	C - C * C - O - O	# 0.71
133	AS	C - C - C - O - O	# 1.20
131	AS	C * C - C - O - S	# 0.48
132	AS	C - C * C - O - S	# 0.71
133	AS	C - C - C - O - S	# 1.20
134	AS	C C C P	# 4.57
2081	AS	C C C S	# 76.51
116	AS	C * C - C * S	# 4.30
117	AS	C * C - C - S	# 33.04
118	AS	C - C * C * S	# 9.42
119	AS	C - C * C - S	# 18.18
120	AS	C - C - C * S	# 5.21
121	AS	C - C - C - S	# 32.90
122	AS	C * C - C - S - C	# 13.92
123	AS	C - C * C - S - C	# 6.93
124	AS	C - C - C - S - C	# 16.58
125	AS	C * C - C - S - C * C	# 4.07
7	AS	C - C * C - S - C * C	# 6.85
126	AS	C - C * C - S - C * C	# 2.20
127	AS	C - C - C - S - C * C	# 5.20
128	AS	C * C - C - S - C - O	# 3.28
128	AS	C * C - C - S - C - S	# 3.28
129	AS	C * C - C - S - N	# 0.35
130	AS	C - C * C - S - N	# 0.32
131	AS	C * C - C - S - O	# 0.48
132	AS	C - C * C - S - O	# 0.71
133	AS	C - C - C - S - O	# 1.20



# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
131	AS	C * C - C - S - S	# 0.48
132	AS	C - C * C - S - S	# 0.71
133	AS	C - C - C - S - S	# 1.20
134	AS	C C C Se	# 4.57
134	AS	C C C Si	# 4.57
134	AS	C C C Te	# 4.57
2083	AS	C C N C	61.18
135	AS	C * C - N * C	8.07
136	AS	C * C - N - C	18.27
137	AS	C - C * N - C	8.60
138	AS	C - C - N * C	14.80
139	AS	C - C - N - C	29.65
140	AS	C * C * N * C * C	30.93
141	AS	C * C - N * C - C	1.71
142	AS	C * C - N - C * C	1.80
143	AS	C * C - N - C - C	12.19
144	AS	C - C * N * C - C	3.03
141	AS	C - C * N - C * C	1.71
143	AS	C - C - N - C * C	12.19
145	AS	C - C - N - C - C	15.23
21	AS	C * C - N - C * C - Br	# 1.70
102	AS	C * C - N - C * C - Br	# 0.92
7	AS	C * C - N - C * C - C	# 6.85
102	AS	C * C - N - C * C - C	# 0.92
101	AS	C * C - N - C - C * C	4.57
21	AS	C * C - N - C * C - Cl	# 1.70
102	AS	C * C - N - C * C - Cl	# 0.92
21	AS	C * C - N - C * C - F	# 1.70
102	AS	C * C - N - C * C - F	# 0.92
21	AS	C * C - N - C * C - I	# 1.70
102	AS	C * C - N - C * C - I	# 0.92
146	AS	C * C * N * C * C * N	6.79
26	AS	C * C - N - C * C - N	# 1.63
102	AS	C * C - N - C * C - N	# 0.92
147	AS	C * C - N - C - C - N	1.84
148	AS	C * C * N * C * C * O	# 3.85
38	AS	C * C - N - C * C - O	# 5.99
102	AS	C * C - N - C * C - O	# 0.92
149	AS	C * C - N - C - C - O	# 2.49
148	AS	C * C * N * C * C * S	# 3.85
38	AS	C * C - N - C * C - S	# 5.99
102	AS	C * C - N - C * C - S	# 0.92
149	AS	C * C - N - C - C - S	# 2.49
150	AS	C * C * N * C * N	12.29
151	AS	C * C - N - C * N	1.72
152	AS	C * C - N - C - N	2.36
153	AS	C - C * N * C * N	5.44
154	AS	C - C * N * C - N	2.20
155	AS	C - C - N - C - N	3.79
156	AS	C * C - N - C - N - C	1.65
157	AS	C * C * N * C * O	# 6.29
158	AS	C * C - N * C - O	# 3.59
159	AS	C * C - N - C * O	# 0.71
160	AS	C * C - N - C - O	# 11.07
161	AS	C - C * N * C * O	# 3.21

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
162	AS	C - C * N * C - O	# 4.84
163	AS	C - C * N - C - O	# 2.74
164	AS	C - C - N - C - O	# 13.37
165	AS	C * C - N - C - O - C	# 0.83
157	AS	C * C * N * C * S	# 6.29
158	AS	C * C - N * C - S	# 3.59
159	AS	C * C - N - C * S	# 0.71
160	AS	C * C - N - C - S	# 11.07
161	AS	C - C * N * C * S	# 3.21
162	AS	C - C * N * C - S	# 4.84
163	AS	C - C * N - C - S	# 2.74
164	AS	C - C - N - C - S	# 13.37
165	AS	C * C - N - C - S - C	# 0.83
2085	AS	C C N N	# 26.07
166	AS	C * C - N * N	1.79
167	AS	C * C - N - N	2.67
168	AS	C - C * N * N	4.81
169	AS	C - C - N - N	3.78
170	AS	C - C * N * N - C	1.83
171	AS	C - C - N - N - C	2.85
172	AS	C * C - N - N - C * C	1.18
2085	AS	C C N O	# 26.07
173	AS	C * C * N * O	# 1.32
174	AS	C * C - N - O	# 6.36
175	AS	C - C * N - O	# 0.56
176	AS	C - C - N - O	# 3.06
177	AS	C * C - N - O - C	# 1.40
178	AS	C - C - N - O - C	# 2.11
179	AS	C * C - N - O - O	# 1.31
179	AS	C * C - N - O - S	# 1.31
2085	AS	C C N S	# 26.07
173	AS	C * C * N * S	# 1.32
174	AS	C * C - N - S	# 6.36
175	AS	C - C * N - S	# 0.56
176	AS	C - C - N - S	# 3.06
177	AS	C * C - N - S - C	# 1.40
178	AS	C - C - N - S - C	# 2.11
179	AS	C * C - N - S - O	# 1.31
179	AS	C * C - N - S - S	# 1.31
196	AS	C C O Br	# 0.10
2084	AS	C C O C	# 55.24
180	AS	C * C - O - C	# 26.47
181	AS	C * C * O * C * C	# 17.85
182	AS	C * C - O - C * C	# 3.48
183	AS	C * C - O - C - C	# 14.37
184	AS	C - C * O * C - C	# 2.61
183	AS	C - C - O - C * C	# 14.37
185	AS	C - C - O - C - C	# 13.52
186	AS	C C O C C Br	# 2.66
21	AS	C * C - O - C * C - Br	# 1.70
126	AS	C * C - O - C * C - Br	# 2.20
7	AS	C * C - O - C * C - C	# 6.85
126	AS	C * C - O - C * C - C	# 2.20
125	AS	C * C - O - C - C * C	# 4.07
127	AS	C * C - O - C - C - C	# 5.20

# Atom Sequences

Screen Number		Fragment Definition							Frequency Percent	
186	AS	C	C	O	C	C	Cl	#	2.66	
21	AS	C	*	C	-	O	-	C	#	1.70
126	AS	C	*	C	-	O	-	C	#	2.20
186	AS	C	C	O	C	C	F	#	2.66	
21	AS	C	*	C	-	O	-	C	#	1.70
126	AS	C	*	C	-	O	-	C	#	2.20
186	AS	C	C	O	C	C	I	#	2.66	
21	AS	C	*	C	-	O	-	C	#	1.70
126	AS	C	*	C	-	O	-	C	#	2.20
26	AS	C	*	C	-	O	-	C	#	1.63
126	AS	C	*	C	-	O	-	C	#	2.20
38	AS	C	*	C	-	O	-	C	#	5.99
126	AS	C	*	C	-	O	-	C	#	2.20
187	AS	C	*	C	-	O	-	C	#	3.29
38	AS	C	*	C	-	O	-	C	#	5.99
126	AS	C	*	C	-	O	-	C	#	2.20
187	AS	C	*	C	-	O	-	C	#	3.29
188	AS	C	*	C	-	O	-	C	#	0.61
189	AS	C	*	C	-	O	-	C	#	0.58
190	AS	C	-	C	*	O	*	C	#	2.79
191	AS	C	-	C	*	O	*	C	#	2.04
192	AS	C	*	C	-	O	-	C	#	1.20
193	AS	C	*	C	-	O	-	C	#	4.71
194	AS	C	-	C	*	O	*	C	#	3.38
195	AS	C	-	C	-	O	-	C	#	13.48
192	AS	C	*	C	-	O	-	C	#	1.20
193	AS	C	*	C	-	O	-	C	#	4.71
194	AS	C	-	C	*	O	*	C	#	3.38
195	AS	C	-	C	-	O	-	C	#	13.48
196	AS	C	C	O	Cl			#	0.10	
196	AS	C	C	O	F			#	0.10	
196	AS	C	C	O	I			#	0.10	
2085	AS	C	C	O	N			#	26.07	
197	AS	C	*	C	-	O	-	N	#	3.51
198	AS	C	-	C	*	O	*	N	#	0.77
199	AS	C	-	C	-	O	-	N	#	1.12
200	AS	C	*	C	-	O	-	N	#	2.34
2085	AS	C	C	O	O			#	26.07	
201	AS	C	*	C	-	O	-	O	#	6.11
202	AS	C	-	C	-	O	-	O	#	2.21
203	AS	C	*	C	-	O	-	O	#	0.20
2085	AS	C	C	O	S			#	26.07	
201	AS	C	*	C	-	O	-	S	#	6.11
202	AS	C	-	C	-	O	-	S	#	2.21
203	AS	C	*	C	-	O	-	S	#	0.20
196	AS	C	C	S	Br			#	0.10	
2084	AS	C	C	S	C			#	55.24	
180	AS	C	*	C	-	S	-	C	#	26.47
181	AS	C	*	C	*	S	*	C	#	17.85
182	AS	C	*	C	-	S	-	C	#	3.48
183	AS	C	*	C	-	S	-	C	#	14.37
184	AS	C	-	C	*	S	*	C	#	2.61
183	AS	C	-	C	-	S	-	C	#	14.37
185	AS	C	-	C	-	S	-	C	#	13.52
186	AS	C	C	S	C	C	Br	#	2.66	

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
21	AS	C * C - S - C * C - Br	# 1.70
126	AS	C * C - S - C * C - Br	# 2.20
7	AS	C * C - S - C * C - C	# 6.85
126	AS	C * C - S - C * C - C	# 2.20
125	AS	C * C - S - C - C * C	# 4.07
127	AS	C * C - S - C - C - C	# 5.20
186	AS	C C S C C Cl	# 2.66
21	AS	C * C - S - C * C - Cl	# 1.70
126	AS	C * C - S - C * C - Cl	# 2.20
186	AS	C C S C C F	# 2.66
21	AS	C * C - S - C * C - F	# 1.70
126	AS	C * C - S - C * C - F	# 2.20
186	AS	C C S C C I	# 2.66
21	AS	C * C - S - C * C - I	# 1.70
126	AS	C * C - S - C * C - I	# 2.20
26	AS	C * C - S - C * C - N	# 1.63
126	AS	C * C - S - C * C - N	# 2.20
38	AS	C * C - S - C * C - O	# 5.99
126	AS	C * C - S - C * C - O	# 2.20
187	AS	C * C - S - C - C - O	# 3.29
38	AS	C * C - S - C * C - S	# 5.99
126	AS	C * C - S - C * C - S	# 2.20
187	AS	C * C - S - C - C - S	# 3.29
188	AS	C * C - S - C * N	# 0.61
189	AS	C * C - S - C - N	# 0.58
190	AS	C - C * S * C * N	# 2.79
191	AS	C - C * S * C - N	# 2.04
192	AS	C * C - S - C * O	# 1.20
193	AS	C * C - S - C - O	# 4.71
194	AS	C - C * S * C - O	# 3.38
195	AS	C - C - S - C - O	# 13.48
192	AS	C * C - S - C * S	# 1.20
193	AS	C * C - S - C - S	# 4.71
194	AS	C - C * S * C - S	# 3.38
195	AS	C - C - S - C - S	# 13.48
196	AS	C C S Cl	# 0.10
196	AS	C C S F	# 0.10
196	AS	C C S I	# 0.10
2085	AS	C C S N	# 26.07
197	AS	C * C - S - N	# 3.51
198	AS	C - C * S * N	# 0.77
199	AS	C - C - S - N	# 1.12
200	AS	C * C - S - N - C	# 2.34
2085	AS	C C S O	# 26.07
201	AS	C * C - S - O	# 6.11
202	AS	C - C - S - O	# 2.21
203	AS	C * C - S - O - C * C	# 0.20
2085	AS	C C S S	# 26.07
201	AS	C * C - S - S	# 6.11
202	AS	C - C - S - S	# 2.21
203	AS	C * C - S - S - C * C	# 0.20
2083	AS	C N C C	61.18
135	AS	C * N - C * C	8.07
138	AS	C * N - C - C	14.80
137	AS	C - N * C - C	8.60

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
136 AS	C - N - C * C	18.27
139 AS	C - N - C - C	29.65
212 AS	C - N - C C Br	# 4.26
96 AS	C * N - C - C * C	4.61
100 AS	C * N - C - C - C	7.00
98 AS	C - N * C * C - C	5.92
99 AS	C - N - C * C - C	1.84
97 AS	C - N - C - C * C	12.91
62 AS	C * N - C - C - C * C	1.14
64 AS	C - N * C * C * C - C	5.71
65 AS	C - N - C * C * C - C	2.97
66 AS	C - N - C - C * C - C	1.27
63 AS	C - N - C - C - C * C	5.95
204 AS	C * N - C * C * C * N	0.75
205 AS	C * N - C - C - C - N	0.86
206 AS	C - N * C * C - C - N	1.01
207 AS	C - N - C * C * C - N	0.82
208 AS	C - N * C * C * C - O	# 3.76
209 AS	C - N - C * C * C - O	# 2.16
210 AS	C - N - C * C - C - O	# 1.11
211 AS	C - N - C - C * C - O	# 1.57
208 AS	C - N * C * C * C - S	# 3.76
209 AS	C - N - C * C * C - S	# 2.16
210 AS	C - N - C * C - C - S	# 1.11
211 AS	C - N - C - C * C - S	# 1.57
212 AS	C N C C Cl	# 4.26
212 AS	C N C C F	# 4.26
212 AS	C N C C I	# 4.26
213 AS	C * N - C * C * N	0.36
214 AS	C * N - C - C - N	3.24
215 AS	C - N * C * C * N	6.81
216 AS	C - N * C * C - N	1.18
217 AS	C - N * C - C - N	2.43
218 AS	C - N - C * C - N	0.85
219 AS	C - N - C - C - N	7.91
220 AS	C - N * C * C * N - C	2.77
221 AS	C N C C N N	2.85
222 AS	C - N - C * C - N - O	# 0.32
222 AS	C - N - C * C - N - S	# 0.32
223 AS	C * N - C * C - O	# 0.96
224 AS	C * N - C - C - O	# 2.89
225 AS	C - N * C * C * O	# 3.33
226 AS	C - N * C * C - O	# 1.88
227 AS	C - N * C - C - O	# 2.68
228 AS	C - N - C * C - O	# 3.06
229 AS	C - N - C - C - O	# 12.06
230 AS	C - N - C * C - O - C	# 1.28
223 AS	C * N - C * C - S	# 0.96
224 AS	C * N - C - C - S	# 2.89
225 AS	C - N * C * C * S	# 3.33
226 AS	C - N * C * C - S	# 1.88
227 AS	C - N * C - C - S	# 2.68
228 AS	C - N - C * C - S	# 3.06
229 AS	C - N - C - C - S	# 12.06
230 AS	C - N - C * C - S - C	# 1.28

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
2086	AS	C N C N	# 30.95
231	AS	C * N - C * N	1.29
232	AS	C * N - C - N	0.93
233	AS	C - N * C * N	7.12
234	AS	C - N - C * N	4.77
235	AS	C - N - C - N	5.46
236	AS	C - N * C * N - C	1.19
237	AS	C - N - C - N - C	2.24
156	AS	C - N - C - N - C * C	1.65
238	AS	C * N * C * N * C * N	2.92
2087	AS	C N C O	# 39.80
239	AS	C * N - C * O	# 1.30
240	AS	C * N - C - O	# 5.80
241	AS	C - N * C * O	# 1.96
242	AS	C - N * C - O	# 8.74
243	AS	C - N - C - O	# 23.15
244	AS	C * N - C - O - C	# 1.06
245	AS	C - N * C - O - C	# 1.08
246	AS	C - N - C - O - C	# 3.12
2087	AS	C N C S	# 39.80
239	AS	C * N - C * S	# 1.30
240	AS	C * N - C - S	# 5.80
241	AS	C - N * C * S	# 1.96
242	AS	C - N * C - S	# 8.74
243	AS	C - N - C - S	# 23.15
244	AS	C * N - C - S - C	# 1.06
245	AS	C - N * C - S - C	# 1.08
246	AS	C - N - C - S - C	# 3.12
2093	AS	C N N C	# 24.67
247	AS	C - N * N - C	0.23
248	AS	C - N - N - C	4.27
170	AS	C - N * N * C - C	1.83
171	AS	C - N - N - C - C	2.85
249	AS	C - N * N * C - O	# 0.35
249	AS	C - N * N * C - S	# 0.35
250	AS	C N N N	1.47
2092	AS	C N O C	# 13.08
251	AS	C * N - O - C	# 1.09
252	AS	C - N - O - C	# 3.76
200	AS	C - N - O - C * C	# 2.34
2092	AS	C N O O	# 13.08
253	AS	C * N - O - O	# 0.97
254	AS	C - N - O * O	# 0.00
255	AS	C - N - O - O	# 2.96
2092	AS	C N O S	# 13.08
253	AS	C * N - O - S	# 0.97
254	AS	C - N - O * S	# 0.00
255	AS	C - N - O - S	# 2.96
2092	AS	C N S C	# 13.08
251	AS	C * N - S - C	# 1.09
252	AS	C - N - S - C	# 3.76
200	AS	C - N - S - C * C	# 2.34
2092	AS	C N S O	# 13.08
253	AS	C * N - S - O	# 0.97
254	AS	C - N - S * O	# 0.00

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
255	AS	C - N - S - O	# 2.96
2092	AS	C - N - S - S	# 13.08
253	AS	C * N - S - S	# 0.97
254	AS	C - N - S * S	# 0.00
255	AS	C - N - S - S	# 2.96
2084	AS	C - O - C - C	# 55.24
180	AS	C - O - C * C	# 26.47
265	AS	C - O - C * C - Br	# 1.77
123	AS	C - O - C * C - C	# 6.93
122	AS	C - O - C - C * C	# 13.92
124	AS	C - O - C - C - C	# 16.58
256	AS	C - O - C - C - C - Br	# 3.02
82	AS	C - O - C * C * C - C	# 7.34
84	AS	C - O - C * C - C - C	# 1.91
83	AS	C - O - C - C * C - C	# 2.79
81	AS	C - O - C - C - C * C	# 2.56
256	AS	C - O - C - C - C - Cl	# 3.02
256	AS	C - O - C - C - C - F	# 3.02
256	AS	C - O - C - C - C - I	# 3.02
257	AS	C - O - C * C * C - N	# 1.86
258	AS	C - O - C * C - C - N	# 1.12
259	AS	C - O - C - C * C - N	# 0.72
260	AS	C - O - C - C - C - N	# 2.88
261	AS	C - O - C * C * C - O	# 4.46
262	AS	C - O - C * C - C - O	# 2.33
263	AS	C - O - C - C * C - O	# 2.05
264	AS	C - O - C - C - C - O	# 3.09
261	AS	C - O - C * C * C - S	# 4.46
262	AS	C - O - C * C - C - S	# 2.33
263	AS	C - O - C - C * C - S	# 2.05
264	AS	C - O - C - C - C - S	# 3.09
265	AS	C - O - C * C - Cl	# 1.77
265	AS	C - O - C * C - F	# 1.77
265	AS	C - O - C * C - I	# 1.77
266	AS	C - O - C * C * N	# 1.56
267	AS	C - O - C * C - N	# 2.37
268	AS	C - O - C - C * N	# 1.79
269	AS	C - O - C - C - N	# 6.99
230	AS	C - O - C * C - N - C	# 1.28
270	AS	C - O - C - C - N - N	# 2.19
271	AS	C - O - C * C - N - O	# 0.42
271	AS	C - O - C * C - N - S	# 0.42
272	AS	C - O - C * C - O	# 6.16
273	AS	C - O - C - C - O	# 8.01
272	AS	C - O - C * C - S	# 6.16
273	AS	C - O - C - C - S	# 8.01
2086	AS	C - O - C - N	# 30.95
2093	AS	C - O - C - N	# 24.67
274	AS	C - O - C * N	# 3.68
275	AS	C - O - C - N	# 4.54
245	AS	C - O - C * N - C	# 1.08
244	AS	C - O - C - N * C	# 1.06
246	AS	C - O - C - N - C	# 3.12
165	AS	C - O - C - N - C * C	# 0.83
276	AS	C - O - C * N * N	# 1.23

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
2088	AS	C O C O	# 27.26
2094	AS	C O C O	# 27.26
277	AS	C - O - C * O	# 2.86
278	AS	C - O - C - O - C	# 1.42
2088	AS	C O C S	# 27.26
2094	AS	C O C S	# 27.26
277	AS	C - O - C * S	# 2.86
278	AS	C - O - C - S - C	# 1.42
2092	AS	C O N C	# 13.08
251	AS	C - O - N * C	# 1.09
252	AS	C - O - N - C	# 3.76
177	AS	C - O - N - C * C	# 1.40
178	AS	C - O - N - C - C	# 2.11
279	AS	C O N O	# 0.17
279	AS	C O N S	# 0.17
2092	AS	C O O C	# 13.08
2093	AS	C O O C	# 24.67
280	AS	C - O - O - C	# 0.81
281	AS	C O O N	# 0.09
282	AS	C O O O	# 1.03
282	AS	C O O S	# 1.03
2092	AS	C O S C	# 13.08
2093	AS	C O S C	# 24.67
280	AS	C - O - S - C	# 0.81
281	AS	C O S N	# 0.09
282	AS	C O S O	# 1.03
282	AS	C O S S	# 1.03
2084	AS	C S C C	# 55.24
180	AS	C - S - C * C	# 26.47
265	AS	C - S - C * C - Br	# 1.77
123	AS	C - S - C * C - C	# 6.93
122	AS	C - S - C - C * C	# 13.92
124	AS	C - S - C - C - C	# 16.58
256	AS	C S C C C Br	# 3.02
82	AS	C - S - C * C * C - C	# 7.34
84	AS	C - S - C * C - C - C	# 1.91
83	AS	C - S - C - C * C - C	# 2.79
81	AS	C - S - C - C - C * C	# 2.56
256	AS	C S C C C Cl	# 3.02
256	AS	C S C C C F	# 3.02
256	AS	C S C C C I	# 3.02
257	AS	C - S - C * C * C - N	# 1.86
258	AS	C - S - C * C - C - N	# 1.12
259	AS	C - S - C - C * C - N	# 0.72
260	AS	C - S - C - C - C - N	# 2.88
261	AS	C - S - C * C * C - O	# 4.46
262	AS	C - S - C * C - C - O	# 2.33
263	AS	C - S - C - C * C - O	# 2.05
264	AS	C - S - C - C - C - O	# 3.09
261	AS	C - S - C * C * C - S	# 4.46
262	AS	C - S - C * C - C - S	# 2.33
263	AS	C - S - C - C * C - S	# 2.05
264	AS	C - S - C - C - C - S	# 3.09
265	AS	C - S - C * C - Cl	# 1.77
265	AS	C - S - C * C - F	# 1.77



# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
265	AS	C - S - C * C - I	# 1.77
266	AS	C - S - C * C * N	# 1.56
267	AS	C - S - C * C - N	# 2.37
268	AS	C - S - C - C * N	# 1.79
269	AS	C - S - C - C - N	# 6.99
230	AS	C - S - C * C - N - C	# 1.28
270	AS	C S C C N N	# 2.19
271	AS	C - S - C * C - N - O	# 0.42
271	AS	C - S - C * C - N - S	# 0.42
272	AS	C - S - C * C - O	# 6.16
273	AS	C - S - C - C - O	# 8.01
272	AS	C - S - C * C - S	# 6.16
273	AS	C - S - C - C - S	# 8.01
2086	AS	C S C N	# 30.95
2093	AS	C S C N	# 24.67
274	AS	C - S - C * N	# 3.68
275	AS	C - S - C - N	# 4.54
245	AS	C - S - C * N - C	# 1.08
244	AS	C - S - C - N * C	# 1.06
246	AS	C - S - C - N - C	# 3.12
165	AS	C - S - C - N - C * C	# 0.83
276	AS	C - S - C * N * N	# 1.23
2088	AS	C S C O	# 27.26
2094	AS	C S C O	# 27.26
277	AS	C - S - C * O	# 2.86
278	AS	C - S - C - O - C	# 1.42
2088	AS	C S C S	# 27.26
2094	AS	C S C S	# 27.26
277	AS	C - S - C * S	# 2.86
278	AS	C - S - C - S - C	# 1.42
2092	AS	C S N C	# 13.08
251	AS	C - S - N * C	# 1.09
252	AS	C - S - N - C	# 3.76
177	AS	C - S - N - C * C	# 1.40
178	AS	C - S - N - C - C	# 2.11
279	AS	C S N O	# 0.17
279	AS	C S N S	# 0.17
2092	AS	C S O C	# 13.08
2093	AS	C S O C	# 24.67
280	AS	C - S - O - C	# 0.81
281	AS	C S O N	# 0.09
282	AS	C S O O	# 1.03
282	AS	C S O S	# 1.03
2092	AS	C S S C	# 13.08
2093	AS	C S S C	# 24.67
280	AS	C - S - S - C	# 0.81
281	AS	C S S N	# 0.09
282	AS	C S S O	# 1.03
282	AS	C S S S	# 1.03
331	AS	Cl C C As	# 1.39
331	AS	Cl C C B	# 1.39
312	AS	Cl- C * C - Br	# 2.00
313	AS	Cl- C - C - Br	# 0.90
88	AS	Cl- C * C - C	# 4.80
87	AS	Cl- C - C * C	# 3.30

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
89	AS	Cl- C - C - C	# 2.86
311	AS	Cl C C C As	# 1.14
311	AS	Cl C C C B	# 1.14
292	AS	Cl- C * C * C - Br	# 3.37
293	AS	Cl- C * C - C - Br	# 0.20
293	AS	Cl- C - C * C - Br	# 0.20
294	AS	Cl- C - C - C - Br	# 0.74
49	AS	Cl- C * C * C - C	# 4.52
6	AS	Cl- C * C - C * C	# 7.08
21	AS	Cl- C * C - C * C	# 1.70
50	AS	Cl- C * C - C - C	# 1.14
48	AS	Cl- C - C - C * C	# 0.77
51	AS	Cl- C - C - C - C	# 1.49
291	AS	Cl C C C C As	# 0.79
291	AS	Cl C C C C B	# 0.79
283	AS	Cl- C * C * C * C - Br	# 1.11
284	AS	Cl- C - C - C - C - Br	# 0.36
22	AS	Cl- C * C * C * C - C	# 5.91
14	AS	Cl- C * C - C - C * C	# 3.46
21	AS	Cl- C * C - C - C * C	# 1.70
23	AS	Cl- C - C - C - C - C	# 0.96
283	AS	Cl- C * C * C * C - Cl	# 1.11
284	AS	Cl- C - C - C - C - Cl	# 0.36
283	AS	Cl- C * C * C * C - F	# 1.11
284	AS	Cl- C - C - C - C - F	# 0.36
283	AS	Cl- C * C * C * C - I	# 1.11
284	AS	Cl- C - C - C - C - I	# 0.36
285	AS	Cl C C C C N	# 7.02
286	AS	Cl- C * C * C * C - N	# 2.55
287	AS	Cl- C * C * C - C - N	# 1.22
288	AS	Cl C C C C O	# 6.39
289	AS	Cl- C * C * C * C - O	# 3.00
290	AS	Cl- C * C * C - C - O	# 1.30
291	AS	Cl C C C C P	# 0.79
288	AS	Cl C C C C S	# 6.39
289	AS	Cl- C * C * C * C - S	# 3.00
290	AS	Cl- C * C * C - C - S	# 1.30
291	AS	Cl C C C C Se	# 0.79
291	AS	Cl C C C C Si	# 0.79
291	AS	Cl C C C C Te	# 0.79
292	AS	Cl- C * C * C - Cl	# 3.37
293	AS	Cl- C * C - C - Cl	# 0.20
293	AS	Cl- C - C * C - Cl	# 0.20
294	AS	Cl- C - C - C - Cl	# 0.74
292	AS	Cl- C * C * C - F	# 3.37
293	AS	Cl- C * C - C - F	# 0.20
293	AS	Cl- C - C * C - F	# 0.20
294	AS	Cl- C - C - C - F	# 0.74
292	AS	Cl- C * C * C - I	# 3.37
293	AS	Cl- C * C - C - I	# 0.20
293	AS	Cl- C - C * C - I	# 0.20
294	AS	Cl- C - C - C - I	# 0.74
295	AS	Cl C C C N	# 5.58
296	AS	Cl- C * C * C * N	# 1.36
297	AS	Cl- C * C * C - N	# 1.96

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
298	AS	Cl- C * C - C - N	# 1.26
299	AS	Cl- C - C - C - N	# 0.37
302	AS	Cl C C C N As	# 0.44
302	AS	Cl C C C N B	# 0.44
300	AS	Cl C C C N N	# 0.84
301	AS	Cl C C C N O	# 0.55
302	AS	Cl C C C N P	# 0.44
301	AS	Cl C C C N S	# 0.55
302	AS	Cl C C C N Se	# 0.44
302	AS	Cl C C C N Si	# 0.44
302	AS	Cl C C C N Te	# 0.44
303	AS	Cl C C C O	# 5.10
304	AS	Cl- C * C * C * O	# 0.64
305	AS	Cl- C * C * C - O	# 1.72
306	AS	Cl- C * C - C - O	# 1.61
307	AS	Cl- C - C - C - O	# 0.86
310	AS	Cl C C C O As	# 2.38
310	AS	Cl C C C O B	# 2.38
256	AS	Cl C C C O C	# 3.02
308	AS	Cl C C C O N	# 0.26
309	AS	Cl C C C O O	# 0.37
310	AS	Cl C C C O P	# 2.38
309	AS	Cl C C C O S	# 0.37
310	AS	Cl C C C O Se	# 2.38
310	AS	Cl C C C O Si	# 2.38
310	AS	Cl C C C O Te	# 2.38
311	AS	Cl C C C P	# 1.14
303	AS	Cl C C C S	# 5.10
304	AS	Cl- C * C * C * S	# 0.64
305	AS	Cl- C * C * C - S	# 1.72
306	AS	Cl- C * C - C - S	# 1.61
307	AS	Cl- C - C - C - S	# 0.86
310	AS	Cl C C C S As	# 2.38
310	AS	Cl C C C S B	# 2.38
256	AS	Cl C C C S C	# 3.02
308	AS	Cl C C C S N	# 0.26
309	AS	Cl C C C S O	# 0.37
310	AS	Cl C C C S P	# 2.38
309	AS	Cl C C C S S	# 0.37
310	AS	Cl C C C S Se	# 2.38
310	AS	Cl C C C S Si	# 2.38
310	AS	Cl C C C S Te	# 2.38
311	AS	Cl C C C Se	# 1.14
311	AS	Cl C C C Si	# 1.14
311	AS	Cl C C C Te	# 1.14
312	AS	Cl- C * C - Cl	# 2.00
313	AS	Cl- C - C - Cl	# 0.90
312	AS	Cl- C * C - F	# 2.00
313	AS	Cl- C - C - F	# 0.90
312	AS	Cl- C * C - I	# 2.00
313	AS	Cl- C - C - I	# 0.90
314	AS	Cl- C * C * N	# 1.48
315	AS	Cl- C * C - N	# 2.34
316	AS	Cl- C - C * N	# 0.64
317	AS	Cl- C - C - N	# 1.12

# Atom Sequences

Screen Number		Fragment Definition						Frequency Percent
302	AS	Cl	C	C	N	As	#	0.44
302	AS	Cl	C	C	N	B	#	0.44
212	AS	Cl	C	C	N	C	#	4.26
21	AS	Cl-	C *	C -	N -	C * C	#	1.70
102	AS	Cl-	C *	C -	N -	C * C	#	0.92
318	AS	Cl	C	C	N	C N	#	1.48
319	AS	Cl	C	C	N	C O	#	1.84
320	AS	Cl-	C *	C -	N -	C - O	#	0.72
319	AS	Cl	C	C	N	C S	#	1.84
320	AS	Cl-	C *	C -	N -	C - S	#	0.72
321	AS	Cl	C	C	N	N	#	0.82
322	AS	Cl	C	C	N	O	#	0.39
302	AS	Cl	C	C	N	P	#	0.44
322	AS	Cl	C	C	N	S	#	0.39
302	AS	Cl	C	C	N	Se	#	0.44
302	AS	Cl	C	C	N	Si	#	0.44
302	AS	Cl	C	C	N	Te	#	0.44
323	AS	Cl-	C *	C *	O		#	0.61
324	AS	Cl-	C *	C -	O		#	2.95
325	AS	Cl-	C -	C *	O		#	0.45
326	AS	Cl-	C -	C -	O		#	2.53
310	AS	Cl	C	C	O	As	#	2.38
310	AS	Cl	C	C	O	B	#	2.38
265	AS	Cl-	C *	C -	O -	C	#	1.77
186	AS	Cl	C	C	O	C C	#	2.66
21	AS	Cl-	C *	C -	O -	C * C	#	1.70
126	AS	Cl-	C *	C -	O -	C * C	#	2.20
327	AS	Cl	C	C	O	C N	#	0.27
328	AS	Cl	C	C	O	C O	#	0.64
328	AS	Cl	C	C	O	C S	#	0.64
329	AS	Cl	C	C	O	N	#	0.30
330	AS	Cl	C	C	O	O	#	0.43
310	AS	Cl	C	C	O	P	#	2.38
330	AS	Cl	C	C	O	S	#	0.43
310	AS	Cl	C	C	O	Se	#	2.38
310	AS	Cl	C	C	O	Si	#	2.38
310	AS	Cl	C	C	O	Te	#	2.38
331	AS	Cl	C	C	P		#	1.39
323	AS	Cl-	C *	C *	S		#	0.61
324	AS	Cl-	C *	C -	S		#	2.95
325	AS	Cl-	C -	C *	S		#	0.45
326	AS	Cl-	C -	C -	S		#	2.53
310	AS	Cl	C	C	S	As	#	2.38
310	AS	Cl	C	C	S	B	#	2.38
265	AS	Cl-	C *	C -	S -	C	#	1.77
186	AS	Cl	C	C	S	C C	#	2.66
21	AS	Cl-	C *	C -	S -	C * C	#	1.70
126	AS	Cl-	C *	C -	S -	C * C	#	2.20
327	AS	Cl	C	C	S	C N	#	0.27
328	AS	Cl	C	C	S	C O	#	0.64
328	AS	Cl	C	C	S	C S	#	0.64
329	AS	Cl	C	C	S	N	#	0.30
330	AS	Cl	C	C	S	O	#	0.43
310	AS	Cl	C	C	S	P	#	2.38
330	AS	Cl	C	C	S	S	#	0.43

# Atom Sequences

Screen Number		Fragment Definition						Frequency	Percent
310	AS	Cl	C	C	S	Se	#	2.38	
310	AS	Cl	C	C	S	Si	#	2.38	
310	AS	Cl	C	C	S	Te	#	2.38	
331	AS	Cl	C	C	Se		#	1.39	
331	AS	Cl	C	C	Si		#	1.39	
331	AS	Cl	C	C	Te		#	1.39	
332	AS	Cl	C	N	C	Br	#	0.12	
332	AS	Cl	C	N	C	Cl	#	0.12	
332	AS	Cl	C	N	C	F	#	0.12	
332	AS	Cl	C	N	C	I	#	0.12	
333	AS	Cl	C	N	C	N	#	0.53	
334	AS	Cl	C	N	C	O	#	0.18	
334	AS	Cl	C	N	C	S	#	0.18	
335	AS	Cl	C	N	O		#	0.09	
335	AS	Cl	C	N	S		#	0.09	
336	AS	Cl	C	O	O		#	0.37	
336	AS	Cl	C	O	S		#	0.37	
336	AS	Cl	C	S	O		#	0.37	
336	AS	Cl	C	S	S		#	0.37	
196	AS	Cl	O	C	C		#	0.10	
196	AS	Cl	S	C	C		#	0.10	
331	AS	F	C	C	As		#	1.39	
331	AS	F	C	C	B		#	1.39	
312	AS	F - C	* C -	Br			#	2.00	
313	AS	F - C -	C -	Br			#	0.90	
88	AS	F - C	* C -	C			#	4.80	
87	AS	F - C -	C *	C			#	3.30	
89	AS	F - C -	C -	C			#	2.86	
311	AS	F	C	C	C	As	#	1.14	
311	AS	F	C	C	C	B	#	1.14	
292	AS	F - C	* C *	C -	Br		#	3.37	
293	AS	F - C	* C -	C -	Br		#	0.20	
293	AS	F - C -	C *	C -	Br		#	0.20	
294	AS	F - C -	C -	C -	Br		#	0.74	
49	AS	F - C	* C *	C -	C		#	4.52	
6	AS	F - C	* C -	C *	C		#	7.08	
21	AS	F - C	* C -	C *	C		#	1.70	
50	AS	F - C	* C -	C -	C		#	1.14	
48	AS	F - C -	C -	C *	C		#	0.77	
51	AS	F - C -	C -	C -	C		#	1.49	
291	AS	F	C	C	C	C As	#	0.79	
291	AS	F	C	C	C	C B	#	0.79	
283	AS	F - C	* C *	C *	C -	Br	#	1.11	
284	AS	F - C -	C -	C -	C -	Br	#	0.36	
22	AS	F - C	* C *	C *	C -	C	#	5.91	
14	AS	F - C	* C -	C -	C *	C	#	3.46	
21	AS	F - C	* C -	C -	C *	C	#	1.70	
23	AS	F - C -	C -	C -	C -	C	#	0.96	
283	AS	F - C	* C *	C *	C -	Cl	#	1.11	
284	AS	F - C -	C -	C -	C -	Cl	#	0.36	
283	AS	F - C	* C *	C *	C -	F	#	1.11	
284	AS	F - C -	C -	C -	C -	F	#	0.36	
283	AS	F - C	* C *	C *	C -	I	#	1.11	
284	AS	F - C -	C -	C -	C -	I	#	0.36	
285	AS	F	C	C	C	C N	#	7.02	

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
286	AS F - C * C * C * C - N	# 2.55
287	AS F - C * C * C - C - N	# 1.22
288	AS F - C C C C O	# 6.39
289	AS F - C * C * C * C - O	# 3.00
290	AS F - C * C * C - C - O	# 1.30
291	AS F C C C C P	# 0.79
288	AS F C C C C S	# 6.39
289	AS F - C * C * C * C - S	# 3.00
290	AS F - C * C * C - C - S	# 1.30
291	AS F C C C C Se	# 0.79
291	AS F C C C C Si	# 0.79
291	AS F C C C C Te	# 0.79
292	AS F - C * C * C - Cl	# 3.37
293	AS F - C * C - C - Cl	# 0.20
293	AS F - C - C * C - Cl	# 0.20
294	AS F - C - C - C - Cl	# 0.74
292	AS F - C * C * C - F	# 3.37
293	AS F - C * C - C - F	# 0.20
293	AS F - C - C * C - F	# 0.20
294	AS F - C - C - C - F	# 0.74
292	AS F - C * C * C - I	# 3.37
293	AS F - C * C - C - I	# 0.20
293	AS F - C - C * C - I	# 0.20
294	AS F - C - C - C - I	# 0.74
295	AS F C C C N	# 5.58
296	AS F - C * C * C * N	# 1.36
297	AS F - C * C * C - N	# 1.96
298	AS F - C * C - C - N	# 1.26
299	AS F - C - C - C - N	# 0.37
302	AS F C C C N As	# 0.44
302	AS F C C C N B	# 0.44
300	AS F C C C N N	# 0.84
301	AS F C C C N O	# 0.55
302	AS F C C C N P	# 0.44
301	AS F C C C N S	# 0.55
302	AS F C C C N Se	# 0.44
302	AS F C C C N Si	# 0.44
302	AS F C C C N Te	# 0.44
303	AS F C C C O	# 5.10
304	AS F - C * C * C * O	# 0.64
305	AS F - C * C * C - O	# 1.72
306	AS F - C * C - C - O	# 1.61
307	AS F - C - C - C - O	# 0.86
310	AS F C C C O As	# 2.38
310	AS F C C C O B	# 2.38
256	AS F C C C O C	# 3.02
308	AS F C C C O N	# 0.26
309	AS F C C C O O	# 0.37
310	AS F C C C O P	# 2.38
309	AS F C C C O S	# 0.37
310	AS F C C C O Se	# 2.38
310	AS F C C C O Si	# 2.38
310	AS F C C C O Te	# 2.38
311	AS F C C C P	# 1.14
303	AS F C C C S	# 5.10

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
304	AS	F - C * C * C * S	# 0.64
305	AS	F - C * C * C - S	# 1.72
306	AS	F - C * C - C - S	# 1.61
307	AS	F - C - C - C - S	# 0.86
310	AS	F C C C S As	# 2.38
310	AS	F C C C S B	# 2.38
256	AS	F C C C S C	# 3.02
308	AS	F C C C S N	# 0.26
309	AS	F C C C S O	# 0.37
310	AS	F C C C S P	# 2.38
309	AS	F C C C S S	# 0.37
310	AS	F C C C S Se	# 2.38
310	AS	F C C C S Si	# 2.38
310	AS	F C C C S Te	# 2.38
311	AS	F C C C Se	# 1.14
311	AS	F C C C Si	# 1.14
311	AS	F C C C Te	# 1.14
312	AS	F - C * C - Cl	# 2.00
313	AS	F - C - C - Cl	# 0.90
312	AS	F - C * C - F	# 2.00
313	AS	F - C - C - F	# 0.90
312	AS	F - C * C - I	# 2.00
313	AS	F - C - C - I	# 0.90
314	AS	F - C * C * N	# 1.48
315	AS	F - C * C - N	# 2.34
316	AS	F - C - C * N	# 0.64
317	AS	F - C - C - N	# 1.12
302	AS	F C C N As	# 0.44
302	AS	F C C N B	# 0.44
212	AS	F C C N C	# 4.26
21	AS	F - C * C - N - C * C	# 1.70
102	AS	F - C * C - N - C * C	# 0.92
318	AS	F C C N C N	# 1.48
319	AS	F C C N C O	# 1.84
320	AS	F - C * C - N - C - O	# 0.72
319	AS	F C C N C S	# 1.84
320	AS	F - C * C - N - C - S	# 0.72
321	AS	F C C N N	# 0.82
322	AS	F C C N O	# 0.39
302	AS	F C C N P	# 0.44
322	AS	F C C N S	# 0.39
302	AS	F C C N Se	# 0.44
302	AS	F C C N Si	# 0.44
302	AS	F C C N Te	# 0.44
323	AS	F - C * C * O	# 0.61
324	AS	F - C * C - O	# 2.95
325	AS	F - C - C * O	# 0.45
326	AS	F - C - C - O	# 2.53
310	AS	F C C O As	# 2.38
310	AS	F C C O B	# 2.38
265	AS	F - C * C - O - C	# 1.77
186	AS	F C C O C C	# 2.66
21	AS	F - C * C - O - C * C	# 1.70
126	AS	F - C * C - O - C * C	# 2.20
327	AS	F C C O C N	# 0.27

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
328	AS F C C O C O	# 0.64
328	AS F C C O C S	# 0.64
329	AS F C C O N	# 0.30
330	AS F C C O O	# 0.43
310	AS F C C O P	# 2.38
330	AS F C C O S	# 0.43
310	AS F C C O Se	# 2.38
310	AS F C C O Si	# 2.38
310	AS F C C O Te	# 2.38
331	AS F C C P	# 1.39
323	AS F - C * C * S	# 0.61
324	AS F - C * C - S	# 2.95
325	AS F - C - C * S	# 0.45
326	AS F - C - C - S	# 2.53
310	AS F C C S As	# 2.38
310	AS F C C S B	# 2.38
265	AS F - C * C - S - C	# 1.77
186	AS F C C S C C	# 2.66
21	AS F - C * C - S - C * C	# 1.70
126	AS F - C * C - S - C * C	# 2.20
327	AS F C C S C N	# 0.27
328	AS F C C S C O	# 0.64
328	AS F C C S C S	# 0.64
329	AS F C C S N	# 0.30
330	AS F C C S O	# 0.43
310	AS F C C S P	# 2.38
330	AS F C C S S	# 0.43
310	AS F C C S Se	# 2.38
310	AS F C C S Si	# 2.38
310	AS F C C S Te	# 2.38
331	AS F C C Se	# 1.39
331	AS F C C Si	# 1.39
331	AS F C C Te	# 1.39
332	AS F C N C Br	# 0.12
332	AS F C N C Cl	# 0.12
332	AS F C N C F	# 0.12
332	AS F C N C I	# 0.12
333	AS F C N C N	# 0.53
334	AS F C N C O	# 0.18
334	AS F C N C S	# 0.18
335	AS F C N O	# 0.09
335	AS F C N S	# 0.09
336	AS F C O O	# 0.37
336	AS F C O S	# 0.37
336	AS F C S O	# 0.37
336	AS F C S S	# 0.37
196	AS F O C C	# 0.10
196	AS F S C C	# 0.10
331	AS I C C As	# 1.39
331	AS I C C B	# 1.39
312	AS I - C * C - Br	# 2.00
313	AS I - C - C - Br	# 0.90
88	AS I - C * C - C	# 4.80
87	AS I - C - C * C	# 3.30
89	AS I - C - C - C	# 2.86



# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
311	AS I C C C As	# 1.14
311	AS I C C C B	# 1.14
292	AS I - C * C * C - Br	# 3.37
293	AS I - C * C - C - Br	# 0.20
293	AS I - C - C * C - Br	# 0.20
294	AS I - C - C - C - Br	# 0.74
49	AS I - C * C * C - C	# 4.52
6	AS I - C * C - C * C	# 7.08
21	AS I - C * C - C * C	# 1.70
50	AS I - C * C - C - C	# 1.14
48	AS I - C - C - C * C	# 0.77
51	AS I - C - C - C - C	# 1.49
291	AS I C C C C As	# 0.79
291	AS I C C C C B	# 0.79
283	AS I - C * C * C * C - Br	# 1.11
284	AS I - C - C - C - C - Br	# 0.36
22	AS I - C * C * C * C - C	# 5.91
14	AS I - C * C - C - C * C	# 3.46
21	AS I - C * C - C - C * C	# 1.70
23	AS I - C - C - C - C - C	# 0.96
283	AS I - C * C * C * C - Cl	# 1.11
284	AS I - C - C - C - C - Cl	# 0.36
283	AS I - C * C * C * C - F	# 1.11
284	AS I - C - C - C - C - F	# 0.36
283	AS I - C * C * C * C - I	# 1.11
284	AS I - C - C - C - C - I	# 0.36
285	AS I C C C C N	# 7.02
286	AS I - C * C * C * C - N	# 2.55
287	AS I - C * C * C - C - N	# 1.22
288	AS I C C C C O	# 6.39
289	AS I - C * C * C * C - O	# 3.00
290	AS I - C * C * C - C - O	# 1.30
291	AS I C C C C P	# 0.79
288	AS I C C C C S	# 6.39
289	AS I - C * C * C * C - S	# 3.00
290	AS I - C * C * C - C - S	# 1.30
291	AS I C C C C Se	# 0.79
291	AS I C C C C Si	# 0.79
291	AS I C C C C Te	# 0.79
292	AS I - C * C * C - Cl	# 3.37
293	AS I - C * C - C - Cl	# 0.20
293	AS I - C - C * C - Cl	# 0.20
294	AS I - C - C - C - Cl	# 0.74
292	AS I - C * C * C - F	# 3.37
293	AS I - C * C - C - F	# 0.20
293	AS I - C - C * C - F	# 0.20
294	AS I - C - C - C - F	# 0.74
292	AS I - C * C * C - I	# 3.37
293	AS I - C * C - C - I	# 0.20
293	AS I - C - C * C - I	# 0.20
294	AS I - C - C - C - I	# 0.74
295	AS I C C C N	# 5.58
296	AS I - C * C * C * N	# 1.36
297	AS I - C * C * C - N	# 1.96
298	AS I - C * C - C - N	# 1.26

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
299 AS	I - C - C - C - N	# 0.37
302 AS	I C C C N As	# 0.44
302 AS	I C C C N B	# 0.44
300 AS	I C C C N N	# 0.84
301 AS	I C C C N O	# 0.55
302 AS	I C C C N P	# 0.44
301 AS	I C C C N S	# 0.55
302 AS	I C C C N Se	# 0.44
302 AS	I C C C N Si	# 0.44
302 AS	I C C C N Te	# 0.44
303 AS	I C C C O	# 5.10
304 AS	I - C * C * C * O	# 0.64
305 AS	I - C * C * C - O	# 1.72
306 AS	I - C * C - C - O	# 1.61
307 AS	I - C - C - C - O	# 0.86
310 AS	I C C C O As	# 2.38
310 AS	I C C C O B	# 2.38
256 AS	I C C C O C	# 3.02
308 AS	I C C C O N	# 0.26
309 AS	I C C C O O	# 0.37
310 AS	I C C C O P	# 2.38
309 AS	I C C C O S	# 0.37
310 AS	I C C C O Se	# 2.38
310 AS	I C C C O Si	# 2.38
310 AS	I C C C O Te	# 2.38
311 AS	I C C C P	# 1.14
303 AS	I C C C S	# 5.10
304 AS	I - C * C * C * S	# 0.64
305 AS	I - C * C * C - S	# 1.72
306 AS	I - C * C - C - S	# 1.61
307 AS	I - C - C - C - S	# 0.86
310 AS	I C C C S As	# 2.38
310 AS	I C C C S B	# 2.38
256 AS	I C C C S C	# 3.02
308 AS	I C C C S N	# 0.26
309 AS	I C C C S O	# 0.37
310 AS	I C C C S P	# 2.38
309 AS	I C C C S S	# 0.37
310 AS	I C C C S Se	# 2.38
310 AS	I C C C S Si	# 2.38
310 AS	I C C C S Te	# 2.38
311 AS	I C C C Se	# 1.14
311 AS	I C C C Si	# 1.14
311 AS	I C C C Te	# 1.14
312 AS	I - C * C - Cl	# 2.00
313 AS	I - C - C - Cl	# 0.90
312 AS	I - C * C - F	# 2.00
313 AS	I - C - C - F	# 0.90
312 AS	I - C * C - I	# 2.00
313 AS	I - C - C - I	# 0.90
314 AS	I - C * C * N	# 1.48
315 AS	I - C * C - N	# 2.34
316 AS	I - C - C * N	# 0.64
317 AS	I - C - C - N	# 1.12
302 AS	I C C N As	# 0.44

# Atom Sequences

Screen Number		Fragment Definition						Frequency Percent
302	AS	I	C	C	N	B		# 0.44
212	AS	I	C	C	N	C		# 4.26
21	AS	I	- C *	C - N - C *	C			# 1.70
102	AS	I	- C *	C - N - C *	C			# 0.92
318	AS	I	C	C	N	C	N	# 1.48
319	AS	I	C	C	N	C	O	# 1.84
320	AS	I	- C *	C - N - C - O				# 0.72
319	AS	I	C	C	N	C	S	# 1.84
320	AS	I	- C *	C - N - C - S				# 0.72
321	AS	I	C	C	N	N		# 0.82
322	AS	I	C	C	N	O		# 0.39
302	AS	I	C	C	N	P		# 0.44
322	AS	I	C	C	N	S		# 0.39
302	AS	I	C	C	N	Se		# 0.44
302	AS	I	C	C	N	Si		# 0.44
302	AS	I	C	C	N	Te		# 0.44
323	AS	I	- C *	C * O				# 0.61
324	AS	I	- C *	C - O				# 2.95
325	AS	I	- C - C *	O				# 0.45
326	AS	I	- C - C - O					# 2.53
310	AS	I	C	C	O	As		# 2.38
310	AS	I	C	C	O	B		# 2.38
265	AS	I	- C *	C - O - C				# 1.77
186	AS	I	C	C	O	C	C	# 2.66
21	AS	I	- C *	C - O - C *	C			# 1.70
126	AS	I	- C *	C - O - C *	C			# 2.20
327	AS	I	C	C	O	C	N	# 0.27
328	AS	I	C	C	O	C	O	# 0.64
328	AS	I	C	C	O	C	S	# 0.64
329	AS	I	C	C	O	N		# 0.30
330	AS	I	C	C	O	O		# 0.43
310	AS	I	C	C	O	P		# 2.38
330	AS	I	C	C	O	S		# 0.43
310	AS	I	C	C	O	Se		# 2.38
310	AS	I	C	C	O	Si		# 2.38
310	AS	I	C	C	O	Te		# 2.38
331	AS	I	C	C	P			# 1.39
323	AS	I	- C *	C * S				# 0.61
324	AS	I	- C *	C - S				# 2.95
325	AS	I	- C - C *	S				# 0.45
326	AS	I	- C - C - S					# 2.53
310	AS	I	C	C	S	As		# 2.38
310	AS	I	C	C	S	B		# 2.38
265	AS	I	- C *	C - S - C				# 1.77
186	AS	I	C	C	S	C	C	# 2.66
21	AS	I	- C *	C - S - C *	C			# 1.70
126	AS	I	- C *	C - S - C *	C			# 2.20
327	AS	I	C	C	S	C	N	# 0.27
328	AS	I	C	C	S	C	O	# 0.64
328	AS	I	C	C	S	C	S	# 0.64
329	AS	I	C	C	S	N		# 0.30
330	AS	I	C	C	S	O		# 0.43
310	AS	I	C	C	S	P		# 2.38
330	AS	I	C	C	S	S		# 0.43
310	AS	I	C	C	S	Se		# 2.38

# Atom Sequences

Screen Number		Fragment Definition					Frequency Percent
310	AS	I	C	C	S	Si	# 2.38
310	AS	I	C	C	S	Te	# 2.38
331	AS	I	C	C	Se		# 1.39
331	AS	I	C	C	Si		# 1.39
331	AS	I	C	C	Te		# 1.39
332	AS	I	C	N	C	Br	# 0.12
332	AS	I	C	N	C	Cl	# 0.12
332	AS	I	C	N	C	F	# 0.12
332	AS	I	C	N	C	I	# 0.12
333	AS	I	C	N	C	N	# 0.53
334	AS	I	C	N	C	O	# 0.18
334	AS	I	C	N	C	S	# 0.18
335	AS	I	C	N	O		# 0.09
335	AS	I	C	N	S		# 0.09
336	AS	I	C	O	O		# 0.37
336	AS	I	C	O	S		# 0.37
336	AS	I	C	S	O		# 0.37
336	AS	I	C	S	S		# 0.37
196	AS	I	O	C	C		# 0.10
196	AS	I	S	C	C		# 0.10
331	AS	N	C	C	C	As	# 1.39
331	AS	N	C	C	C	B	# 1.39
314	AS	N	* C	* C	-	Br	# 1.48
316	AS	N	* C	-	C	- Br	# 0.64
315	AS	N	-	C	* C	- Br	# 2.34
317	AS	N	-	C	-	C - Br	# 1.12
2080	AS	N	C	C	C		67.06
92	AS	N	* C	* C	-	C	16.85
90	AS	N	* C	-	C	* C	8.61
94	AS	N	* C	-	C	- C	6.85
93	AS	N	-	C	* C	- C	6.37
91	AS	N	-	C	-	C * C	22.25
95	AS	N	-	C	-	C - C	24.66
311	AS	N	C	C	C	As	# 1.14
311	AS	N	C	C	C	B	# 1.14
295	AS	N	C	C	C	Br	# 5.58
296	AS	N	* C	* C	* C	- Br	# 1.36
297	AS	N	-	C	* C	* C - Br	# 1.96
298	AS	N	-	C	-	C * C - Br	# 1.26
299	AS	N	-	C	-	C - C - Br	# 0.37
52	AS	N	* C	* C	* C	* C	31.81
56	AS	N	* C	* C	* C	- C	13.91
53	AS	N	* C	* C	-	C * C	2.97
59	AS	N	* C	* C	-	C - C	7.01
54	AS	N	* C	-	C	- C * C	1.62
57	AS	N	-	C	* C	* C - C	6.09
6	AS	N	-	C	* C	- C * C	# 7.08
26	AS	N	-	C	* C	- C * C	# 1.63
60	AS	N	-	C	* C	- C - C	1.24
58	AS	N	-	C	-	C * C - C	2.87
55	AS	N	-	C	-	C - C * C	8.56
61	AS	N	-	C	-	C - C - C	14.08
291	AS	N	C	C	C	C As	# 0.79
291	AS	N	C	C	C	C B	# 0.79
285	AS	N	C	C	C	C Br	# 7.02

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
286 AS	N - C * C * C * C - Br	# 2.55
287 AS	N - C - C * C * C - Br	# 1.22
24 AS	N * C * C * C * C * C	27.22
28 AS	N * C * C * C * C - C	11.69
25 AS	N * C * C * C - C * C	4.17
29 AS	N - C * C * C * C - C	8.40
32 AS	N - C * C * C - C - C	0.92
14 AS	N - C * C - C - C * C	# 3.46
26 AS	N - C * C - C - C * C	# 1.63
30 AS	N - C - C * C * C - C	2.36
33 AS	N - C - C * C - C - C	0.34
31 AS	N - C - C - C * C - C	0.41
27 AS	N - C - C - C - C * C	5.29
34 AS	N - C - C - C - C - C	7.98
285 AS	N C C C C Cl	# 7.02
286 AS	N - C * C * C * C - Cl	# 2.55
287 AS	N - C - C * C * C - Cl	# 1.22
285 AS	N C C C C F	# 7.02
286 AS	N - C * C * C * C - F	# 2.55
287 AS	N - C - C * C * C - F	# 1.22
285 AS	N C C C C I	# 7.02
286 AS	N - C * C * C * C - I	# 2.55
287 AS	N - C - C * C * C - I	# 1.22
337 AS	N C C C C N	14.57
338 AS	N * C * C * C * C - N	2.18
339 AS	N * C * C * C - C * N	0.58
340 AS	N * C * C * C - C - N	1.89
341 AS	N * C * C - C * C * N	0.18
339 AS	N * C - C * C * C * N	0.58
338 AS	N - C * C * C * C * N	2.18
342 AS	N - C * C * C * C - N	2.33
343 AS	N - C * C * C - C - N	1.25
340 AS	N - C - C * C * C * N	1.89
343 AS	N - C - C * C * C - N	1.25
344 AS	N - C - C - C - C - N	3.17
345 AS	N C C C C O	# 25.91
346 AS	N * C * C * C * C - O	# 5.92
347 AS	N - C * C * C * C * O	# 2.82
348 AS	N - C * C * C * C - O	# 5.24
349 AS	N - C * C * C - C - O	# 1.64
350 AS	N - C - C * C * C - O	# 1.95
351 AS	N - C - C * C - C - O	# 0.50
352 AS	N - C - C - C * C - O	# 0.41
353 AS	N - C - C - C - C - O	# 4.12
291 AS	N C C C C P	# 0.79
345 AS	N C C C C S	# 25.91
346 AS	N * C * C * C * C - S	# 5.92
347 AS	N - C * C * C * C * S	# 2.82
348 AS	N - C * C * C * C - S	# 5.24
349 AS	N - C * C * C - C - S	# 1.64
350 AS	N - C - C * C * C - S	# 1.95
351 AS	N - C - C * C - C - S	# 0.50
352 AS	N - C - C - C * C - S	# 0.41
353 AS	N - C - C - C - C - S	# 4.12
291 AS	N C C C C Se	# 0.79

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
291 AS	N C C C C Si	# 0.79
291 AS	N C C C C Te	# 0.79
295 AS	N C C C Cl	# 5.58
296 AS	N * C * C * C - Cl	# 1.36
297 AS	N - C * C * C - Cl	# 1.96
298 AS	N - C - C * C - Cl	# 1.26
299 AS	N - C - C - C - Cl	# 0.37
295 AS	N C C C F	# 5.58
296 AS	N * C * C * C - F	# 1.36
297 AS	N - C * C * C - F	# 1.96
298 AS	N - C - C * C - F	# 1.26
299 AS	N - C - C - C - F	# 0.37
295 AS	N C C C I	# 5.58
296 AS	N * C * C * C - I	# 1.36
297 AS	N - C * C * C - I	# 1.96
298 AS	N - C - C * C - I	# 1.26
299 AS	N - C - C - C - I	# 0.37
2098 AS	N C C C N	# 22.43
354 AS	N * C * C * C * N	11.18
355 AS	N * C * C * C - N	4.85
356 AS	N * C * C - C * N	0.63
357 AS	N * C * C - C - N	3.16
356 AS	N * C - C * C * N	0.63
358 AS	N * C - C * C - N	0.16
359 AS	N * C - C - C * N	0.19
360 AS	N * C - C - C - N	1.65
355 AS	N - C * C * C * N	4.85
361 AS	N - C * C * C - N	1.84
358 AS	N - C * C - C * N	0.16
362 AS	N - C * C - C - N	1.32
357 AS	N - C - C * C * N	3.16
362 AS	N - C - C * C - N	1.32
360 AS	N - C - C - C * N	1.65
363 AS	N - C - C - C - N	3.46
302 AS	N C C C N As	# 0.44
302 AS	N C C C N B	# 0.44
204 AS	N * C * C * C - N * C	0.75
207 AS	N - C * C * C - N - C	0.82
206 AS	N - C - C * C * N - C	1.01
205 AS	N - C - C - C - N * C	0.86
364 AS	N C C C N N	3.16
365 AS	N C C C N O	# 2.43
366 AS	N * C * C * C - N - O	# 0.35
367 AS	N - C * C * C - N - O	# 1.02
302 AS	N C C C N P	# 0.44
365 AS	N C C C N S	# 2.43
366 AS	N * C * C * C - N - S	# 0.35
367 AS	N - C * C * C - N - S	# 1.02
302 AS	N C C C N Se	# 0.44
302 AS	N C C C N Si	# 0.44
302 AS	N C C C N Te	# 0.44
368 AS	N * C * C * C * O	# 4.16
369 AS	N * C * C * C - O	# 9.05
370 AS	N * C * C - C * O	# 2.56
371 AS	N * C * C - C - O	# 4.73

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
370	AS	N * C - C * C * O	# 2.56
372	AS	N * C - C * C - O	# 0.73
370	AS	N * C - C - C * O	# 2.56
373	AS	N * C - C - C - O	# 1.07
374	AS	N - C * C * C * O	# 1.65
375	AS	N - C * C * C - O	# 4.45
370	AS	N - C * C - C * O	# 2.56
376	AS	N - C * C - C - O	# 1.92
370	AS	N - C - C * C * O	# 2.56
377	AS	N - C - C * C - O	# 2.93
370	AS	N - C - C - C * O	# 2.56
378	AS	N - C - C - C - O	# 7.21
310	AS	N C C C O As	# 2.38
310	AS	N C C C O B	# 2.38
257	AS	N - C * C * C - O - C	# 1.86
259	AS	N - C * C - C - O - C	# 0.72
258	AS	N - C - C * C - O - C	# 1.12
260	AS	N - C - C - C - O - C	# 2.88
379	AS	N C C C O N	# 0.80
380	AS	N C C C O O	# 1.74
381	AS	N - C * C * C - O - O	# 0.76
310	AS	N C C C O P	# 2.38
380	AS	N C C C O S	# 1.74
381	AS	N - C * C * C - O - S	# 0.76
310	AS	N C C C O Se	# 2.38
310	AS	N C C C O Si	# 2.38
310	AS	N C C C O Te	# 2.38
311	AS	N C C C P	# 1.14
368	AS	N * C * C * C * S	# 4.16
369	AS	N * C * C * C - S	# 9.05
370	AS	N * C * C - C * S	# 2.56
371	AS	N * C * C - C - S	# 4.73
370	AS	N * C - C * C * S	# 2.56
372	AS	N * C - C * C - S	# 0.73
370	AS	N * C - C - C * S	# 2.56
373	AS	N * C - C - C - S	# 1.07
374	AS	N - C * C * C * S	# 1.65
375	AS	N - C * C * C - S	# 4.45
370	AS	N - C * C - C * S	# 2.56
376	AS	N - C * C - C - S	# 1.92
370	AS	N - C - C * C * S	# 2.56
377	AS	N - C - C * C - S	# 2.93
370	AS	N - C - C - C * S	# 2.56
378	AS	N - C - C - C - S	# 7.21
310	AS	N C C C S As	# 2.38
310	AS	N C C C S B	# 2.38
257	AS	N - C * C * C - S - C	# 1.86
259	AS	N - C * C - C - S - C	# 0.72
258	AS	N - C - C * C - S - C	# 1.12
260	AS	N - C - C - C - S - C	# 2.88
379	AS	N C C C S N	# 0.80
380	AS	N C C C S O	# 1.74
381	AS	N - C * C * C - S - O	# 0.76
310	AS	N C C C S P	# 2.38
380	AS	N C C C S S	# 1.74

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
381 AS	N - C * C * C - S - S	# 0.76
310 AS	N C C C S Se	# 2.38
310 AS	N C C C S Si	# 2.38
310 AS	N C C C S Te	# 2.38
311 AS	N C C C Se	# 1.14
311 AS	N C C C Si	# 1.14
311 AS	N C C C Te	# 1.14
314 AS	N * C * C - Cl	# 1.48
316 AS	N * C - C - Cl	# 0.64
315 AS	N - C * C - Cl	# 2.34
317 AS	N - C - C - Cl	# 1.12
314 AS	N * C * C - F	# 1.48
316 AS	N * C - C - F	# 0.64
315 AS	N - C * C - F	# 2.34
317 AS	N - C - C - F	# 1.12
314 AS	N * C * C - I	# 1.48
316 AS	N * C - C - I	# 0.64
315 AS	N - C * C - I	# 2.34
317 AS	N - C - C - I	# 1.12
2089 AS	N C C N	23.97
382 AS	N * C * C * N	12.36
383 AS	N * C * C - N	4.10
384 AS	N * C - C * N	0.52
385 AS	N * C - C - N	4.56
383 AS	N - C * C * N	4.10
386 AS	N - C * C - N	1.42
385 AS	N - C - C * N	4.56
387 AS	N - C - C - N	8.72
302 AS	N C C N As	# 0.44
302 AS	N C C N B	# 0.44
215 AS	N * C * C * N - C	6.81
213 AS	N * C * C - N * C	0.36
216 AS	N - C * C * N - C	1.18
218 AS	N - C * C - N - C	0.85
217 AS	N - C - C * N - C	2.43
214 AS	N - C - C - N * C	3.24
219 AS	N - C - C - N - C	7.91
146 AS	N * C * C * N * C * C	6.79
26 AS	N - C * C - N - C * C	# 1.63
102 AS	N - C * C - N - C * C	# 0.92
147 AS	N - C - C - N - C * C	1.84
388 AS	N C C N C N	5.86
389 AS	N C C N C O	# 12.87
390 AS	N * C * C * N - C - O	# 1.34
391 AS	N - C * C - N - C - O	# 0.42
392 AS	N - C - C - N - C - O	# 5.48
389 AS	N C C N C S	# 12.87
390 AS	N * C * C * N - C - S	# 1.34
391 AS	N - C * C - N - C - S	# 0.42
392 AS	N - C - C - N - C - S	# 5.48
393 AS	N C C N N	3.65
394 AS	N C C N O	# 3.00
395 AS	N * C * C - N - O	# 0.48
396 AS	N - C * C - N - O	# 0.72
397 AS	N - C - C - N - O	# 0.82



# Atom Sequences

Screen Number		Fragment Definition					Frequency Percent
302	AS	N	C	C	N	P	# 0.44
394	AS	N	C	C	N	S	# 3.00
395	AS	N	* C	* C	- N	- S	# 0.48
396	AS	N	- C	* C	- N	- S	# 0.72
397	AS	N	- C	- C	- N	- S	# 0.82
302	AS	N	C	C	N	Se	# 0.44
302	AS	N	C	C	N	Si	# 0.44
302	AS	N	C	C	N	Te	# 0.44
2090	AS	N	C	C	O		# 35.39
398	AS	N	* C	* C	* O		# 8.97
399	AS	N	* C	* C	- O		# 5.41
400	AS	N	* C	- C	* O		# 0.73
401	AS	N	* C	- C	- O		# 6.21
402	AS	N	- C	* C	* O		# 1.91
403	AS	N	- C	* C	- O		# 6.11
404	AS	N	- C	- C	* O		# 2.34
405	AS	N	- C	- C	- O		# 16.92
310	AS	N	C	C	O	As	# 2.38
310	AS	N	C	C	O	B	# 2.38
266	AS	N	* C	* C	- O	- C	# 1.56
268	AS	N	* C	- C	- O	- C	# 1.79
267	AS	N	- C	* C	- O	- C	# 2.37
269	AS	N	- C	- C	- O	- C	# 6.99
26	AS	N	- C	* C	- O	- C * C	# 1.63
126	AS	N	- C	* C	- O	- C * C	# 2.20
406	AS	N	C	C	O	C N	# 4.07
407	AS	N	- C	- C	- O	- C - N	# 0.13
408	AS	N	C	C	O	C O	# 4.14
409	AS	N	- C	* C	- O	- C - O	# 0.36
410	AS	N	- C	- C	- O	- C - O	# 1.42
408	AS	N	C	C	O	C S	# 4.14
409	AS	N	- C	* C	- O	- C - S	# 0.36
410	AS	N	- C	- C	- O	- C - S	# 1.42
411	AS	N	C	C	O	N	# 0.75
412	AS	N	C	C	O	O	# 1.53
413	AS	N	* C	* C	- O	- O	# 0.27
414	AS	N	- C	* C	- O	- O	# 0.52
310	AS	N	C	C	O	P	# 2.38
412	AS	N	C	C	O	S	# 1.53
413	AS	N	* C	* C	- O	- S	# 0.27
414	AS	N	- C	* C	- O	- S	# 0.52
310	AS	N	C	C	O	Se	# 2.38
310	AS	N	C	C	O	Si	# 2.38
310	AS	N	C	C	O	Te	# 2.38
331	AS	N	C	C	P		# 1.39
2090	AS	N	C	C	S		# 35.39
398	AS	N	* C	* C	* S		# 8.97
399	AS	N	* C	* C	- S		# 5.41
400	AS	N	* C	- C	* S		# 0.73
401	AS	N	* C	- C	- S		# 6.21
402	AS	N	- C	* C	* S		# 1.91
403	AS	N	- C	* C	- S		# 6.11
404	AS	N	- C	- C	* S		# 2.34
405	AS	N	- C	- C	- S		# 16.92
310	AS	N	C	C	S	As	# 2.38

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
310 AS	N C C S B	# 2.38
266 AS	N * C * C - S - C	# 1.56
268 AS	N * C - C - S - C	# 1.79
267 AS	N - C * C - S - C	# 2.37
269 AS	N - C - C - S - C	# 6.99
26 AS	N - C * C - S - C * C	# 1.63
126 AS	N - C * C - S - C * C	# 2.20
406 AS	N C C S C N	# 4.07
407 AS	N - C - C - S - C - N	# 0.13
408 AS	N C C S C O	# 4.14
409 AS	N - C * C - S - C - O	# 0.36
410 AS	N - C - C - S - C - O	# 1.42
408 AS	N C C S C S	# 4.14
409 AS	N - C * C - S - C - S	# 0.36
410 AS	N - C - C - S - C - S	# 1.42
411 AS	N C C S N	# 0.75
412 AS	N C C S O	# 1.53
413 AS	N * C * C - S - O	# 0.27
414 AS	N - C * C - S - O	# 0.52
310 AS	N C C S P	# 2.38
412 AS	N C C S S	# 1.53
413 AS	N * C * C - S - S	# 0.27
414 AS	N - C * C - S - S	# 0.52
310 AS	N C C S Se	# 2.38
310 AS	N C C S Si	# 2.38
310 AS	N C C S Te	# 2.38
331 AS	N C C Se	# 1.39
331 AS	N C C Si	# 1.39
331 AS	N C C Te	# 1.39
2086 AS	N C N C	# 30.95
233 AS	N * C * N - C	7.12
231 AS	N * C - N * C	1.29
234 AS	N * C - N - C	4.77
232 AS	N - C - N * C	0.93
235 AS	N - C - N - C	5.46
333 AS	N C N C Br	# 0.53
150 AS	N * C * N * C * C	12.29
153 AS	N * C * N * C - C	5.44
151 AS	N * C - N - C * C	1.72
154 AS	N - C * N * C - C	2.20
152 AS	N - C - N - C * C	2.36
155 AS	N - C - N - C - C	3.79
318 AS	N C N C C Br	# 1.48
103 AS	N * C * N * C * C * C	9.30
105 AS	N - C - N - C * C - C	0.37
104 AS	N - C - N - C - C * C	0.88
318 AS	N C N C C Cl	# 1.48
318 AS	N C N C C F	# 1.48
318 AS	N C N C C I	# 1.48
388 AS	N C N C C N	5.86
415 AS	N C N C C O	# 7.06
416 AS	N * C * N * C * C - O	# 1.32
417 AS	N * C * N * C - C - O	# 0.56
418 AS	N - C - N - C * C - O	# 0.25
419 AS	N - C - N - C - C - O	# 0.42

# Atom Sequences

Screen Number		Fragment Definition						Frequency Percent	
415	AS	N	C	N	C	C	S	#	7.06
416	AS	N	* C	* N	* C	* C	- S	#	1.32
417	AS	N	* C	* N	* C	- C	- S	#	0.56
418	AS	N	- C	- N	- C	* C	- S	#	0.25
419	AS	N	- C	- N	- C	- C	- S	#	0.42
333	AS	N	C	N	C	Cl		#	0.53
333	AS	N	C	N	C	F		#	0.53
333	AS	N	C	N	C	I		#	0.53
420	AS	N	C	N	C	N			6.57
421	AS	N	* C	* N	* C	- N			3.26
422	AS	N	* C	- N	- C	* N			0.08
421	AS	N	- C	* N	* C	* N			3.26
423	AS	N	- C	* N	* C	- N			0.98
424	AS	N	- C	- N	- C	- N			0.19
238	AS	N	* C	* N	* C	* N	* C		2.92
425	AS	N	C	N	C	O		#	9.70
426	AS	N	* C	* N	* C	- O		#	5.47
427	AS	N	* C	* N	- C	- O		#	0.50
428	AS	N	* C	- N	- C	- O		#	1.59
429	AS	N	- C	* N	* C	- O		#	1.44
430	AS	N	- C	- N	- C	- O		#	0.75
425	AS	N	C	N	C	S		#	9.70
426	AS	N	* C	* N	* C	- S		#	5.47
427	AS	N	* C	* N	- C	- S		#	0.50
428	AS	N	* C	- N	- C	- S		#	1.59
429	AS	N	- C	* N	* C	- S		#	1.44
430	AS	N	- C	- N	- C	- S		#	0.75
431	AS	N	C	N	N				3.67
2092	AS	N	C	N	N			#	13.08
432	AS	N	* C	* N	* N				3.24
433	AS	N	* C	- N	- N				0.55
434	AS	N	- C	* N	* N				1.27
435	AS	N	- C	- N	- N				0.73
436	AS	N	C	N	N	C	N		0.65
437	AS	N	C	N	O			#	1.66
438	AS	N	* C	* N	* O			#	0.48
439	AS	N	* C	- N	- O			#	0.35
440	AS	N	- C	- N	- O			#	0.51
437	AS	N	C	N	S			#	1.66
438	AS	N	* C	* N	* S			#	0.48
439	AS	N	* C	- N	- S			#	0.35
440	AS	N	- C	- N	- S			#	0.51
2086	AS	N	C	O	C			#	30.95
2093	AS	N	C	O	C			#	24.67
274	AS	N	* C	- O	- C			#	3.68
275	AS	N	- C	- O	- C			#	4.54
190	AS	N	* C	* O	* C	- C		#	2.79
188	AS	N	* C	- O	- C	* C		#	0.61
191	AS	N	- C	* O	* C	- C		#	2.04
189	AS	N	- C	- O	- C	* C		#	0.58
327	AS	N	C	O	C	C	Br	#	0.27
327	AS	N	C	O	C	C	Cl	#	0.27
327	AS	N	C	O	C	C	F	#	0.27
327	AS	N	C	O	C	C	I	#	0.27
406	AS	N	C	O	C	C	N	#	4.07

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
407 AS	N - C - O - C - C - N	# 0.13
441 AS	N C O C C O	# 4.35
441 AS	N C O C C S	# 4.35
442 AS	N C O C N	# 1.12
443 AS	N C O C O	# 0.95
443 AS	N C O C S	# 0.95
2092 AS	N C O N	# 13.08
444 AS	N * C * O * N	# 0.42
445 AS	N - C - O - N	# 0.06
446 AS	N C O O	# 0.48
446 AS	N C O S	# 0.48
2086 AS	N C S C	# 30.95
2093 AS	N C S C	# 24.67
274 AS	N * C - S - C	# 3.68
275 AS	N - C - S - C	# 4.54
190 AS	N * C * S * C - C	# 2.79
188 AS	N * C - S - C * C	# 0.61
191 AS	N - C * S * C - C	# 2.04
189 AS	N - C - S - C * C	# 0.58
327 AS	N C S C C Br	# 0.27
327 AS	N C S C C Cl	# 0.27
327 AS	N C S C C F	# 0.27
327 AS	N C S C C I	# 0.27
406 AS	N C S C C N	# 4.07
407 AS	N - C - S - C - C - N	# 0.13
441 AS	N C S C C O	# 4.35
441 AS	N C S C C S	# 4.35
442 AS	N C S C N	# 1.12
443 AS	N C S C O	# 0.95
443 AS	N C S C S	# 0.95
2092 AS	N C S N	# 13.08
444 AS	N * C * S * N	# 0.42
445 AS	N - C - S - N	# 0.06
446 AS	N C S O	# 0.48
446 AS	N C S S	# 0.48
2085 AS	N N C C	# 26.07
168 AS	N * N * C - C	4.81
166 AS	N * N - C * C	1.79
167 AS	N - N - C * C	2.67
169 AS	N - N - C - C	3.78
321 AS	N N C C Br	# 0.82
110 AS	N * N * C * C * C	4.61
112 AS	N - N - C * C - C	0.55
111 AS	N - N - C - C * C	2.65
113 AS	N - N - C - C - C	1.14
300 AS	N N C C C Br	# 0.84
67 AS	N * N * C * C * C	2.26
69 AS	N - N - C * C * C - C	0.49
68 AS	N - N - C - C - C * C	0.23
300 AS	N N C C C Cl	# 0.84
300 AS	N N C C C F	# 0.84
300 AS	N N C C C I	# 0.84
364 AS	N N C C C N	3.16
447 AS	N N C C C O	# 3.35
448 AS	N - N - C * C * C - O	# 0.33

# Atom Sequences

Screen Number		Fragment Definition						Frequency Percent	
447	AS	N	N	C	C	C	S	#	3.35
448	AS	N	-	N	-	C	* C * C - S	#	0.33
321	AS	N	N	C	C	C1		#	0.82
321	AS	N	N	C	C	F		#	0.82
321	AS	N	N	C	C	I		#	0.82
393	AS	N	N	C	C	N			3.65
221	AS	N	N	C	C	N	C		2.85
449	AS	N	N	C	C	N	N		0.42
450	AS	N	N	C	C	N	O	#	0.51
450	AS	N	N	C	C	N	S	#	0.51
451	AS	N	N	C	C	O		#	4.22
452	AS	N	*	N	*	C	* C - O	#	0.46
453	AS	N	*	N	*	C	- C - O	#	0.74
454	AS	N	-	N	-	C	* C - O	#	0.91
455	AS	N	-	N	-	C	- C - O	#	0.80
270	AS	N	N	C	C	O	C	#	2.19
456	AS	N	N	C	C	O	O	#	0.36
456	AS	N	N	C	C	O	S	#	0.36
451	AS	N	N	C	C	S		#	4.22
452	AS	N	*	N	*	C	* C - S	#	0.46
453	AS	N	*	N	*	C	- C - S	#	0.74
454	AS	N	-	N	-	C	* C - S	#	0.91
455	AS	N	-	N	-	C	- C - S	#	0.80
270	AS	N	N	C	C	S	C	#	2.19
456	AS	N	N	C	C	S	O	#	0.36
456	AS	N	N	C	C	S	S	#	0.36
431	AS	N	N	C	N				3.67
2092	AS	N	N	C	N			#	13.08
432	AS	N	*	N	*	C	* N		3.24
434	AS	N	*	N	*	C	- N		1.27
433	AS	N	-	N	-	C	* N		0.55
435	AS	N	-	N	-	C	- N		0.73
457	AS	N	N	C	N	N			1.08
458	AS	N	N	C	N	O		#	0.17
458	AS	N	N	C	N	S		#	0.17
459	AS	N	N	C	O			#	6.66
460	AS	N	*	N	*	C	* O	#	1.19
461	AS	N	*	N	*	C	- O	#	2.61
462	AS	N	*	N	-	C	- O	#	0.41
463	AS	N	-	N	-	C	- O	#	2.57
276	AS	N	*	N	*	C	- O - C	#	1.23
459	AS	N	N	C	S			#	6.66
460	AS	N	*	N	*	C	* S	#	1.19
461	AS	N	*	N	*	C	- S	#	2.61
462	AS	N	*	N	-	C	- S	#	0.41
463	AS	N	-	N	-	C	- S	#	2.57
276	AS	N	*	N	*	C	- S - C	#	1.23
250	AS	N	N	N	C				1.47
464	AS	N	N	N	N				0.60
465	AS	N	N	O	O			#	0.17
465	AS	N	N	O	S			#	0.17
465	AS	N	N	S	O			#	0.17
465	AS	N	N	S	S			#	0.17
2085	AS	N	O	C	C			#	26.07
198	AS	N	*	O	*	C	- C	#	0.77

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
197	AS	N - O - C * C	# 3.51
199	AS	N - O - C - C	# 1.12
329	AS	N O C C Br	# 0.30
130	AS	N - O - C * C - C	# 0.32
129	AS	N - O - C - C * C	# 0.35
308	AS	N O C C C Br	# 0.26
85	AS	N - O - C * C * C - C	# 0.42
308	AS	N O C C C Cl	# 0.26
308	AS	N O C C C F	# 0.26
308	AS	N O C C C I	# 0.26
379	AS	N O C C C N	# 0.80
466	AS	N O C C C O	# 0.71
466	AS	N O C C C S	# 0.71
329	AS	N O C C Cl	# 0.30
329	AS	N O C C F	# 0.30
329	AS	N O C C I	# 0.30
411	AS	N O C C N	# 0.75
467	AS	N O C C O	# 0.63
467	AS	N O C C S	# 0.63
2092	AS	N O C N	# 13.08
444	AS	N * O * C * N	# 0.42
445	AS	N - O - C - N	# 0.06
468	AS	N O C O	# 0.58
468	AS	N O C S	# 0.58
281	AS	N O O C	# 0.09
281	AS	N O S C	# 0.09
2085	AS	N S C C	# 26.07
198	AS	N * S * C - C	# 0.77
197	AS	N - S - C * C	# 3.51
199	AS	N - S - C - C	# 1.12
329	AS	N S C C Br	# 0.30
130	AS	N - S - C * C - C	# 0.32
129	AS	N - S - C - C * C	# 0.35
308	AS	N S C C C Br	# 0.26
85	AS	N - S - C * C * C - C	# 0.42
308	AS	N S C C C Cl	# 0.26
308	AS	N S C C C F	# 0.26
308	AS	N S C C C I	# 0.26
379	AS	N S C C C N	# 0.80
466	AS	N S C C C O	# 0.71
466	AS	N S C C C S	# 0.71
329	AS	N S C C Cl	# 0.30
329	AS	N S C C F	# 0.30
329	AS	N S C C I	# 0.30
411	AS	N S C C N	# 0.75
467	AS	N S C C O	# 0.63
467	AS	N S C C S	# 0.63
2092	AS	N S C N	# 13.08
444	AS	N * S * C * N	# 0.42
445	AS	N - S - C - N	# 0.06
468	AS	N S C O	# 0.58
468	AS	N S C S	# 0.58
281	AS	N S O C	# 0.09
281	AS	N S S C	# 0.09
331	AS	O C C As	# 1.39

# Atom Sequences

Screen Number		Fragment Definition					Frequency Percent
331	AS	O	C	C	B		# 1.39
323	AS	O	*	C	*	C - Br	# 0.61
325	AS	O	*	C	- C - Br		# 0.45
324	AS	O	- C	*	C - Br		# 2.95
326	AS	O	- C	- C	- Br		# 2.53
2081	AS	O	C	C	C		# 76.51
118	AS	O	*	C	*	C - C	# 9.42
116	AS	O	*	C	- C	* C	# 4.30
120	AS	O	*	C	- C	- C	# 5.21
119	AS	O	- C	*	C - C		# 18.18
117	AS	O	- C	- C	* C		# 33.04
121	AS	O	- C	- C	- C		# 32.90
311	AS	O	C	C	C	As	# 1.14
311	AS	O	C	C	C	B	# 1.14
303	AS	O	C	C	C	Br	# 5.10
304	AS	O	*	C	*	C * C - Br	# 0.64
305	AS	O	- C	*	C * C - Br		# 1.72
306	AS	O	- C	- C	* C - Br		# 1.61
307	AS	O	- C	- C	- C - Br		# 0.86
72	AS	O	*	C	*	C * C * C	# 19.48
76	AS	O	*	C	*	C * C - C	# 7.10
73	AS	O	*	C	*	C - C * C	# 2.01
74	AS	O	*	C	- C	- C * C	# 1.34
77	AS	O	- C	*	C * C - C		# 14.59
6	AS	O	- C	*	C - C * C		# 7.08
38	AS	O	- C	*	C - C * C		# 5.99
79	AS	O	- C	*	C - C - C		# 6.96
78	AS	O	- C	- C	* C - C		# 6.22
75	AS	O	- C	- C	- C * C		# 6.25
80	AS	O	- C	- C	- C - C		# 21.57
291	AS	O	C	C	C	C As	# 0.79
291	AS	O	C	C	C	C B	# 0.79
288	AS	O	C	C	C	C Br	# 6.39
289	AS	O	- C	*	C * C * C - Br		# 3.00
290	AS	O	- C	- C	* C * C - Br		# 1.30
35	AS	O	*	C	*	C * C * C * C	# 14.10
40	AS	O	*	C	*	C * C * C - C	# 9.53
36	AS	O	*	C	*	C * C - C * C	# 1.56
41	AS	O	- C	*	C * C * C - C		# 19.86
37	AS	O	- C	*	C * C - C * C		# 2.60
44	AS	O	- C	*	C * C - C - C		# 4.16
14	AS	O	- C	*	C - C - C * C		# 3.46
38	AS	O	- C	*	C - C - C * C		# 5.99
42	AS	O	- C	- C	* C * C - C		# 4.15
45	AS	O	- C	- C	* C - C - C		# 1.26
43	AS	O	- C	- C	- C * C - C		# 1.01
39	AS	O	- C	- C	- C - C * C		# 7.78
46	AS	O	- C	- C	- C - C - C		# 12.64
288	AS	O	C	C	C	C Cl	# 6.39
289	AS	O	- C	*	C * C * C - Cl		# 3.00
290	AS	O	- C	- C	* C * C - Cl		# 1.30
288	AS	O	C	C	C	C F	# 6.39
289	AS	O	- C	*	C * C * C - F		# 3.00
290	AS	O	- C	- C	* C * C - F		# 1.30
288	AS	O	C	C	C	C I	# 6.39

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
289 AS	O - C * C * C * C - I	# 3.00
290 AS	O - C - C * C * C - I	# 1.30
345 AS	O - C - C - C - N	# 25.91
347 AS	O * C * C * C * C - N	# 2.82
346 AS	O - C * C * C * C * N	# 5.92
348 AS	O - C * C * C * C - N	# 5.24
350 AS	O - C * C * C - C - N	# 1.95
352 AS	O - C * C - C - C - N	# 0.41
349 AS	O - C - C * C * C - N	# 1.64
351 AS	O - C - C * C - C - N	# 0.50
353 AS	O - C - C - C - C - N	# 4.12
469 AS	O * C * C * C * C - O	# 5.73
469 AS	O - C * C * C * C * O	# 5.73
470 AS	O - C * C * C * C - O	# 7.27
471 AS	O - C * C * C - C - O	# 4.77
472 AS	O - C * C - C * C - O	# 0.22
473 AS	O - C * C - C - C - O	# 0.86
471 AS	O - C - C * C * C - O	# 4.77
474 AS	O - C - C * C - C - O	# 1.17
473 AS	O - C - C - C * C - O	# 0.86
475 AS	O - C - C - C - C - O	# 4.56
291 AS	O - C - C - C - C - P	# 0.79
469 AS	O * C * C * C * C - S	# 5.73
469 AS	O - C * C * C * C * S	# 5.73
470 AS	O - C * C * C * C - S	# 7.27
471 AS	O - C * C * C - C - S	# 4.77
472 AS	O - C * C - C * C - S	# 0.22
473 AS	O - C * C - C - C - S	# 0.86
471 AS	O - C - C * C * C - S	# 4.77
474 AS	O - C - C * C - C - S	# 1.17
473 AS	O - C - C - C * C - S	# 0.86
475 AS	O - C - C - C - C - S	# 4.56
291 AS	O C C C C Se	# 0.79
291 AS	O C C C C Si	# 0.79
291 AS	O C C C C Te	# 0.79
303 AS	O C C C Cl	# 5.10
304 AS	O * C * C * C - Cl	# 0.64
305 AS	O - C * C * C - Cl	# 1.72
306 AS	O - C - C * C - Cl	# 1.61
307 AS	O - C - C - C - Cl	# 0.86
303 AS	O C C C F	# 5.10
304 AS	O * C * C * C - F	# 0.64
305 AS	O - C * C * C - F	# 1.72
306 AS	O - C - C * C - F	# 1.61
307 AS	O - C - C - C - F	# 0.86
303 AS	O C C C I	# 5.10
304 AS	O * C * C * C - I	# 0.64
305 AS	O - C * C * C - I	# 1.72
306 AS	O - C - C * C - I	# 1.61
307 AS	O - C - C - C - I	# 0.86
368 AS	O * C * C * C * N	# 4.16
374 AS	O * C * C * C - N	# 1.65
370 AS	O * C * C - C * N	# 2.56
370 AS	O * C * C - C - N	# 2.56
370 AS	O * C - C * C * N	# 2.56



# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
370 AS	O * C - C * C - N	# 2.56
370 AS	O * C - C - C * N	# 2.56
370 AS	O * C - C - C - N	# 2.56
369 AS	O - C * C * C * N	# 9.05
375 AS	O - C * C * C - N	# 4.45
372 AS	O - C * C - C * N	# 0.73
377 AS	O - C * C - C - N	# 2.93
371 AS	O - C - C * C * N	# 4.73
376 AS	O - C - C * C - N	# 1.92
373 AS	O - C - C - C * N	# 1.07
378 AS	O - C - C - C - N	# 7.21
302 AS	O C C C N As	# 0.44
302 AS	O C C C N B	# 0.44
208 AS	O - C * C * C * N - C	# 3.76
209 AS	O - C * C * C - N - C	# 2.16
211 AS	O - C * C - C - N - C	# 1.57
210 AS	O - C - C * C - N - C	# 1.11
447 AS	O C C C N N	# 3.35
448 AS	O - C * C * C - N - N	# 0.33
476 AS	O C C C N O	# 2.08
477 AS	O - C * C * C - N - O	# 0.52
302 AS	O C C C N P	# 0.44
476 AS	O C C C N S	# 2.08
477 AS	O - C * C * C - N - S	# 0.52
302 AS	O C C C N Se	# 0.44
302 AS	O C C C N Si	# 0.44
302 AS	O C C C N Te	# 0.44
2096 AS	O C C C O	# 20.23
478 AS	O * C * C * C * O	# 2.29
479 AS	O * C * C * C - O	# 7.38
480 AS	O * C * C - C - O	# 3.12
481 AS	O * C - C - C * O	# 0.19
479 AS	O - C * C * C * O	# 7.38
482 AS	O - C * C * C - O	# 6.67
483 AS	O - C * C - C - O	# 6.12
480 AS	O - C - C * C * O	# 3.12
483 AS	O - C - C * C - O	# 6.12
484 AS	O - C - C - C - O	# 6.65
310 AS	O C C C O As	# 2.38
310 AS	O C C C O B	# 2.38
261 AS	O - C * C * C - O - C	# 4.46
263 AS	O - C * C - C - O - C	# 2.05
262 AS	O - C - C * C - O - C	# 2.33
264 AS	O - C - C - C - O - C	# 3.09
466 AS	O C C C O N	# 0.71
485 AS	O C C C O O	# 1.62
310 AS	O C C C O P	# 2.38
485 AS	O C C C O S	# 1.62
310 AS	O C C C O Se	# 2.38
310 AS	O C C C O Si	# 2.38
310 AS	O C C C O Te	# 2.38
311 AS	O C C C P	# 1.14
478 AS	O * C * C * C * S	# 2.29
479 AS	O * C * C * C - S	# 7.38
480 AS	O * C * C - C - S	# 3.12

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
481 AS	O * C - C - C * S	# 0.19
479 AS	O - C * C * C * S	# 7.38
482 AS	O - C * C * C - S	# 6.67
483 AS	O - C * C - C - S	# 6.12
480 AS	O - C - C * C * S	# 3.12
483 AS	O - C - C * C - S	# 6.12
484 AS	O - C - C - C - S	# 6.65
310 AS	O C C C S As	# 2.38
310 AS	O C C C S B	# 2.38
261 AS	O - C * C * C - S - C	# 4.46
263 AS	O - C * C - C - S - C	# 2.05
262 AS	O - C - C * C - S - C	# 2.33
264 AS	O - C - C - C - S - C	# 3.09
466 AS	O C C C S N	# 0.71
485 AS	O C C C S O	# 1.62
310 AS	O C C C S P	# 2.38
485 AS	O C C C S S	# 1.62
310 AS	O C C C S Se	# 2.38
310 AS	O C C C S Si	# 2.38
310 AS	O C C C S Te	# 2.38
311 AS	O C C C Se	# 1.14
311 AS	O C C C Si	# 1.14
311 AS	O C C C Te	# 1.14
323 AS	O * C * C - Cl	# 0.61
325 AS	O * C - C - Cl	# 0.45
324 AS	O - C * C - Cl	# 2.95
326 AS	O - C - C - Cl	# 2.53
323 AS	O * C * C - F	# 0.61
325 AS	O * C - C - F	# 0.45
324 AS	O - C * C - F	# 2.95
326 AS	O - C - C - F	# 2.53
323 AS	O * C * C - I	# 0.61
325 AS	O * C - C - I	# 0.45
324 AS	O - C * C - I	# 2.95
326 AS	O - C - C - I	# 2.53
2090 AS	O C C N	# 35.39
398 AS	O * C * C * N	# 8.97
402 AS	O * C * C - N	# 1.91
400 AS	O * C - C * N	# 0.73
404 AS	O * C - C - N	# 2.34
399 AS	O - C * C * N	# 5.41
403 AS	O - C * C - N	# 6.11
401 AS	O - C - C * N	# 6.21
405 AS	O - C - C - N	# 16.92
302 AS	O C C N As	# 0.44
302 AS	O C C N B	# 0.44
225 AS	O * C * C * N - C	# 3.33
226 AS	O - C * C * N - C	# 1.88
223 AS	O - C * C - N * C	# 0.96
228 AS	O - C * C - N - C	# 3.06
227 AS	O - C - C * N - C	# 2.68
224 AS	O - C - C - N * C	# 2.89
229 AS	O - C - C - N - C	# 12.06
148 AS	O * C * C * N * C * C	# 3.85
38 AS	O - C * C - N - C * C	# 5.99

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
102 AS	O - C * C - N - C * C	# 0.92
149 AS	O - C - C - N - C * C	# 2.49
415 AS	O C C N C N	# 7.06
416 AS	O - C * C * N * C * N	# 1.32
418 AS	O - C * C - N - C - N	# 0.25
417 AS	O - C - C * N * C * N	# 0.56
419 AS	O - C - C - N - C - N	# 0.42
486 AS	O C C N C O	# 14.96
487 AS	O - C * C - N - C - O	# 2.07
488 AS	O - C - C - N - C - O	# 7.07
486 AS	O C C N C S	# 14.96
487 AS	O - C * C - N - C - S	# 2.07
488 AS	O - C - C - N - C - S	# 7.07
451 AS	O C C N N	# 4.22
452 AS	O - C * C * N * N	# 0.46
454 AS	O - C * C - N - N	# 0.91
453 AS	O - C - C * N * N	# 0.74
455 AS	O - C - C - N - N	# 0.80
489 AS	O C C N O	# 2.88
490 AS	O - C * C - N - O	# 0.94
491 AS	O - C - C - N - O	# 1.05
302 AS	O C C N P	# 0.44
489 AS	O C C N S	# 2.88
490 AS	O - C * C - N - S	# 0.94
491 AS	O - C - C - N - S	# 1.05
302 AS	O C C N Se	# 0.44
302 AS	O C C N Si	# 0.44
302 AS	O C C N Te	# 0.44
2091 AS	O C C O	# 24.29
492 AS	O * C * C * O	# 4.00
493 AS	O * C * C - O	# 6.17
494 AS	O * C - C * O	# 0.42
495 AS	O * C - C - O	# 5.40
493 AS	O - C * C * O	# 6.17
496 AS	O - C * C - O	# 7.98
495 AS	O - C - C * O	# 5.40
497 AS	O - C - C - O	# 9.90
310 AS	O C C O As	# 2.38
310 AS	O C C O B	# 2.38
272 AS	O - C * C - O - C	# 6.16
273 AS	O - C - C - O - C	# 8.01
38 AS	O - C * C - O - C * C	# 5.99
126 AS	O - C * C - O - C * C	# 2.20
187 AS	O - C - C - O - C * C	# 3.29
441 AS	O C C O C N	# 4.35
498 AS	O C C O C O	# 7.30
498 AS	O C C O C S	# 7.30
467 AS	O C C O N	# 0.63
499 AS	O C C O O	# 1.31
310 AS	O C C O P	# 2.38
499 AS	O C C O S	# 1.31
310 AS	O C C O Se	# 2.38
310 AS	O C C O Si	# 2.38
310 AS	O C C O Te	# 2.38
331 AS	O C C P	# 1.39

# Atom Sequences

Screen Number		Fragment Definition						Frequency Percent
2091	AS	O	C	C	S			# 24.29
492	AS	O	*	C	*	C	*	# 4.00
493	AS	O	*	C	*	C	-	# 6.17
494	AS	O	*	C	-	C	*	# 0.42
495	AS	O	*	C	-	C	-	# 5.40
493	AS	O	-	C	*	C	*	# 6.17
496	AS	O	-	C	*	C	-	# 7.98
495	AS	O	-	C	-	C	*	# 5.40
497	AS	O	-	C	-	C	-	# 9.90
310	AS	O	C	C	S	As		# 2.38
310	AS	O	C	C	S	B		# 2.38
272	AS	O	-	C	*	C	-	# 6.16
273	AS	O	-	C	-	C	-	# 8.01
38	AS	O	-	C	*	C	-	# 5.99
126	AS	O	-	C	*	C	-	# 2.20
187	AS	O	-	C	-	C	-	# 3.29
441	AS	O	C	C	S	C	N	# 4.35
498	AS	O	C	C	S	C	O	# 7.30
498	AS	O	C	C	S	C	S	# 7.30
467	AS	O	C	C	S	N		# 0.63
499	AS	O	C	C	S	O		# 1.31
310	AS	O	C	C	S	P		# 2.38
499	AS	O	C	C	S	S		# 1.31
310	AS	O	C	C	S	Se		# 2.38
310	AS	O	C	C	S	Si		# 2.38
310	AS	O	C	C	S	Te		# 2.38
331	AS	O	C	C	Se			# 1.39
331	AS	O	C	C	Si			# 1.39
331	AS	O	C	C	Te			# 1.39
2087	AS	O	C	N	C			# 39.80
241	AS	O	*	C	*	N	-	# 1.96
239	AS	O	*	C	-	N	*	# 1.30
242	AS	O	-	C	*	N	-	# 8.74
240	AS	O	-	C	-	N	*	# 5.80
243	AS	O	-	C	-	N	-	# 23.15
334	AS	O	C	N	C	Br		# 0.18
157	AS	O	*	C	*	N	*	# 6.29
161	AS	O	*	C	*	N	*	# 3.21
159	AS	O	*	C	-	N	-	# 0.71
162	AS	O	-	C	*	N	*	# 4.84
158	AS	O	-	C	*	N	-	# 3.59
163	AS	O	-	C	-	N	*	# 2.74
160	AS	O	-	C	-	N	-	# 11.07
164	AS	O	-	C	-	N	-	# 13.37
319	AS	O	C	N	C	C	Br	# 1.84
320	AS	O	-	C	-	N	-	# 0.72
106	AS	O	*	C	*	N	*	# 2.79
107	AS	O	-	C	*	N	-	# 1.02
109	AS	O	-	C	-	N	-	# 2.05
108	AS	O	-	C	-	N	-	# 3.00
319	AS	O	C	N	C	C	Cl	# 1.84
320	AS	O	-	C	-	N	-	# 0.72
319	AS	O	C	N	C	C	F	# 1.84
320	AS	O	-	C	-	N	-	# 0.72
319	AS	O	C	N	C	C	I	# 1.84

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
320	AS	O - C - N - C * C - I	# 0.72
389	AS	O C N C C N	# 12.87
390	AS	O - C - N * C * C * N	# 1.34
391	AS	O - C - N - C * C - N	# 0.42
392	AS	O - C - N - C - C - N	# 5.48
486	AS	O C N C C O	# 14.96
487	AS	O - C - N - C * C - O	# 2.07
488	AS	O - C - N - C - C - O	# 7.07
486	AS	O C N C C S	# 14.96
487	AS	O - C - N - C * C - S	# 2.07
488	AS	O - C - N - C - C - S	# 7.07
334	AS	O C N C Cl	# 0.18
334	AS	O C N C F	# 0.18
334	AS	O C N C I	# 0.18
425	AS	O C N C N	# 9.70
426	AS	O - C * N * C * N	# 5.47
429	AS	O - C * N * C - N	# 1.44
427	AS	O - C - N * C * N	# 0.50
428	AS	O - C - N - C * N	# 1.59
430	AS	O - C - N - C - N	# 0.75
500	AS	O C N C O	# 8.18
501	AS	O - C * N * C - O	# 4.24
502	AS	O - C * N - C - O	# 0.50
502	AS	O - C - N * C - O	# 0.50
503	AS	O - C - N - C - O	# 0.77
500	AS	O C N C S	# 8.18
501	AS	O - C * N * C - S	# 4.24
502	AS	O - C * N - C - S	# 0.50
502	AS	O - C - N * C - S	# 0.50
503	AS	O - C - N - C - S	# 0.77
459	AS	O C N N	# 6.66
460	AS	O * C * N * N	# 1.19
461	AS	O - C * N * N	# 2.61
462	AS	O - C - N * N	# 0.41
463	AS	O - C - N - N	# 2.57
249	AS	O - C * N * N - C	# 0.35
504	AS	O C N N C O	# 1.09
504	AS	O C N N C S	# 1.09
505	AS	O C N O	# 1.66
2092	AS	O C N O	# 13.08
506	AS	O * C * N * O	# 0.08
507	AS	O * C - N - O	# 0.24
508	AS	O - C * N * O	# 0.24
509	AS	O - C - N - O	# 0.83
505	AS	O C N S	# 1.66
2092	AS	O C N S	# 13.08
506	AS	O * C * N * S	# 0.08
507	AS	O * C - N - S	# 0.24
508	AS	O - C * N * S	# 0.24
509	AS	O - C - N - S	# 0.83
2088	AS	O C O C	# 27.26
2094	AS	O C O C	# 27.26
277	AS	O * C - O - C	# 2.86
192	AS	O * C - O - C * C	# 1.20
194	AS	O - C * O * C - C	# 3.38

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
193 AS	O - C - O - C * C	# 4.71
195 AS	O - C - O - C - C	# 13.48
328 AS	O C O C C Br	# 0.64
128 AS	O - C - O - C - C * C	# 3.28
328 AS	O C O C C Cl	# 0.64
328 AS	O C O C C F	# 0.64
328 AS	O C O C C I	# 0.64
408 AS	O C O C C N	# 4.14
409 AS	O - C - O - C * C - N	# 0.36
410 AS	O - C - O - C - C - N	# 1.42
498 AS	O C O C C O	# 7.30
498 AS	O C O C C S	# 7.30
443 AS	O C O C N	# 0.95
510 AS	O C O C O	# 1.46
510 AS	O C O C S	# 1.46
468 AS	O C O N	# 0.58
511 AS	O C O O	# 0.48
511 AS	O C O S	# 0.48
2088 AS	O C S C	# 27.26
2094 AS	O C S C	# 27.26
277 AS	O * C - S - C	# 2.86
192 AS	O * C - S - C * C	# 1.20
194 AS	O - C * S * C - C	# 3.38
193 AS	O - C - S - C * C	# 4.71
195 AS	O - C - S - C - C	# 13.48
328 AS	O C S C C Br	# 0.64
128 AS	O - C - S - C - C * C	# 3.28
328 AS	O C S C C Cl	# 0.64
328 AS	O C S C C F	# 0.64
328 AS	O C S C C I	# 0.64
408 AS	O C S C C N	# 4.14
409 AS	O - C - S - C * C - N	# 0.36
410 AS	O - C - S - C - C - N	# 1.42
498 AS	O C S C C O	# 7.30
498 AS	O C S C C S	# 7.30
443 AS	O C S C N	# 0.95
510 AS	O C S C O	# 1.46
510 AS	O C S C S	# 1.46
468 AS	O C S N	# 0.58
511 AS	O C S O	# 0.48
511 AS	O C S S	# 0.48
335 AS	O N C Br	# 0.09
2085 AS	O N C C	# 26.07
173 AS	O * N * C * C	# 1.32
175 AS	O - N * C - C	# 0.56
174 AS	O - N - C * C	# 6.36
176 AS	O - N - C - C	# 3.06
322 AS	O N C C Br	# 0.39
115 AS	O - N - C * C - C	# 0.94
114 AS	O - N - C - C * C	# 1.22
301 AS	O N C C C Br	# 0.55
71 AS	O - N - C * C * C - C	# 1.36
70 AS	O - N - C - C - C * C	# 0.32
301 AS	O N C C C Cl	# 0.55
301 AS	O N C C C F	# 0.55

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
301 AS	O N C C C I	# 0.55
365 AS	O N C C C N	# 2.43
366 AS	O - N - C * C * C * N	# 0.35
367 AS	O - N - C * C * C - N	# 1.02
476 AS	O N C C C O	# 2.08
477 AS	O - N - C * C * C - O	# 0.52
476 AS	O N C C C S	# 2.08
477 AS	O - N - C * C * C - S	# 0.52
322 AS	O N C C Cl	# 0.39
322 AS	O N C C F	# 0.39
322 AS	O N C C I	# 0.39
394 AS	O N C C N	# 3.00
395 AS	O - N - C * C * N	# 0.48
396 AS	O - N - C * C - N	# 0.72
397 AS	O - N - C - C - N	# 0.82
222 AS	O - N - C * C - N - C	# 0.32
450 AS	O N C C N N	# 0.51
512 AS	O N C C N O	# 0.33
512 AS	O N C C N S	# 0.33
489 AS	O N C C O	# 2.88
490 AS	O - N - C * C - O	# 0.94
491 AS	O - N - C - C - O	# 1.05
271 AS	O - N - C * C - O - C	# 0.42
489 AS	O N C C S	# 2.88
490 AS	O - N - C * C - S	# 0.94
491 AS	O - N - C - C - S	# 1.05
271 AS	O - N - C * C - S - C	# 0.42
335 AS	O N C Cl	# 0.09
335 AS	O N C F	# 0.09
335 AS	O N C I	# 0.09
437 AS	O N C N	# 1.66
438 AS	O * N * C * N	# 0.48
439 AS	O - N - C * N	# 0.35
440 AS	O - N - C - N	# 0.51
458 AS	O N C N N	# 0.17
505 AS	O N C O	# 1.66
2092 AS	O N C O	# 13.08
506 AS	O * N * C * O	# 0.08
508 AS	O * N * C - O	# 0.24
507 AS	O - N - C * O	# 0.24
509 AS	O - N - C - O	# 0.83
505 AS	O N C S	# 1.66
506 AS	O * N * C * S	# 0.08
508 AS	O * N * C - S	# 0.24
507 AS	O - N - C * S	# 0.24
509 AS	O - N - C - S	# 0.83
279 AS	O N O C	# 0.17
279 AS	O N S C	# 0.17
336 AS	O O C Br	# 0.37
2085 AS	O O C C	# 26.07
201 AS	O - O - C * C	# 6.11
202 AS	O - O - C - C	# 2.21
330 AS	O O C C Br	# 0.43
132 AS	O - O - C * C - C	# 0.71
131 AS	O - O - C - C * C	# 0.48

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
133	AS	O - O - C - C - C	# 1.20
309	AS	O O C C C Br	# 0.37
86	AS	O - O - C * C * C - C	# 0.75
309	AS	O O C C C Cl	# 0.37
309	AS	O O C C C F	# 0.37
309	AS	O O C C C I	# 0.37
380	AS	O O C C C N	# 1.74
381	AS	O - O - C * C * C - N	# 0.76
485	AS	O O C C C O	# 1.62
485	AS	O O C C C S	# 1.62
330	AS	O O C C Cl	# 0.43
330	AS	O O C C F	# 0.43
330	AS	O O C C I	# 0.43
412	AS	O O C C N	# 1.53
413	AS	O - O - C * C * N	# 0.27
414	AS	O - O - C * C - N	# 0.52
456	AS	O O C C N N	# 0.36
499	AS	O O C C O	# 1.31
499	AS	O O C C S	# 1.31
336	AS	O O C Cl	# 0.37
336	AS	O O C F	# 0.37
336	AS	O O C I	# 0.37
446	AS	O O C N	# 0.48
511	AS	O O C O	# 0.48
511	AS	O O C S	# 0.48
2092	AS	O O N C	# 13.08
254	AS	O * O - N - C	# 0.00
253	AS	O - O - N * C	# 0.97
255	AS	O - O - N - C	# 2.96
179	AS	O - O - N - C * C	# 1.31
465	AS	O O N N	# 0.17
282	AS	O O O C	# 1.03
282	AS	O O S C	# 1.03
336	AS	O S C Br	# 0.37
2085	AS	O S C C	# 26.07
201	AS	O - S - C * C	# 6.11
202	AS	O - S - C - C	# 2.21
330	AS	O S C C Br	# 0.43
132	AS	O - S - C * C - C	# 0.71
131	AS	O - S - C - C * C	# 0.48
133	AS	O - S - C - C - C	# 1.20
309	AS	O S C C C Br	# 0.37
86	AS	O - S - C * C * C - C	# 0.75
309	AS	O S C C C Cl	# 0.37
309	AS	O S C C C F	# 0.37
309	AS	O S C C C I	# 0.37
380	AS	O S C C C N	# 1.74
381	AS	O - S - C * C * C - N	# 0.76
485	AS	O S C C C O	# 1.62
485	AS	O S C C C S	# 1.62
330	AS	O S C C Cl	# 0.43
330	AS	O S C C F	# 0.43
330	AS	O S C C I	# 0.43
412	AS	O S C C N	# 1.53
413	AS	O - S - C * C * N	# 0.27



# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
414 AS	O - S - C * C - N	# 0.52
456 AS	O S C C N N	# 0.36
499 AS	O S C C O	# 1.31
499 AS	O S C C S	# 1.31
336 AS	O S C Cl	# 0.37
336 AS	O S C F	# 0.37
336 AS	O S C I	# 0.37
446 AS	O S C N	# 0.48
511 AS	O S C O	# 0.48
511 AS	O S C S	# 0.48
2092 AS	O S N C	# 13.08
254 AS	O * S - N - C	# 0.00
253 AS	O - S - N * C	# 0.97
255 AS	O - S - N - C	# 2.96
179 AS	O - S - N - C * C	# 1.31
465 AS	O S N N	# 0.17
282 AS	O S O C	# 1.03
282 AS	O S S C	# 1.03
331 AS	P C C As	# 1.39
331 AS	P C C B	# 1.39
331 AS	P C C Br	# 1.39
134 AS	P C C C	# 4.57
311 AS	P C C C As	# 1.14
311 AS	P C C C B	# 1.14
311 AS	P C C C Br	# 1.14
291 AS	P C C C C As	# 0.79
291 AS	P C C C C B	# 0.79
291 AS	P C C C C Br	# 0.79
47 AS	P C C C C C	# 3.83
291 AS	P C C C C Cl	# 0.79
291 AS	P C C C C F	# 0.79
291 AS	P C C C C I	# 0.79
291 AS	P C C C C N	# 0.79
291 AS	P C C C C O	# 0.79
291 AS	P C C C C P	# 0.79
291 AS	P C C C C S	# 0.79
291 AS	P C C C C Se	# 0.79
291 AS	P C C C C Si	# 0.79
291 AS	P C C C C Te	# 0.79
311 AS	P C C C Cl	# 1.14
311 AS	P C C C F	# 1.14
311 AS	P C C C I	# 1.14
311 AS	P C C C N	# 1.14
302 AS	P C C C N As	# 0.44
302 AS	P C C C N B	# 0.44
302 AS	P C C C N P	# 0.44
302 AS	P C C C N Se	# 0.44
302 AS	P C C C N Si	# 0.44
302 AS	P C C C N Te	# 0.44
311 AS	P C C C O	# 1.14
310 AS	P C C C O As	# 2.38
310 AS	P C C C O B	# 2.38
310 AS	P C C C O P	# 2.38
310 AS	P C C C O Se	# 2.38
310 AS	P C C C O Si	# 2.38

# Atom Sequences

Screen Number	Fragment Definition							Frequency Percent
310	AS	P	C	C	C	O	Te	# 2.38
311	AS	P	C	C	C	P		# 1.14
311	AS	P	C	C	C	S		# 1.14
310	AS	P	C	C	C	S	As	# 2.38
310	AS	P	C	C	C	S	B	# 2.38
310	AS	P	C	C	C	S	P	# 2.38
310	AS	P	C	C	C	S	Se	# 2.38
310	AS	P	C	C	C	S	Si	# 2.38
310	AS	P	C	C	C	S	Te	# 2.38
311	AS	P	C	C	C	Se		# 1.14
311	AS	P	C	C	C	Si		# 1.14
311	AS	P	C	C	C	Te		# 1.14
331	AS	P	C	C	Cl			# 1.39
331	AS	P	C	C	F			# 1.39
331	AS	P	C	C	I			# 1.39
331	AS	P	C	C	N			# 1.39
302	AS	P	C	C	N	As		# 0.44
302	AS	P	C	C	N	B		# 0.44
302	AS	P	C	C	N	P		# 0.44
302	AS	P	C	C	N	Se		# 0.44
302	AS	P	C	C	N	Si		# 0.44
302	AS	P	C	C	N	Te		# 0.44
331	AS	P	C	C	O			# 1.39
310	AS	P	C	C	O	As		# 2.38
310	AS	P	C	C	O	B		# 2.38
310	AS	P	C	C	O	P		# 2.38
310	AS	P	C	C	O	Se		# 2.38
310	AS	P	C	C	O	Si		# 2.38
310	AS	P	C	C	O	Te		# 2.38
331	AS	P	C	C	P			# 1.39
331	AS	P	C	C	S			# 1.39
310	AS	P	C	C	S	As		# 2.38
310	AS	P	C	C	S	B		# 2.38
310	AS	P	C	C	S	P		# 2.38
310	AS	P	C	C	S	Se		# 2.38
310	AS	P	C	C	S	Si		# 2.38
310	AS	P	C	C	S	Te		# 2.38
331	AS	P	C	C	Se			# 1.39
331	AS	P	C	C	Si			# 1.39
331	AS	P	C	C	Te			# 1.39
302	AS	P	N	C	C	As		# 0.44
302	AS	P	N	C	C	B		# 0.44
302	AS	P	N	C	C	Br		# 0.44
302	AS	P	N	C	C	C	As	# 0.44
302	AS	P	N	C	C	C	B	# 0.44
302	AS	P	N	C	C	C	Br	# 0.44
302	AS	P	N	C	C	C	Cl	# 0.44
302	AS	P	N	C	C	C	F	# 0.44
302	AS	P	N	C	C	C	I	# 0.44
302	AS	P	N	C	C	C	N	# 0.44
302	AS	P	N	C	C	C	O	# 0.44
302	AS	P	N	C	C	C	P	# 0.44
302	AS	P	N	C	C	C	S	# 0.44
302	AS	P	N	C	C	C	Se	# 0.44
302	AS	P	N	C	C	C	Si	# 0.44

# Atom Sequences

Screen Number	Fragment Definition							Frequency Percent
302	AS	P	N	C	C	C	Te	# 0.44
302	AS	P	N	C	C	Cl		# 0.44
302	AS	P	N	C	C	F		# 0.44
302	AS	P	N	C	C	I		# 0.44
302	AS	P	N	C	C	N		# 0.44
302	AS	P	N	C	C	O		# 0.44
302	AS	P	N	C	C	P		# 0.44
302	AS	P	N	C	C	S		# 0.44
302	AS	P	N	C	C	Se		# 0.44
302	AS	P	N	C	C	Si		# 0.44
302	AS	P	N	C	C	Te		# 0.44
310	AS	P	O	C	C	As		# 2.38
310	AS	P	O	C	C	B		# 2.38
310	AS	P	O	C	C	Br		# 2.38
310	AS	P	O	C	C	C	As	# 2.38
310	AS	P	O	C	C	C	B	# 2.38
310	AS	P	O	C	C	C	Br	# 2.38
310	AS	P	O	C	C	C	Cl	# 2.38
310	AS	P	O	C	C	C	F	# 2.38
310	AS	P	O	C	C	C	I	# 2.38
310	AS	P	O	C	C	C	N	# 2.38
310	AS	P	O	C	C	C	O	# 2.38
310	AS	P	O	C	C	C	P	# 2.38
310	AS	P	O	C	C	C	S	# 2.38
310	AS	P	O	C	C	C	Se	# 2.38
310	AS	P	O	C	C	C	Si	# 2.38
310	AS	P	O	C	C	C	Te	# 2.38
310	AS	P	O	C	C	Cl		# 2.38
310	AS	P	O	C	C	F		# 2.38
310	AS	P	O	C	C	I		# 2.38
310	AS	P	O	C	C	N		# 2.38
310	AS	P	O	C	C	O		# 2.38
310	AS	P	O	C	C	P		# 2.38
310	AS	P	O	C	C	S		# 2.38
310	AS	P	O	C	C	Se		# 2.38
310	AS	P	O	C	C	Si		# 2.38
310	AS	P	O	C	C	Te		# 2.38
310	AS	P	S	C	C	As		# 2.38
310	AS	P	S	C	C	B		# 2.38
310	AS	P	S	C	C	Br		# 2.38
310	AS	P	S	C	C	C	As	# 2.38
310	AS	P	S	C	C	C	B	# 2.38
310	AS	P	S	C	C	C	Br	# 2.38
310	AS	P	S	C	C	C	As	# 2.38
310	AS	P	S	C	C	C	B	# 2.38
310	AS	P	S	C	C	C	Br	# 2.38
310	AS	P	S	C	C	C	Cl	# 2.38
310	AS	P	S	C	C	C	F	# 2.38
310	AS	P	S	C	C	C	I	# 2.38
310	AS	P	S	C	C	C	N	# 2.38
310	AS	P	S	C	C	C	O	# 2.38
310	AS	P	S	C	C	C	P	# 2.38
310	AS	P	S	C	C	C	S	# 2.38
310	AS	P	S	C	C	C	Se	# 2.38
310	AS	P	S	C	C	C	Si	# 2.38
310	AS	P	S	C	C	C	Te	# 2.38
310	AS	P	S	C	C	Cl		# 2.38
310	AS	P	S	C	C	F		# 2.38

# Atom Sequences

Screen Number		Fragment Definition					Frequency Percent
310	AS	P	S	C	C	I	# 2.38
310	AS	P	S	C	C	N	# 2.38
310	AS	P	S	C	C	O	# 2.38
310	AS	P	S	C	C	P	# 2.38
310	AS	P	S	C	C	S	# 2.38
310	AS	P	S	C	C	Se	# 2.38
310	AS	P	S	C	C	Si	# 2.38
310	AS	P	S	C	C	Te	# 2.38
331	AS	S	C	C		As	# 1.39
331	AS	S	C	C		B	# 1.39
323	AS	S	*	C	*	C - Br	# 0.61
325	AS	S	*	C	- C -	Br	# 0.45
324	AS	S	- C	*	C -	Br	# 2.95
326	AS	S	- C	- C	-	Br	# 2.53
2081	AS	S	C	C	C		# 76.51
118	AS	S	*	C	*	C - C	# 9.42
116	AS	S	*	C	- C *	C	# 4.30
120	AS	S	*	C	- C -	C	# 5.21
119	AS	S	- C	*	C -	C	# 18.18
117	AS	S	- C	- C	*	C	# 33.04
121	AS	S	- C	- C	-	C	# 32.90
311	AS	S	C	C	C	As	# 1.14
311	AS	S	C	C	C	B	# 1.14
303	AS	S	C	C	C	Br	# 5.10
304	AS	S	*	C	*	C * C - Br	# 0.64
305	AS	S	- C	*	C * C -	Br	# 1.72
306	AS	S	- C	- C	*	C - Br	# 1.61
307	AS	S	- C	- C	- C -	Br	# 0.86
72	AS	S	*	C	*	C * C * C	# 19.48
76	AS	S	*	C	*	C * C - C	# 7.10
73	AS	S	*	C	*	C - C * C	# 2.01
74	AS	S	*	C	- C -	C * C	# 1.34
77	AS	S	- C	*	C * C -	C	# 14.59
6	AS	S	- C	*	C -	C * C	# 7.08
38	AS	S	- C	*	C -	C * C	# 5.99
79	AS	S	- C	*	C -	C - C	# 6.96
78	AS	S	- C	- C	*	C - C	# 6.22
75	AS	S	- C	- C	- C *	C	# 6.25
80	AS	S	- C	- C	- C -	C	# 21.57
291	AS	S	C	C	C	C As	# 0.79
291	AS	S	C	C	C	C B	# 0.79
288	AS	S	C	C	C	C Br	# 6.39
289	AS	S	- C	*	C * C * C -	Br	# 3.00
290	AS	S	- C	- C	*	C * C - Br	# 1.30
35	AS	S	*	C	*	C * C * C * C	# 14.10
40	AS	S	*	C	*	C * C * C - C	# 9.53
36	AS	S	*	C	*	C * C - C * C	# 1.56
41	AS	S	- C	*	C * C * C -	C	# 19.86
37	AS	S	- C	*	C * C -	C * C	# 2.60
44	AS	S	- C	*	C * C -	C - C	# 4.16
14	AS	S	- C	*	C -	C - C * C	# 3.46
38	AS	S	- C	*	C -	C - C * C	# 5.99
42	AS	S	- C	- C	*	C * C - C	# 4.15
45	AS	S	- C	- C	*	C - C - C	# 1.26
43	AS	S	- C	- C	- C *	C - C	# 1.01

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
39	AS	S - C - C - C - C * C	# 7.78
46	AS	S - C - C - C - C - C	# 12.64
288	AS	S - C - C - C - C - Cl	# 6.39
289	AS	S - C * C * C * C - Cl	# 3.00
290	AS	S - C - C * C * C - Cl	# 1.30
288	AS	S - C - C - C - C - F	# 6.39
289	AS	S - C * C * C * C - F	# 3.00
290	AS	S - C - C * C * C - F	# 1.30
288	AS	S - C - C - C - C - I	# 6.39
289	AS	S - C * C * C * C - I	# 3.00
290	AS	S - C - C * C * C - I	# 1.30
345	AS	S - C - C - C - C - N	# 25.91
347	AS	S * C * C * C * C - N	# 2.82
346	AS	S - C * C * C * C * N	# 5.92
348	AS	S - C * C * C * C - N	# 5.24
350	AS	S - C * C * C - C - N	# 1.95
352	AS	S - C * C - C - C - N	# 0.41
349	AS	S - C - C * C * C - N	# 1.64
351	AS	S - C - C * C - C - N	# 0.50
353	AS	S - C - C - C - C - N	# 4.12
469	AS	S * C * C * C * C - O	# 5.73
469	AS	S - C * C * C * C * O	# 5.73
470	AS	S - C * C * C * C - O	# 7.27
471	AS	S - C * C * C - C - O	# 4.77
472	AS	S - C * C - C * C - O	# 0.22
473	AS	S - C * C - C - C - O	# 0.86
471	AS	S - C - C * C * C - O	# 4.77
474	AS	S - C - C * C - C - O	# 1.17
473	AS	S - C - C - C * C - O	# 0.86
475	AS	S - C - C - C - C - O	# 4.56
291	AS	S - C - C - C - C - P	# 0.79
469	AS	S * C * C * C * C - S	# 5.73
469	AS	S - C * C * C * C * S	# 5.73
470	AS	S - C * C * C * C - S	# 7.27
471	AS	S - C * C * C - C - S	# 4.77
472	AS	S - C * C - C * C - S	# 0.22
473	AS	S - C * C - C - C - S	# 0.86
471	AS	S - C - C * C * C - S	# 4.77
474	AS	S - C - C * C - C - S	# 1.17
473	AS	S - C - C - C * C - S	# 0.86
475	AS	S - C - C - C - C - S	# 4.56
291	AS	S - C - C - C - C - Se	# 0.79
291	AS	S - C - C - C - C - Si	# 0.79
291	AS	S - C - C - C - C - Te	# 0.79
303	AS	S - C - C - C - Cl	# 5.10
304	AS	S * C * C * C - Cl	# 0.64
305	AS	S - C * C * C - Cl	# 1.72
306	AS	S - C - C * C - Cl	# 1.61
307	AS	S - C - C - C - Cl	# 0.86
303	AS	S - C - C - C - F	# 5.10
304	AS	S * C * C * C - F	# 0.64
305	AS	S - C * C * C - F	# 1.72
306	AS	S - C - C * C - F	# 1.61
307	AS	S - C - C - C - F	# 0.86
303	AS	S - C - C - C - I	# 5.10

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
304	AS	S * C * C * C - I	# 0.64
305	AS	S - C * C * C - I	# 1.72
306	AS	S - C - C * C - I	# 1.61
307	AS	S - C - C - C - I	# 0.86
368	AS	S * C * C * C * N	# 4.16
374	AS	S * C * C * C - N	# 1.65
370	AS	S * C * C - C * N	# 2.56
370	AS	S * C * C - C - N	# 2.56
370	AS	S * C - C * C * N	# 2.56
370	AS	S * C - C * C - N	# 2.56
370	AS	S * C - C - C * N	# 2.56
370	AS	S * C - C - C - N	# 2.56
369	AS	S - C * C * C * N	# 9.05
375	AS	S - C * C * C - N	# 4.45
372	AS	S - C * C - C * N	# 0.73
377	AS	S - C * C - C - N	# 2.93
371	AS	S - C - C * C * N	# 4.73
376	AS	S - C - C * C - N	# 1.92
373	AS	S - C - C - C * N	# 1.07
378	AS	S - C - C - C - N	# 7.21
302	AS	S C C C N As	# 0.44
302	AS	S C C C N B	# 0.44
208	AS	S - C * C * C * N - C	# 3.76
209	AS	S - C * C * C - N - C	# 2.16
211	AS	S - C * C - C - N - C	# 1.57
210	AS	S - C - C * C - N - C	# 1.11
447	AS	S C C C N N	# 3.35
448	AS	S - C * C * C - N - N	# 0.33
476	AS	S C C C N O	# 2.08
477	AS	S - C * C * C - N - O	# 0.52
302	AS	S C C C N P	# 0.44
476	AS	S C C C N S	# 2.08
477	AS	S - C * C * C - N - S	# 0.52
302	AS	S C C C N Se	# 0.44
302	AS	S C C C N Si	# 0.44
302	AS	S C C C N Te	# 0.44
478	AS	S * C * C * C * O	# 2.29
479	AS	S * C * C * C - O	# 7.38
480	AS	S * C * C - C - O	# 3.12
481	AS	S * C - C - C * O	# 0.19
479	AS	S - C * C * C * O	# 7.38
482	AS	S - C * C * C - O	# 6.67
483	AS	S - C * C - C - O	# 6.12
480	AS	S - C - C * C * O	# 3.12
483	AS	S - C - C * C - O	# 6.12
484	AS	S - C - C - C - O	# 6.65
310	AS	S C C C O As	# 2.38
310	AS	S C C C O B	# 2.38
261	AS	S - C * C * C - O - C	# 4.46
263	AS	S - C * C - C - O - C	# 2.05
262	AS	S - C - C * C - O - C	# 2.33
264	AS	S - C - C - C - O - C	# 3.09
466	AS	S C C C O N	# 0.71
485	AS	S C C C O O	# 1.62
310	AS	S C C C O P	# 2.38

# Atom Sequences

Screen Number		Fragment Definition						Frequency Percent
485	AS	S	C	C	C	O	S	# 1.62
310	AS	S	C	C	C	O	Se	# 2.38
310	AS	S	C	C	C	O	Si	# 2.38
310	AS	S	C	C	C	O	Te	# 2.38
311	AS	S	C	C	C	P		# 1.14
2096	AS	S	C	C	C	S		# 20.23
478	AS	S	* C	* C	* C	* S		# 2.29
479	AS	S	* C	* C	* C	- S		# 7.38
480	AS	S	* C	* C	- C	- S		# 3.12
481	AS	S	* C	- C	- C	* S		# 0.19
479	AS	S	- C	* C	* C	* S		# 7.38
482	AS	S	- C	* C	* C	- S		# 6.67
483	AS	S	- C	* C	- C	- S		# 6.12
480	AS	S	- C	- C	* C	* S		# 3.12
483	AS	S	- C	- C	* C	- S		# 6.12
484	AS	S	- C	- C	- C	- S		# 6.65
310	AS	S	C	C	C	S	As	# 2.38
310	AS	S	C	C	C	S	B	# 2.38
261	AS	S	- C	* C	* C	- S	- C	# 4.46
263	AS	S	- C	* C	- C	- S	- C	# 2.05
262	AS	S	- C	- C	* C	- S	- C	# 2.33
264	AS	S	- C	- C	- C	- S	- C	# 3.09
466	AS	S	C	C	C	S	N	# 0.71
485	AS	S	C	C	C	S	O	# 1.62
310	AS	S	C	C	C	S	P	# 2.38
485	AS	S	C	C	C	S	S	# 1.62
310	AS	S	C	C	C	S	Se	# 2.38
310	AS	S	C	C	C	S	Si	# 2.38
310	AS	S	C	C	C	S	Te	# 2.38
311	AS	S	C	C	C	Se		# 1.14
311	AS	S	C	C	C	Si		# 1.14
311	AS	S	C	C	C	Te		# 1.14
323	AS	S	* C	* C	- Cl			# 0.61
325	AS	S	* C	- C	- Cl			# 0.45
324	AS	S	- C	* C	- Cl			# 2.95
326	AS	S	- C	- C	- Cl			# 2.53
323	AS	S	* C	* C	- F			# 0.61
325	AS	S	* C	- C	- F			# 0.45
324	AS	S	- C	* C	- F			# 2.95
326	AS	S	- C	- C	- F			# 2.53
323	AS	S	* C	* C	- I			# 0.61
325	AS	S	* C	- C	- I			# 0.45
324	AS	S	- C	* C	- I			# 2.95
326	AS	S	- C	- C	- I			# 2.53
2090	AS	S	C	C	N			# 35.39
398	AS	S	* C	* C	* N			# 8.97
402	AS	S	* C	* C	- N			# 1.91
400	AS	S	* C	- C	* N			# 0.73
404	AS	S	* C	- C	- N			# 2.34
399	AS	S	- C	* C	* N			# 5.41
403	AS	S	- C	* C	- N			# 6.11
401	AS	S	- C	- C	* N			# 6.21
405	AS	S	- C	- C	- N			# 16.92
302	AS	S	C	C	N	As		# 0.44
302	AS	S	C	C	N	B		# 0.44

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
225	AS	S * C * C * N - C	# 3.33
226	AS	S - C * C * N - C	# 1.88
223	AS	S - C * C - N * C	# 0.96
228	AS	S - C * C - N - C	# 3.06
227	AS	S - C - C * N - C	# 2.68
224	AS	S - C - C - N * C	# 2.89
229	AS	S - C - C - N - C	# 12.06
148	AS	S * C * C * N * C * C	# 3.85
38	AS	S - C * C - N - C * C	# 5.99
102	AS	S - C * C - N - C * C	# 0.92
149	AS	S - C - C - N - C * C	# 2.49
415	AS	S - C - C - N - C - N	# 7.06
416	AS	S - C * C * N * C * N	# 1.32
418	AS	S - C * C - N - C - N	# 0.25
417	AS	S - C - C * N * C * N	# 0.56
419	AS	S - C - C - N - C - N	# 0.42
486	AS	S - C - C - N - C - O	# 14.96
487	AS	S - C * C - N - C - O	# 2.07
488	AS	S - C - C - N - C - O	# 7.07
486	AS	S - C - C - N - C - S	# 14.96
487	AS	S - C * C - N - C - S	# 2.07
488	AS	S - C - C - N - C - S	# 7.07
451	AS	S - C - C - N - N	# 4.22
452	AS	S - C * C * N * N	# 0.46
454	AS	S - C * C - N - N	# 0.91
453	AS	S - C - C * N * N	# 0.74
455	AS	S - C - C - N - N	# 0.80
489	AS	S - C - C - N - O	# 2.88
490	AS	S - C * C - N - O	# 0.94
491	AS	S - C - C - N - O	# 1.05
302	AS	S - C - C - N - P	# 0.44
489	AS	S - C - C - N - S	# 2.88
490	AS	S - C * C - N - S	# 0.94
491	AS	S - C - C - N - S	# 1.05
302	AS	S - C - C - N - Se	# 0.44
302	AS	S - C - C - N - Si	# 0.44
302	AS	S - C - C - N - Te	# 0.44
2091	AS	S - C - C - O	# 24.29
492	AS	S * C * C * O	# 4.00
493	AS	S * C * C - O	# 6.17
494	AS	S * C - C * O	# 0.42
495	AS	S * C - C - O	# 5.40
493	AS	S - C * C * O	# 6.17
496	AS	S - C * C - O	# 7.98
495	AS	S - C - C * O	# 5.40
497	AS	S - C - C - O	# 9.90
310	AS	S - C - C - O - As	# 2.38
310	AS	S - C - C - O - B	# 2.38
272	AS	S - C * C - O - C	# 6.16
273	AS	S - C - C - O - C	# 8.01
38	AS	S - C * C - O - C * C	# 5.99
126	AS	S - C * C - O - C * C	# 2.20
187	AS	S - C - C - O - C * C	# 3.29
441	AS	S - C - C - O - C - N	# 4.35
498	AS	S - C - C - O - C - O	# 7.30



# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
498 AS	S C C O C S	# 7.30
467 AS	S C C O N	# 0.63
499 AS	S C C O O	# 1.31
310 AS	S C C O P	# 2.38
499 AS	S C C O S	# 1.31
310 AS	S C C O Se	# 2.38
310 AS	S C C O Si	# 2.38
310 AS	S C C O Te	# 2.38
331 AS	S C C P	# 1.39
2091 AS	S C C S	# 24.29
492 AS	S * C * C * S	# 4.00
493 AS	S * C * C - S	# 6.17
494 AS	S * C - C * S	# 0.42
495 AS	S * C - C - S	# 5.40
493 AS	S - C * C * S	# 6.17
496 AS	S - C * C - S	# 7.98
495 AS	S - C - C * S	# 5.40
497 AS	S - C - C - S	# 9.90
310 AS	S C C S As	# 2.38
310 AS	S C C S B	# 2.38
272 AS	S - C * C - S - C	# 6.16
273 AS	S - C - C - S - C	# 8.01
38 AS	S - C * C - S - C * C	# 5.99
126 AS	S - C * C - S - C * C	# 2.20
187 AS	S - C - C - S - C * C	# 3.29
441 AS	S C C S C N	# 4.35
498 AS	S C C S C O	# 7.30
498 AS	S C C S C S	# 7.30
467 AS	S C C S N	# 0.63
499 AS	S C C S O	# 1.31
310 AS	S C C S P	# 2.38
499 AS	S C C S S	# 1.31
310 AS	S C C S Se	# 2.38
310 AS	S C C S Si	# 2.38
310 AS	S C C S Te	# 2.38
331 AS	S C C Se	# 1.39
331 AS	S C C Si	# 1.39
331 AS	S C C Te	# 1.39
2087 AS	S C N C	# 39.80
241 AS	S * C * N - C	# 1.96
239 AS	S * C - N * C	# 1.30
242 AS	S - C * N - C	# 8.74
240 AS	S - C - N * C	# 5.80
243 AS	S - C - N - C	# 23.15
334 AS	S C N C Br	# 0.18
157 AS	S * C * N * C * C	# 6.29
161 AS	S * C * N * C - C	# 3.21
159 AS	S * C - N - C * C	# 0.71
162 AS	S - C * N * C - C	# 4.84
158 AS	S - C * N - C * C	# 3.59
163 AS	S - C - N * C - C	# 2.74
160 AS	S - C - N - C * C	# 11.07
164 AS	S - C - N - C - C	# 13.37
319 AS	S C N C C Br	# 1.84
320 AS	S - C - N - C * C - Br	# 0.72

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
106	AS	S * C * N * C * C * C	# 2.79
107	AS	S - C * N - C - C * C	# 1.02
109	AS	S - C - N - C * C - C	# 2.05
108	AS	S - C - N - C - C * C	# 3.00
319	AS	S C N C C Cl	# 1.84
320	AS	S - C - N - C * C - Cl	# 0.72
319	AS	S C N C C F	# 1.84
320	AS	S - C - N - C * C - F	# 0.72
319	AS	S C N C C I	# 1.84
320	AS	S - C - N - C * C - I	# 0.72
389	AS	S C N C C N	# 12.87
390	AS	S - C - N * C * C * N	# 1.34
391	AS	S - C - N - C * C - N	# 0.42
392	AS	S - C - N - C - C - N	# 5.48
486	AS	S C N C C O	# 14.96
487	AS	S - C - N - C * C - O	# 2.07
488	AS	S - C - N - C - C - O	# 7.07
486	AS	S C N C C S	# 14.96
487	AS	S - C - N - C * C - S	# 2.07
488	AS	S - C - N - C - C - S	# 7.07
334	AS	S C N C Cl	# 0.18
334	AS	S C N C F	# 0.18
334	AS	S C N C I	# 0.18
425	AS	S C N C N	# 9.70
426	AS	S - C * N * C * N	# 5.47
429	AS	S - C * N * C - N	# 1.44
427	AS	S - C - N * C * N	# 0.50
428	AS	S - C - N - C * N	# 1.59
430	AS	S - C - N - C - N	# 0.75
500	AS	S C N C O	# 8.18
501	AS	S - C * N * C - O	# 4.24
502	AS	S - C * N - C - O	# 0.50
502	AS	S - C - N * C - O	# 0.50
503	AS	S - C - N - C - O	# 0.77
500	AS	S C N C S	# 8.18
501	AS	S - C * N * C - S	# 4.24
502	AS	S - C * N - C - S	# 0.50
502	AS	S - C - N * C - S	# 0.50
503	AS	S - C - N - C - S	# 0.77
459	AS	S C N N	# 6.66
460	AS	S * C * N * N	# 1.19
461	AS	S - C * N * N	# 2.61
462	AS	S - C - N * N	# 0.41
463	AS	S - C - N - N	# 2.57
249	AS	S - C * N * N - C	# 0.35
504	AS	S C N N C O	# 1.09
504	AS	S C N N C S	# 1.09
505	AS	S C N O	# 1.66
506	AS	S * C * N * O	# 0.08
507	AS	S * C - N - O	# 0.24
508	AS	S - C * N * O	# 0.24
509	AS	S - C - N - O	# 0.83
505	AS	S C N S	# 1.66
2092	AS	S C N S	# 13.08
506	AS	S * C * N * S	# 0.08

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
507 AS	S * C - N - S	# 0.24
508 AS	S - C * N * S	# 0.24
509 AS	S - C - N - S	# 0.83
2088 AS	S C O C	# 27.26
2094 AS	S C O C	# 27.26
277 AS	S * C - O - C	# 2.86
192 AS	S * C - O - C * C	# 1.20
194 AS	S - C * O * C - C	# 3.38
193 AS	S - C - O - C * C	# 4.71
195 AS	S - C - O - C - C	# 13.48
328 AS	S C O C C Br	# 0.64
128 AS	S - C - O - C - C * C	# 3.28
328 AS	S C O C C Cl	# 0.64
328 AS	S C O C C F	# 0.64
328 AS	S C O C C I	# 0.64
408 AS	S C O C C N	# 4.14
409 AS	S - C - O - C * C - N	# 0.36
410 AS	S - C - O - C - C - N	# 1.42
498 AS	S C O C C O	# 7.30
498 AS	S C O C C S	# 7.30
443 AS	S C O C N	# 0.95
510 AS	S C O C O	# 1.46
510 AS	S C O C S	# 1.46
468 AS	S C O N	# 0.58
511 AS	S C O O	# 0.48
511 AS	S C O S	# 0.48
2088 AS	S C S C	# 27.26
2094 AS	S C S C	# 27.26
277 AS	S * C - S - C	# 2.86
192 AS	S * C - S - C * C	# 1.20
194 AS	S - C * S * C - C	# 3.38
193 AS	S - C - S - C * C	# 4.71
195 AS	S - C - S - C - C	# 13.48
328 AS	S C S C C Br	# 0.64
128 AS	S - C - S - C - C * C	# 3.28
328 AS	S C S C C Cl	# 0.64
328 AS	S C S C C F	# 0.64
328 AS	S C S C C I	# 0.64
408 AS	S C S C C N	# 4.14
409 AS	S - C - S - C * C - N	# 0.36
410 AS	S - C - S - C - C - N	# 1.42
498 AS	S C S C C O	# 7.30
498 AS	S C S C C S	# 7.30
443 AS	S C S C N	# 0.95
510 AS	S C S C O	# 1.46
510 AS	S C S C S	# 1.46
468 AS	S C S N	# 0.58
511 AS	S C S O	# 0.48
511 AS	S C S S	# 0.48
335 AS	S N C Br	# 0.09
2085 AS	S N C C	# 26.07
173 AS	S * N * C * C	# 1.32
175 AS	S - N * C - C	# 0.56
174 AS	S - N - C * C	# 6.36
176 AS	S - N - C - C	# 3.06

# Atom Sequences

Screen Number		Fragment Definition	Frequency Percent
322	AS	S N C C Br	# 0.39
115	AS	S - N - C * C - C	# 0.94
114	AS	S - N - C - C * C	# 1.22
301	AS	S N C C Br	# 0.55
71	AS	S - N - C * C * C - C	# 1.36
70	AS	S - N - C - C - C * C	# 0.32
301	AS	S N C C C Cl	# 0.55
301	AS	S N C C C F	# 0.55
301	AS	S N C C C I	# 0.55
365	AS	S N C C C N	# 2.43
366	AS	S - N - C * C * C * N	# 0.35
367	AS	S - N - C * C * C - N	# 1.02
476	AS	S N C C C O	# 2.08
477	AS	S - N - C * C * C - O	# 0.52
476	AS	S N C C C S	# 2.08
477	AS	S - N - C * C * C - S	# 0.52
322	AS	S N C C Cl	# 0.39
322	AS	S N C C F	# 0.39
322	AS	S N C C I	# 0.39
394	AS	S N C C N	# 3.00
395	AS	S - N - C * C * N	# 0.48
396	AS	S - N - C * C - N	# 0.72
397	AS	S - N - C - C - N	# 0.82
222	AS	S - N - C * C - N - C	# 0.32
450	AS	S N C C N N	# 0.51
512	AS	S N C C N O	# 0.33
512	AS	S N C C N S	# 0.33
489	AS	S N C C O	# 2.88
490	AS	S - N - C * C - O	# 0.94
491	AS	S - N - C - C - O	# 1.05
271	AS	S - N - C * C - O - C	# 0.42
489	AS	S N C C S	# 2.88
490	AS	S - N - C * C - S	# 0.94
491	AS	S - N - C - C - S	# 1.05
271	AS	S - N - C * C - S - C	# 0.42
335	AS	S N C Cl	# 0.09
335	AS	S N C F	# 0.09
335	AS	S N C I	# 0.09
437	AS	S N C N	# 1.66
438	AS	S * N * C * N	# 0.48
439	AS	S - N - C * N	# 0.35
440	AS	S - N - C - N	# 0.51
458	AS	S N C N N	# 0.17
505	AS	S N C O	# 1.66
2092	AS	S N C O	# 13.08
506	AS	S * N * C * O	# 0.08
508	AS	S * N * C - O	# 0.24
507	AS	S - N - C * O	# 0.24
509	AS	S - N - C - O	# 0.83
505	AS	S N C S	# 1.66
2092	AS	S N C S	# 13.08
506	AS	S * N * C * S	# 0.08
508	AS	S * N * C - S	# 0.24
507	AS	S - N - C * S	# 0.24
509	AS	S - N - C - S	# 0.83

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
279 AS	S N O C	# 0.17
279 AS	S N S C	# 0.17
336 AS	S O C Br	# 0.37
2085 AS	S O C C	# 26.07
201 AS	S - O - C * C	# 6.11
202 AS	S - O - C - C	# 2.21
330 AS	S O C C Br	# 0.43
132 AS	S - O - C * C - C	# 0.71
131 AS	S - O - C - C * C	# 0.48
133 AS	S - O - C - C - C	# 1.20
309 AS	S O C C C Br	# 0.37
86 AS	S - O - C * C * C - C	# 0.75
309 AS	S O C C C Cl	# 0.37
309 AS	S O C C C F	# 0.37
309 AS	S O C C C I	# 0.37
380 AS	S O C C C N	# 1.74
381 AS	S - O - C * C * C - N	# 0.76
485 AS	S O C C C O	# 1.62
485 AS	S O C C C S	# 1.62
330 AS	S O C C C Cl	# 0.43
330 AS	S O C C C F	# 0.43
330 AS	S O C C C I	# 0.43
412 AS	S O C C C N	# 1.53
413 AS	S - O - C * C * N	# 0.27
414 AS	S - O - C * C - N	# 0.52
456 AS	S O C C N N	# 0.36
499 AS	S O C C O	# 1.31
499 AS	S O C C S	# 1.31
336 AS	S O C Cl	# 0.37
336 AS	S O C F	# 0.37
336 AS	S O C I	# 0.37
446 AS	S O C N	# 0.48
511 AS	S O C O	# 0.48
511 AS	S O C S	# 0.48
2092 AS	S O N C	# 13.08
254 AS	S * O - N - C	# 0.00
253 AS	S - O - N * C	# 0.97
255 AS	S - O - N - C	# 2.96
179 AS	S - O - N - C * C	# 1.31
465 AS	S O N N	# 0.17
282 AS	S O O C	# 1.03
282 AS	S O S C	# 1.03
336 AS	S S C Br	# 0.37
2085 AS	S S C C	# 26.07
201 AS	S - S - C * C	# 6.11
202 AS	S - S - C - C	# 2.21
330 AS	S S C C Br	# 0.43
132 AS	S - S - C * C - C	# 0.71
131 AS	S - S - C - C * C	# 0.48
133 AS	S - S - C - C - C	# 1.20
309 AS	S S C C C Br	# 0.37
86 AS	S - S - C * C * C - C	# 0.75
309 AS	S S C C C Cl	# 0.37
309 AS	S S C C C F	# 0.37
309 AS	S S C C C I	# 0.37

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
380 AS	S S C C C N	# 1.74
381 AS	S - S - C * C * C - N	# 0.76
485 AS	S S C C C O	# 1.62
485 AS	S S C C C S	# 1.62
330 AS	S S C C Cl	# 0.43
330 AS	S S C C F	# 0.43
330 AS	S S C C I	# 0.43
412 AS	S S C C N	# 1.53
413 AS	S - S - C * C * N	# 0.27
414 AS	S - S - C * C - N	# 0.52
456 AS	S S C C N N	# 0.36
499 AS	S S C C O	# 1.31
499 AS	S S C C S	# 1.31
336 AS	S S C Cl	# 0.37
336 AS	S S C F	# 0.37
336 AS	S S C I	# 0.37
446 AS	S S C N	# 0.48
511 AS	S S C O	# 0.48
511 AS	S S C S	# 0.48
2092 AS	S S N C	# 13.08
254 AS	S * S - N - C	# 0.00
253 AS	S - S - N * C	# 0.97
255 AS	S - S - N - C	# 2.96
179 AS	S - S - N - C * C	# 1.31
465 AS	S S N N	# 0.17
282 AS	S S O C	# 1.03
282 AS	S S S C	# 1.03
331 AS	Se C C As	# 1.39
331 AS	Se C C B	# 1.39
331 AS	Se C C Br	# 1.39
134 AS	Se C C C	# 4.57
311 AS	Se C C C As	# 1.14
311 AS	Se C C C B	# 1.14
311 AS	Se C C C Br	# 1.14
291 AS	Se C C C C As	# 0.79
291 AS	Se C C C C B	# 0.79
291 AS	Se C C C C Br	# 0.79
47 AS	Se C C C C C	# 3.83
291 AS	Se C C C C Cl	# 0.79
291 AS	Se C C C C F	# 0.79
291 AS	Se C C C C I	# 0.79
291 AS	Se C C C C N	# 0.79
291 AS	Se C C C C O	# 0.79
291 AS	Se C C C C P	# 0.79
291 AS	Se C C C C S	# 0.79
291 AS	Se C C C C Se	# 0.79
291 AS	Se C C C C Si	# 0.79
291 AS	Se C C C C Te	# 0.79
311 AS	Se C C C Cl	# 1.14
311 AS	Se C C C F	# 1.14
311 AS	Se C C C I	# 1.14
311 AS	Se C C C N	# 1.14
302 AS	Se C C C N As	# 0.44
302 AS	Se C C C N B	# 0.44
302 AS	Se C C C N P	# 0.44

# Atom Sequences

Screen Number	Fragment Definition	Frequency Percent
302	AS Se C C C N Se	# 0.44
302	AS Se C C C N Si	# 0.44
302	AS Se C C C N Te	# 0.44
311	AS Se C C C O	# 1.14
310	AS Se C C C O As	# 2.38
310	AS Se C C C O B	# 2.38
310	AS Se C C C O P	# 2.38
310	AS Se C C C O Se	# 2.38
310	AS Se C C C O Si	# 2.38
310	AS Se C C C O Te	# 2.38
311	AS Se C C C P	# 1.14
311	AS Se C C C S	# 1.14
310	AS Se C C C S As	# 2.38
310	AS Se C C C S B	# 2.38
310	AS Se C C C S P	# 2.38
310	AS Se C C C S Se	# 2.38
310	AS Se C C C S Si	# 2.38
310	AS Se C C C S Te	# 2.38
311	AS Se C C C Se	# 1.14
311	AS Se C C C Si	# 1.14
311	AS Se C C C Te	# 1.14
331	AS Se C C Cl	# 1.39
331	AS Se C C F	# 1.39
331	AS Se C C I	# 1.39
331	AS Se C C N	# 1.39
302	AS Se C C N As	# 0.44
302	AS Se C C N B	# 0.44
302	AS Se C C N P	# 0.44
302	AS Se C C N Se	# 0.44
302	AS Se C C N Si	# 0.44
302	AS Se C C N Te	# 0.44
331	AS Se C C O	# 1.39
310	AS Se C C O As	# 2.38
310	AS Se C C O B	# 2.38
310	AS Se C C O P	# 2.38
310	AS Se C C O Se	# 2.38
310	AS Se C C O Si	# 2.38
310	AS Se C C O Te	# 2.38
331	AS Se C C P	# 1.39
331	AS Se C C S	# 1.39
310	AS Se C C S As	# 2.38
310	AS Se C C S B	# 2.38
310	AS Se C C S P	# 2.38
310	AS Se C C S Se	# 2.38
310	AS Se C C S Si	# 2.38
310	AS Se C C S Te	# 2.38
331	AS Se C C Se	# 1.39
331	AS Se C C Si	# 1.39
331	AS Se C C Te	# 1.39
302	AS Se N C C As	# 0.44
302	AS Se N C C B	# 0.44
302	AS Se N C C Br	# 0.44
302	AS Se N C C C As	# 0.44
302	AS Se N C C C B	# 0.44
302	AS Se N C C C Br	# 0.44

# Atom Sequences

Screen Number	Fragment Definition							Frequency Percent
302	AS	Se	N	C	C	C	Cl	# 0.44
302	AS	Se	N	C	C	C	F	# 0.44
302	AS	Se	N	C	C	C	I	# 0.44
302	AS	Se	N	C	C	C	N	# 0.44
302	AS	Se	N	C	C	C	O	# 0.44
302	AS	Se	N	C	C	C	P	# 0.44
302	AS	Se	N	C	C	C	S	# 0.44
302	AS	Se	N	C	C	C	Se	# 0.44
302	AS	Se	N	C	C	C	Si	# 0.44
302	AS	Se	N	C	C	C	Te	# 0.44
302	AS	Se	N	C	C	C	Cl	# 0.44
302	AS	Se	N	C	C	C	F	# 0.44
302	AS	Se	N	C	C	C	I	# 0.44
302	AS	Se	N	C	C	C	N	# 0.44
302	AS	Se	N	C	C	C	O	# 0.44
302	AS	Se	N	C	C	C	P	# 0.44
302	AS	Se	N	C	C	C	S	# 0.44
302	AS	Se	N	C	C	C	Se	# 0.44
302	AS	Se	N	C	C	C	Si	# 0.44
302	AS	Se	N	C	C	C	Te	# 0.44
310	AS	Se	O	C	C	C	As	# 2.38
310	AS	Se	O	C	C	C	B	# 2.38
310	AS	Se	O	C	C	C	Br	# 2.38
310	AS	Se	O	C	C	C	As	# 2.38
310	AS	Se	O	C	C	C	B	# 2.38
310	AS	Se	O	C	C	C	Br	# 2.38
310	AS	Se	O	C	C	C	Cl	# 2.38
310	AS	Se	O	C	C	C	F	# 2.38
310	AS	Se	O	C	C	C	I	# 2.38
310	AS	Se	O	C	C	C	N	# 2.38
310	AS	Se	O	C	C	C	O	# 2.38
310	AS	Se	O	C	C	C	P	# 2.38
310	AS	Se	O	C	C	C	S	# 2.38
310	AS	Se	O	C	C	C	Se	# 2.38
310	AS	Se	O	C	C	C	Si	# 2.38
310	AS	Se	O	C	C	C	Te	# 2.38
310	AS	Se	O	C	C	C	Cl	# 2.38
310	AS	Se	O	C	C	C	F	# 2.38
310	AS	Se	O	C	C	C	I	# 2.38
310	AS	Se	O	C	C	C	N	# 2.38
310	AS	Se	O	C	C	C	O	# 2.38
310	AS	Se	O	C	C	C	P	# 2.38
310	AS	Se	O	C	C	C	S	# 2.38
310	AS	Se	O	C	C	C	Se	# 2.38
310	AS	Se	O	C	C	C	Si	# 2.38
310	AS	Se	O	C	C	C	Te	# 2.38
310	AS	Se	S	C	C	C	As	# 2.38
310	AS	Se	S	C	C	C	B	# 2.38
310	AS	Se	S	C	C	C	Br	# 2.38
310	AS	Se	S	C	C	C	As	# 2.38
310	AS	Se	S	C	C	C	B	# 2.38
310	AS	Se	S	C	C	C	Br	# 2.38
310	AS	Se	S	C	C	C	Cl	# 2.38
310	AS	Se	S	C	C	C	F	# 2.38
310	AS	Se	S	C	C	C	I	# 2.38



# Atom Sequences

Screen Number	Fragment Definition							Frequency Percent
310	AS	Se	S	C	C	C	N	# 2.38
310	AS	Se	S	C	C	C	O	# 2.38
310	AS	Se	S	C	C	C	P	# 2.38
310	AS	Se	S	C	C	C	S	# 2.38
310	AS	Se	S	C	C	C	Se	# 2.38
310	AS	Se	S	C	C	C	Si	# 2.38
310	AS	Se	S	C	C	C	Te	# 2.38
310	AS	Se	S	C	C	Cl		# 2.38
310	AS	Se	S	C	C	F		# 2.38
310	AS	Se	S	C	C	I		# 2.38
310	AS	Se	S	C	C	N		# 2.38
310	AS	Se	S	C	C	O		# 2.38
310	AS	Se	S	C	C	P		# 2.38
310	AS	Se	S	C	C	S		# 2.38
310	AS	Se	S	C	C	Se		# 2.38
310	AS	Se	S	C	C	Si		# 2.38
310	AS	Se	S	C	C	Te		# 2.38
331	AS	Si	C	C	As			# 1.39
331	AS	Si	C	C	B			# 1.39
331	AS	Si	C	C	Br			# 1.39
134	AS	Si	C	C	C			# 4.57
311	AS	Si	C	C	C	As		# 1.14
311	AS	Si	C	C	C	B		# 1.14
311	AS	Si	C	C	C	Br		# 1.14
291	AS	Si	C	C	C	C	As	# 0.79
291	AS	Si	C	C	C	C	B	# 0.79
291	AS	Si	C	C	C	C	Br	# 0.79
47	AS	Si	C	C	C	C	C	# 3.83
291	AS	Si	C	C	C	C	Cl	# 0.79
291	AS	Si	C	C	C	C	F	# 0.79
291	AS	Si	C	C	C	C	I	# 0.79
291	AS	Si	C	C	C	C	N	# 0.79
291	AS	Si	C	C	C	C	O	# 0.79
291	AS	Si	C	C	C	C	P	# 0.79
291	AS	Si	C	C	C	C	S	# 0.79
291	AS	Si	C	C	C	C	Se	# 0.79
291	AS	Si	C	C	C	C	Si	# 0.79
291	AS	Si	C	C	C	C	Te	# 0.79
311	AS	Si	C	C	C	Cl		# 1.14
311	AS	Si	C	C	C	F		# 1.14
311	AS	Si	C	C	C	I		# 1.14
311	AS	Si	C	C	C	N		# 1.14
302	AS	Si	C	C	C	N	As	# 0.44
302	AS	Si	C	C	C	N	B	# 0.44
302	AS	Si	C	C	C	N	P	# 0.44
302	AS	Si	C	C	C	N	Se	# 0.44
302	AS	Si	C	C	C	N	Si	# 0.44
302	AS	Si	C	C	C	N	Te	# 0.44
311	AS	Si	C	C	C	O		# 1.14
310	AS	Si	C	C	C	O	As	# 2.38
310	AS	Si	C	C	C	O	B	# 2.38
310	AS	Si	C	C	C	O	P	# 2.38
310	AS	Si	C	C	C	O	Se	# 2.38
310	AS	Si	C	C	C	O	Si	# 2.38
310	AS	Si	C	C	C	O	Te	# 2.38

# Atom Sequences

Screen Number	Fragment Definition							Frequency Percent
311	AS	Si	C	C	C	P		# 1.14
311	AS	Si	C	C	C	S		# 1.14
310	AS	Si	C	C	C	S	As	# 2.38
310	AS	Si	C	C	C	S	B	# 2.38
310	AS	Si	C	C	C	S	P	# 2.38
310	AS	Si	C	C	C	S	Se	# 2.38
310	AS	Si	C	C	C	S	Si	# 2.38
310	AS	Si	C	C	C	S	Te	# 2.38
311	AS	Si	C	C	C	Se		# 1.14
311	AS	Si	C	C	C	Si		# 1.14
311	AS	Si	C	C	C	Te		# 1.14
331	AS	Si	C	C	Cl			# 1.39
331	AS	Si	C	C	F			# 1.39
331	AS	Si	C	C	I			# 1.39
331	AS	Si	C	C	N			# 1.39
302	AS	Si	C	C	N	As		# 0.44
302	AS	Si	C	C	N	B		# 0.44
302	AS	Si	C	C	N	P		# 0.44
302	AS	Si	C	C	N	Se		# 0.44
302	AS	Si	C	C	N	Si		# 0.44
302	AS	Si	C	C	N	Te		# 0.44
331	AS	Si	C	C	O			# 1.39
310	AS	Si	C	C	O	As		# 2.38
310	AS	Si	C	C	O	B		# 2.38
310	AS	Si	C	C	O	P		# 2.38
310	AS	Si	C	C	O	Se		# 2.38
310	AS	Si	C	C	O	Si		# 2.38
310	AS	Si	C	C	O	Te		# 2.38
331	AS	Si	C	C	P			# 1.39
331	AS	Si	C	C	S			# 1.39
310	AS	Si	C	C	S	As		# 2.38
310	AS	Si	C	C	S	B		# 2.38
310	AS	Si	C	C	S	P		# 2.38
310	AS	Si	C	C	S	Se		# 2.38
310	AS	Si	C	C	S	Si		# 2.38
310	AS	Si	C	C	S	Te		# 2.38
331	AS	Si	C	C	Se			# 1.39
331	AS	Si	C	C	Si			# 1.39
331	AS	Si	C	C	Te			# 1.39
302	AS	Si	N	C	C	As		# 0.44
302	AS	Si	N	C	C	B		# 0.44
302	AS	Si	N	C	C	Br		# 0.44
302	AS	Si	N	C	C	C	As	# 0.44
302	AS	Si	N	C	C	C	B	# 0.44
302	AS	Si	N	C	C	C	Br	# 0.44
302	AS	Si	N	C	C	C	Cl	# 0.44
302	AS	Si	N	C	C	C	F	# 0.44
302	AS	Si	N	C	C	C	I	# 0.44
302	AS	Si	N	C	C	C	N	# 0.44
302	AS	Si	N	C	C	C	O	# 0.44
302	AS	Si	N	C	C	C	P	# 0.44
302	AS	Si	N	C	C	C	S	# 0.44
302	AS	Si	N	C	C	C	Se	# 0.44
302	AS	Si	N	C	C	C	Si	# 0.44
302	AS	Si	N	C	C	C	Te	# 0.44

# Atom Sequences

Screen Number	Fragment Definition						Frequency Percent
302	AS	Si	N	C	C	Cl	# 0.44
302	AS	Si	N	C	C	F	# 0.44
302	AS	Si	N	C	C	I	# 0.44
302	AS	Si	N	C	C	N	# 0.44
302	AS	Si	N	C	C	O	# 0.44
302	AS	Si	N	C	C	P	# 0.44
302	AS	Si	N	C	C	S	# 0.44
302	AS	Si	N	C	C	Se	# 0.44
302	AS	Si	N	C	C	Si	# 0.44
302	AS	Si	N	C	C	Te	# 0.44
310	AS	Si	O	C	C	As	# 2.38
310	AS	Si	O	C	C	B	# 2.38
310	AS	Si	O	C	C	Br	# 2.38
310	AS	Si	O	C	C	C As	# 2.38
310	AS	Si	O	C	C	C B	# 2.38
310	AS	Si	O	C	C	C Br	# 2.38
310	AS	Si	O	C	C	C Cl	# 2.38
310	AS	Si	O	C	C	C F	# 2.38
310	AS	Si	O	C	C	C I	# 2.38
310	AS	Si	O	C	C	C N	# 2.38
310	AS	Si	O	C	C	C O	# 2.38
310	AS	Si	O	C	C	C P	# 2.38
310	AS	Si	O	C	C	C S	# 2.38
310	AS	Si	O	C	C	C Se	# 2.38
310	AS	Si	O	C	C	C Si	# 2.38
310	AS	Si	O	C	C	C Te	# 2.38
310	AS	Si	O	C	C	Cl	# 2.38
310	AS	Si	O	C	C	F	# 2.38
310	AS	Si	O	C	C	I	# 2.38
310	AS	Si	O	C	C	N	# 2.38
310	AS	Si	O	C	C	O	# 2.38
310	AS	Si	O	C	C	P	# 2.38
310	AS	Si	O	C	C	S	# 2.38
310	AS	Si	O	C	C	Se	# 2.38
310	AS	Si	O	C	C	Si	# 2.38
310	AS	Si	O	C	C	Te	# 2.38
310	AS	Si	S	C	C	As	# 2.38
310	AS	Si	S	C	C	B	# 2.38
310	AS	Si	S	C	C	Br	# 2.38
310	AS	Si	S	C	C	C As	# 2.38
310	AS	Si	S	C	C	C B	# 2.38
310	AS	Si	S	C	C	C Br	# 2.38
310	AS	Si	S	C	C	C Cl	# 2.38
310	AS	Si	S	C	C	C F	# 2.38
310	AS	Si	S	C	C	C I	# 2.38
310	AS	Si	S	C	C	C N	# 2.38
310	AS	Si	S	C	C	C O	# 2.38
310	AS	Si	S	C	C	C P	# 2.38
310	AS	Si	S	C	C	C S	# 2.38
310	AS	Si	S	C	C	C Se	# 2.38
310	AS	Si	S	C	C	C Si	# 2.38
310	AS	Si	S	C	C	C Te	# 2.38
310	AS	Si	S	C	C	Cl	# 2.38
310	AS	Si	S	C	C	F	# 2.38
310	AS	Si	S	C	C	I	# 2.38

# Atom Sequences

Screen Number		Fragment Definition						Frequency Percent	
310	AS	Si	S	C	C	N		#	2.38
310	AS	Si	S	C	C	O		#	2.38
310	AS	Si	S	C	C	P		#	2.38
310	AS	Si	S	C	C	S		#	2.38
310	AS	Si	S	C	C	Se		#	2.38
310	AS	Si	S	C	C	Si		#	2.38
310	AS	Si	S	C	C	Te		#	2.38
331	AS	Te	C	C	As			#	1.39
331	AS	Te	C	C	B			#	1.39
331	AS	Te	C	C	Br			#	1.39
134	AS	Te	C	C	C			#	4.57
311	AS	Te	C	C	C	As		#	1.14
311	AS	Te	C	C	C	B		#	1.14
311	AS	Te	C	C	C	Br		#	1.14
291	AS	Te	C	C	C	C	As	#	0.79
291	AS	Te	C	C	C	C	B	#	0.79
291	AS	Te	C	C	C	C	Br	#	0.79
47	AS	Te	C	C	C	C	C	#	3.83
291	AS	Te	C	C	C	C	Cl	#	0.79
291	AS	Te	C	C	C	C	F	#	0.79
291	AS	Te	C	C	C	C	I	#	0.79
291	AS	Te	C	C	C	C	N	#	0.79
291	AS	Te	C	C	C	C	O	#	0.79
291	AS	Te	C	C	C	C	P	#	0.79
291	AS	Te	C	C	C	C	S	#	0.79
291	AS	Te	C	C	C	C	Se	#	0.79
291	AS	Te	C	C	C	C	Si	#	0.79
291	AS	Te	C	C	C	C	Te	#	0.79
311	AS	Te	C	C	C	Cl		#	1.14
311	AS	Te	C	C	C	F		#	1.14
311	AS	Te	C	C	C	I		#	1.14
311	AS	Te	C	C	C	N		#	1.14
302	AS	Te	C	C	C	N	As	#	0.44
302	AS	Te	C	C	C	N	B	#	0.44
302	AS	Te	C	C	C	N	P	#	0.44
302	AS	Te	C	C	C	N	Se	#	0.44
302	AS	Te	C	C	C	N	Si	#	0.44
302	AS	Te	C	C	C	N	Te	#	0.44
311	AS	Te	C	C	C	O		#	1.14
310	AS	Te	C	C	C	O	As	#	2.38
310	AS	Te	C	C	C	O	B	#	2.38
310	AS	Te	C	C	C	O	P	#	2.38
310	AS	Te	C	C	C	O	Se	#	2.38
310	AS	Te	C	C	C	O	Si	#	2.38
310	AS	Te	C	C	C	O	Te	#	2.38
311	AS	Te	C	C	C	P		#	1.14
311	AS	Te	C	C	C	S		#	1.14
310	AS	Te	C	C	C	S	As	#	2.38
310	AS	Te	C	C	C	S	B	#	2.38
310	AS	Te	C	C	C	S	P	#	2.38
310	AS	Te	C	C	C	S	Se	#	2.38
310	AS	Te	C	C	C	S	Si	#	2.38
310	AS	Te	C	C	C	S	Te	#	2.38
311	AS	Te	C	C	C	Se		#	1.14
311	AS	Te	C	C	C	Si		#	1.14

# Atom Sequences

Screen Number		Fragment Definition						Frequency Percent	
311	AS	Te	C	C	C	Te		#	1.14
331	AS	Te	C	C	Cl			#	1.39
331	AS	Te	C	C	F			#	1.39
331	AS	Te	C	C	I			#	1.39
331	AS	Te	C	C	N			#	1.39
302	AS	Te	C	C	N	As		#	0.44
302	AS	Te	C	C	N	B		#	0.44
302	AS	Te	C	C	N	P		#	0.44
302	AS	Te	C	C	N	Se		#	0.44
302	AS	Te	C	C	N	Si		#	0.44
302	AS	Te	C	C	N	Te		#	0.44
331	AS	Te	C	C	O			#	1.39
310	AS	Te	C	C	O	As		#	2.38
310	AS	Te	C	C	O	B		#	2.38
310	AS	Te	C	C	O	P		#	2.38
310	AS	Te	C	C	O	Se		#	2.38
310	AS	Te	C	C	O	Si		#	2.38
310	AS	Te	C	C	O	Te		#	2.38
331	AS	Te	C	C	P			#	1.39
331	AS	Te	C	C	S			#	1.39
310	AS	Te	C	C	S	As		#	2.38
310	AS	Te	C	C	S	B		#	2.38
310	AS	Te	C	C	S	P		#	2.38
310	AS	Te	C	C	S	Se		#	2.38
310	AS	Te	C	C	S	Si		#	2.38
310	AS	Te	C	C	S	Te		#	2.38
331	AS	Te	C	C	Se			#	1.39
331	AS	Te	C	C	Si			#	1.39
331	AS	Te	C	C	Te			#	1.39
302	AS	Te	N	C	C	As		#	0.44
302	AS	Te	N	C	C	B		#	0.44
302	AS	Te	N	C	C	Br		#	0.44
302	AS	Te	N	C	C	C	As	#	0.44
302	AS	Te	N	C	C	C	B	#	0.44
302	AS	Te	N	C	C	C	Br	#	0.44
302	AS	Te	N	C	C	C	Cl	#	0.44
302	AS	Te	N	C	C	C	F	#	0.44
302	AS	Te	N	C	C	C	I	#	0.44
302	AS	Te	N	C	C	C	N	#	0.44
302	AS	Te	N	C	C	C	O	#	0.44
302	AS	Te	N	C	C	C	P	#	0.44
302	AS	Te	N	C	C	C	S	#	0.44
302	AS	Te	N	C	C	C	Se	#	0.44
302	AS	Te	N	C	C	C	Si	#	0.44
302	AS	Te	N	C	C	C	Te	#	0.44
302	AS	Te	N	C	C	Cl		#	0.44
302	AS	Te	N	C	C	F		#	0.44
302	AS	Te	N	C	C	I		#	0.44
302	AS	Te	N	C	C	N		#	0.44
302	AS	Te	N	C	C	O		#	0.44
302	AS	Te	N	C	C	P		#	0.44
302	AS	Te	N	C	C	S		#	0.44
302	AS	Te	N	C	C	Se		#	0.44
302	AS	Te	N	C	C	Si		#	0.44
302	AS	Te	N	C	C	Te		#	0.44

# Atom Sequences

Screen Number	Fragment Definition						Frequency Percent
310	AS	Te	O	C	C	As	# 2.38
310	AS	Te	O	C	C	B	# 2.38
310	AS	Te	O	C	C	Br	# 2.38
310	AS	Te	O	C	C	C As	# 2.38
310	AS	Te	O	C	C	C B	# 2.38
310	AS	Te	O	C	C	C Br	# 2.38
310	AS	Te	O	C	C	C Cl	# 2.38
310	AS	Te	O	C	C	C F	# 2.38
310	AS	Te	O	C	C	C I	# 2.38
310	AS	Te	O	C	C	C N	# 2.38
310	AS	Te	O	C	C	C O	# 2.38
310	AS	Te	O	C	C	C P	# 2.38
310	AS	Te	O	C	C	C S	# 2.38
310	AS	Te	O	C	C	C Si	# 2.38
310	AS	Te	O	C	C	C Se	# 2.38
310	AS	Te	O	C	C	C Te	# 2.38
310	AS	Te	O	C	C	Cl	# 2.38
310	AS	Te	O	C	C	F	# 2.38
310	AS	Te	O	C	C	I	# 2.38
310	AS	Te	O	C	C	N	# 2.38
310	AS	Te	O	C	C	O	# 2.38
310	AS	Te	O	C	C	P	# 2.38
310	AS	Te	O	C	C	S	# 2.38
310	AS	Te	O	C	C	Se	# 2.38
310	AS	Te	O	C	C	Si	# 2.38
310	AS	Te	O	C	C	Te	# 2.38
310	AS	Te	S	C	C	As	# 2.38
310	AS	Te	S	C	C	B	# 2.38
310	AS	Te	S	C	C	Br	# 2.38
310	AS	Te	S	C	C	C As	# 2.38
310	AS	Te	S	C	C	C B	# 2.38
310	AS	Te	S	C	C	C Br	# 2.38
310	AS	Te	S	C	C	C Cl	# 2.38
310	AS	Te	S	C	C	C F	# 2.38
310	AS	Te	S	C	C	C I	# 2.38
310	AS	Te	S	C	C	C N	# 2.38
310	AS	Te	S	C	C	C O	# 2.38
310	AS	Te	S	C	C	C P	# 2.38
310	AS	Te	S	C	C	C S	# 2.38
310	AS	Te	S	C	C	C Se	# 2.38
310	AS	Te	S	C	C	C Si	# 2.38
310	AS	Te	S	C	C	C Te	# 2.38
310	AS	Te	S	C	C	Cl	# 2.38
310	AS	Te	S	C	C	F	# 2.38
310	AS	Te	S	C	C	I	# 2.38
310	AS	Te	S	C	C	N	# 2.38
310	AS	Te	S	C	C	O	# 2.38
310	AS	Te	S	C	C	P	# 2.38
310	AS	Te	S	C	C	S	# 2.38
310	AS	Te	S	C	C	Se	# 2.38
310	AS	Te	S	C	C	Si	# 2.38
310	AS	Te	S	C	C	Te	# 2.38
310	AS	Te	S	C	C	Cl	# 2.38
310	AS	Te	S	C	C	F	# 2.38
310	AS	Te	S	C	C	I	# 2.38
310	AS	Te	S	C	C	N	# 2.38
310	AS	Te	S	C	C	O	# 2.38
310	AS	Te	S	C	C	P	# 2.38
310	AS	Te	S	C	C	S	# 2.38
310	AS	Te	S	C	C	Se	# 2.38
310	AS	Te	S	C	C	Si	# 2.38
310	AS	Te	S	C	C	Te	# 2.38

# Bond Sequences

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## BS Screens

A **bond sequence (BS)** screen specifies both type and value for the bonds between the string atoms but uses only dummy "A" element symbols to represent the atoms, as in:

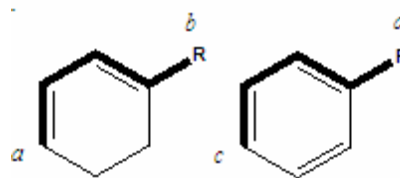
BS    1    A   \*1   A   \*1   A   \*1   A   -2   A

These screens are descriptions of linear sequences of 3, 4, or 5 bonds, always specifying the bond types and often the bond values.

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## BS Screen Definitions

**Note:** bond sequence definitions are exact and do not imply alternative bond specifications. Where tautomer or alternating bonds exist, \*4 and -4 bond symbols must be used in BS descriptions, not the usual "fixed" \*1 and -1 single and \*2 and -2 double bond symbols. Thus, for example, the BS Screen BS A \*2 A \*1 A \*2 A -1 A would Be used to describe the indicated bond Path (*a – b*) in the structure containing a cyclohexadiene ring but not in the structure (*c – d*) containing the benzene ring; the screen BS A \*4 A \*4 A \*4 A -1 A would have to be used to describe the path in that substance.



# Bond Sequences

Screen Number		Fragment Definition	Frequency Percent
795	BS	A * A - A * A	24.19
803	BS	A * A - A * A * A - A	16.99
804	BS	A * A - A * A - A	15.25
805	BS	A * A - A * A - A * A	1.90
811	BS	A * A - A - A * A	20.58
820	BS	A * A - A - A * A - A	11.11
833	BS	A * A - A - A - A * A	16.30
846	BS	A * A - A - A - A - A	49.89
734	BS	A *1A *1A *1A *1A	46.26
744	BS	A *1A *1A *1A *1A *1A	32.33
745	BS	A *1A *1A *1A *1A *2A	11.68
735	BS	A *1A *1A *1A *2A	18.26
736	BS	A *1A *1A *1A *4A	15.85
763	BS	A *1A *1A *1A -1A	43.32
774	BS	A *1A *1A *1A -1A -1A	31.09
775	BS	A *1A *1A *1A -1A -2A	# 15.47
775	BS	A *1A *1A *1A -1A -4A	# 15.47
764	BS	A *1A *1A *1A -2A	# 16.95
764	BS	A *1A *1A *1A -4A	# 16.95
728	BS	A *1A *1A *2A	33.57
746	BS	A *1A *1A *2A *1A *1A	12.39
765	BS	A *1A *1A *2A -1A	# 24.92
729	BS	A *1A *1A *4A	25.91
737	BS	A *1A *1A *4A *1A	23.12
747	BS	A *1A *1A *4A *1A *1A	8.65
765	BS	A *1A *1A *4A -1A	# 24.92
765	BS	A *1A *1A *4A -4A	# 24.92
784	BS	A *1A *1A -1A -1A	38.04
785	BS	A *1A *1A -1A -2A	# 19.91
785	BS	A *1A *1A -1A -4A	# 19.91
786	BS	A *1A *1A -2A -1A	# 4.41
786	BS	A *1A *1A -4A -1A	# 4.41
730	BS	A *1A *4A *1A	23.66
737	BS	A *1A *4A *1A *1A	23.12
738	BS	A *1A *4A *1A *4A	3.11
766	BS	A *1A *4A *1A -1A	# 15.89
766	BS	A *1A *4A *1A -2A	# 15.89
766	BS	A *1A *4A *1A -4A	# 15.89
739	BS	A *1A *4A *4A *1A	5.55
748	BS	A *1A *4A *4A *4A *1A	1.67
753	BS	A *1A *4A *4A *4A -1A	# 11.30
753	BS	A *1A *4A *4A *4A -4A	# 11.30
767	BS	A *1A *4A *4A -1A	# 14.13
776	BS	A *1A *4A *4A -1A -2A	# 3.05
776	BS	A *1A *4A *4A -1A -4A	# 3.05
767	BS	A *1A *4A *4A -4A	# 14.13
787	BS	A *1A *4A -1A -1A	2.71
788	BS	A *1A *4A -1A -2A	# 0.92
788	BS	A *1A *4A -1A -4A	# 0.92
796	BS	A *1A -1A *1A	4.83
797	BS	A *1A -1A *2A	2.29
798	BS	A *1A -1A *4A	17.07
812	BS	A *1A -1A -1A *1A	3.71
813	BS	A *1A -1A -1A *2A	1.34
814	BS	A *1A -1A -1A *4A	8.26



# Bond Sequences

Screen Number		Fragment Definition	Frequency Percent
821	BS	A *1A -1A -1A -1A	# 29.59
834	BS	A *1A -1A -1A -1A *1A	# 9.08
835	BS	A *1A -1A -1A -1A *1A	# 2.29
834	BS	A *1A -1A -1A -1A *2A	# 9.08
836	BS	A *1A -1A -1A -1A *2A	# 1.05
834	BS	A *1A -1A -1A -1A *4A	# 9.08
837	BS	A *1A -1A -1A -1A *4A	# 7.61
847	BS	A *1A -1A -1A -1A -1A	# 19.15
848	BS	A *1A -1A -1A -1A -2A	# 7.95
849	BS	A *1A -1A -1A -1A -3A	# 1.26
848	BS	A *1A -1A -1A -1A -4A	# 7.95
822	BS	A *1A -1A -1A -2A	# 6.54
835	BS	A *1A -1A -1A -2A *1A	# 2.29
838	BS	A *1A -1A -1A -2A *1A	# 0.72
850	BS	A *1A -1A -1A -2A -1A	# 6.05
824	BS	A *1A -1A -1A -3A	# 1.16
823	BS	A *1A -1A -1A -4A	# 3.08
835	BS	A *1A -1A -1A -4A *1A	# 2.29
838	BS	A *1A -1A -1A -4A *1A	# 0.72
838	BS	A *1A -1A -1A -4A *4A	# 0.72
850	BS	A *1A -1A -1A -4A -1A	# 6.05
851	BS	A *1A -1A -1A -4A -4A	# 4.86
815	BS	A *1A -1A -2A *1A	# 1.79
825	BS	A *1A -1A -2A -1A	# 9.84
835	BS	A *1A -1A -2A -1A *1A	# 2.29
839	BS	A *1A -1A -2A -1A *1A	# 3.00
836	BS	A *1A -1A -2A -1A *2A	# 1.05
839	BS	A *1A -1A -2A -1A *2A	# 3.00
837	BS	A *1A -1A -2A -1A *4A	# 7.61
839	BS	A *1A -1A -2A -1A *4A	# 3.00
852	BS	A *1A -1A -2A -1A -1A	# 9.56
853	BS	A *1A -1A -2A -1A -2A	# 3.89
849	BS	A *1A -1A -2A -1A -3A	# 1.26
853	BS	A *1A -1A -2A -1A -4A	# 3.89
806	BS	A *1A -1A -3A	# 3.87
849	BS	A *1A -1A -3A -1A -3A	# 1.26
815	BS	A *1A -1A -4A *1A	# 1.79
815	BS	A *1A -1A -4A *4A	# 1.79
825	BS	A *1A -1A -4A -1A	# 9.84
835	BS	A *1A -1A -4A -1A *1A	# 2.29
840	BS	A *1A -1A -4A -1A *1A	# 3.51
836	BS	A *1A -1A -4A -1A *2A	# 1.05
840	BS	A *1A -1A -4A -1A *2A	# 3.51
837	BS	A *1A -1A -4A -1A *4A	# 7.61
840	BS	A *1A -1A -4A -1A *4A	# 3.51
854	BS	A *1A -1A -4A -1A -1A	# 5.30
855	BS	A *1A -1A -4A -1A -2A	# 1.69
849	BS	A *1A -1A -4A -1A -3A	# 1.26
855	BS	A *1A -1A -4A -1A -4A	# 1.69
826	BS	A *1A -1A -4A -4A	# 3.47
835	BS	A *1A -1A -4A -4A *1A	# 2.29
841	BS	A *1A -1A -4A -4A *1A	# 0.60
837	BS	A *1A -1A -4A -4A *4A	# 7.61
841	BS	A *1A -1A -4A -4A *4A	# 0.60
851	BS	A *1A -1A -4A -4A -1A	# 4.86

# Bond Sequences

Screen Number		Fragment Definition	Frequency Percent
851	BS	A *1A -1A -4A -4A -4A	# 4.86
799	BS	A *1A -2A *1A	# 0.27
815	BS	A *1A -2A -1A *1A	# 1.79
816	BS	A *1A -2A -1A *2A	# 2.34
816	BS	A *1A -2A -1A *4A	# 2.34
835	BS	A *1A -2A -1A -1A *1A	# 2.29
838	BS	A *1A -2A -1A -1A *1A	# 0.72
836	BS	A *1A -2A -1A -1A *2A	# 1.05
838	BS	A *1A -2A -1A -1A *2A	# 0.72
837	BS	A *1A -2A -1A -1A *4A	# 7.61
838	BS	A *1A -2A -1A -1A *4A	# 0.72
854	BS	A *1A -2A -1A -1A -1A	# 5.30
856	BS	A *1A -2A -1A -1A -2A	# 0.24
849	BS	A *1A -2A -1A -1A -3A	# 1.26
856	BS	A *1A -2A -1A -1A -4A	# 0.24
835	BS	A *1A -2A -1A -2A *1A	# 2.29
842	BS	A *1A -2A -1A -2A *1A	# 0.16
857	BS	A *1A -2A -1A -2A -1A	# 0.76
824	BS	A *1A -2A -1A -3A	# 1.16
835	BS	A *1A -2A -1A -4A *1A	# 2.29
842	BS	A *1A -2A -1A -4A *1A	# 0.16
837	BS	A *1A -2A -1A -4A *4A	# 7.61
842	BS	A *1A -2A -1A -4A *4A	# 0.16
857	BS	A *1A -2A -1A -4A -1A	# 0.76
851	BS	A *1A -2A -1A -4A -4A	# 4.86
815	BS	A *1A -4A -1A *1A	# 1.79
816	BS	A *1A -4A -1A *2A	# 2.34
816	BS	A *1A -4A -1A *4A	# 2.34
835	BS	A *1A -4A -1A -1A *1A	# 2.29
838	BS	A *1A -4A -1A -1A *1A	# 0.72
836	BS	A *1A -4A -1A -1A *2A	# 1.05
838	BS	A *1A -4A -1A -1A *2A	# 0.72
837	BS	A *1A -4A -1A -1A *4A	# 7.61
838	BS	A *1A -4A -1A -1A *4A	# 0.72
854	BS	A *1A -4A -1A -1A -1A	# 5.30
856	BS	A *1A -4A -1A -1A -2A	# 0.24
849	BS	A *1A -4A -1A -1A -3A	# 1.26
856	BS	A *1A -4A -1A -1A -4A	# 0.24
835	BS	A *1A -4A -1A -2A *1A	# 2.29
842	BS	A *1A -4A -1A -2A *1A	# 0.16
857	BS	A *1A -4A -1A -2A -1A	# 0.76
824	BS	A *1A -4A -1A -3A	# 1.16
835	BS	A *1A -4A -1A -4A *1A	# 2.29
842	BS	A *1A -4A -1A -4A *1A	# 0.16
837	BS	A *1A -4A -1A -4A *4A	# 7.61
842	BS	A *1A -4A -1A -4A *4A	# 0.16
857	BS	A *1A -4A -1A -4A -1A	# 0.76
851	BS	A *1A -4A -1A -4A -4A	# 4.86
807	BS	A *1A -4A -4A	# 1.54
815	BS	A *1A -4A -4A *1A	# 1.79
815	BS	A *1A -4A -4A *4A	# 1.79
835	BS	A *1A -4A -4A -1A *1A	# 2.29
841	BS	A *1A -4A -4A -1A *1A	# 0.60
836	BS	A *1A -4A -4A -1A *2A	# 1.05
841	BS	A *1A -4A -4A -1A *2A	# 0.60

# Bond Sequences

Screen Number		Fragment Definition						Frequency Percent	
837	BS	A	*1A	-4A	-4A	-1A	*4A	#	7.61
841	BS	A	*1A	-4A	-4A	-1A	*4A	#	0.60
851	BS	A	*1A	-4A	-4A	-1A	-1A	#	4.86
851	BS	A	*1A	-4A	-4A	-1A	-2A	#	4.86
849	BS	A	*1A	-4A	-4A	-1A	-3A	#	1.26
851	BS	A	*1A	-4A	-4A	-1A	-4A	#	4.86
835	BS	A	*1A	-4A	-4A	-4A	*1A	#	2.29
841	BS	A	*1A	-4A	-4A	-4A	*1A	#	0.60
837	BS	A	*1A	-4A	-4A	-4A	*4A	#	7.61
841	BS	A	*1A	-4A	-4A	-4A	*4A	#	0.60
851	BS	A	*1A	-4A	-4A	-4A	-1A	#	4.86
851	BS	A	*1A	-4A	-4A	-4A	-4A	#	4.86
728	BS	A	*2A	*1A	*1A				33.57
735	BS	A	*2A	*1A	*1A	*1A			18.26
745	BS	A	*2A	*1A	*1A	*1A	*1A		11.68
749	BS	A	*2A	*1A	*1A	*1A	*2A		4.86
750	BS	A	*2A	*1A	*1A	*1A	*4A	#	5.71
754	BS	A	*2A	*1A	*1A	*1A	-1A	#	16.45
755	BS	A	*2A	*1A	*1A	*1A	-2A	#	7.52
755	BS	A	*2A	*1A	*1A	*1A	-4A	#	7.52
740	BS	A	*2A	*1A	*1A	*2A			15.67
756	BS	A	*2A	*1A	*1A	*2A	-1A	#	8.46
741	BS	A	*2A	*1A	*1A	*4A			10.64
757	BS	A	*2A	*1A	*1A	*4A	-1A	#	7.07
758	BS	A	*2A	*1A	*1A	*4A	-4A	#	0.97
768	BS	A	*2A	*1A	*1A	-1A		#	26.83
777	BS	A	*2A	*1A	*1A	-1A	-2A	#	4.54
777	BS	A	*2A	*1A	*1A	-1A	-4A	#	4.54
769	BS	A	*2A	*1A	*1A	-2A		#	10.73
769	BS	A	*2A	*1A	*1A	-4A		#	10.73
731	BS	A	*2A	*1A	*2A				14.60
751	BS	A	*2A	*1A	*2A	*1A	*2A		1.80
752	BS	A	*2A	*1A	*2A	*1A	*4A	#	1.61
759	BS	A	*2A	*1A	*2A	*1A	-1A	#	13.23
760	BS	A	*2A	*1A	*2A	*1A	-2A	#	4.14
760	BS	A	*2A	*1A	*2A	*1A	-4A	#	4.14
770	BS	A	*2A	*1A	*2A	-1A		#	17.24
732	BS	A	*2A	*1A	*4A				12.99
752	BS	A	*2A	*1A	*4A	*1A	*2A	#	1.61
752	BS	A	*2A	*1A	*4A	*1A	*4A	#	1.61
759	BS	A	*2A	*1A	*4A	*1A	-1A	#	13.23
760	BS	A	*2A	*1A	*4A	*1A	-2A	#	4.14
760	BS	A	*2A	*1A	*4A	*1A	-4A	#	4.14
761	BS	A	*2A	*1A	*4A	*4A	-1A	#	3.88
762	BS	A	*2A	*1A	*4A	*4A	-4A	#	0.88
770	BS	A	*2A	*1A	*4A	-1A		#	17.24
771	BS	A	*2A	*1A	*4A	-4A		#	3.22
781	BS	A	*2A	*1A	-1A				20.76
789	BS	A	*2A	*1A	-1A	-1A		#	15.32
790	BS	A	*2A	*1A	-1A	-2A		#	6.14
790	BS	A	*2A	*1A	-1A	-4A		#	6.14
782	BS	A	*2A	*1A	-2A				7.00
791	BS	A	*2A	*1A	-2A	-1A		#	2.06
783	BS	A	*2A	*1A	-4A				1.11
791	BS	A	*2A	*1A	-4A	-1A		#	2.06

# Bond Sequences

Screen Number		Fragment Definition	Frequency Percent
797	BS	A *2A -1A *1A	2.29
800	BS	A *2A -1A *2A	0.82
801	BS	A *2A -1A *4A	6.81
808	BS	A *2A -1A -1A	# 14.59
813	BS	A *2A -1A -1A *1A	1.34
817	BS	A *2A -1A -1A *2A	0.35
818	BS	A *2A -1A -1A *4A	1.80
821	BS	A *2A -1A -1A -1A	# 29.59
834	BS	A *2A -1A -1A -1A *1A	# 9.08
836	BS	A *2A -1A -1A -1A *1A	# 1.05
834	BS	A *2A -1A -1A -1A *2A	# 9.08
843	BS	A *2A -1A -1A -1A *2A	# 0.38
834	BS	A *2A -1A -1A -1A *4A	# 9.08
844	BS	A *2A -1A -1A -1A *4A	# 2.50
847	BS	A *2A -1A -1A -1A -1A	# 19.15
848	BS	A *2A -1A -1A -1A -2A	# 7.95
849	BS	A *2A -1A -1A -1A -3A	# 1.26
848	BS	A *2A -1A -1A -1A -4A	# 7.95
822	BS	A *2A -1A -1A -2A	# 6.54
836	BS	A *2A -1A -1A -2A *1A	# 1.05
838	BS	A *2A -1A -1A -2A *1A	# 0.72
850	BS	A *2A -1A -1A -2A -1A	# 6.05
824	BS	A *2A -1A -1A -3A	# 1.16
823	BS	A *2A -1A -1A -4A	# 3.08
836	BS	A *2A -1A -1A -4A *1A	# 1.05
838	BS	A *2A -1A -1A -4A *1A	# 0.72
838	BS	A *2A -1A -1A -4A *4A	# 0.72
844	BS	A *2A -1A -1A -4A *4A	# 2.50
850	BS	A *2A -1A -1A -4A -1A	# 6.05
851	BS	A *2A -1A -1A -4A -4A	# 4.86
809	BS	A *2A -1A -2A	# 8.95
816	BS	A *2A -1A -2A *1A	# 2.34
825	BS	A *2A -1A -2A -1A	# 9.84
836	BS	A *2A -1A -2A -1A *1A	# 1.05
839	BS	A *2A -1A -2A -1A *1A	# 3.00
839	BS	A *2A -1A -2A -1A *2A	# 3.00
843	BS	A *2A -1A -2A -1A *2A	# 0.38
839	BS	A *2A -1A -2A -1A *4A	# 3.00
844	BS	A *2A -1A -2A -1A *4A	# 2.50
852	BS	A *2A -1A -2A -1A -1A	# 9.56
853	BS	A *2A -1A -2A -1A -2A	# 3.89
849	BS	A *2A -1A -2A -1A -3A	# 1.26
853	BS	A *2A -1A -2A -1A -4A	# 3.89
806	BS	A *2A -1A -3A	# 3.87
849	BS	A *2A -1A -3A -1A -3A	# 1.26
809	BS	A *2A -1A -4A	# 8.95
816	BS	A *2A -1A -4A *1A	# 2.34
815	BS	A *2A -1A -4A *4A	# 1.79
825	BS	A *2A -1A -4A -1A	# 9.84
836	BS	A *2A -1A -4A -1A *1A	# 1.05
840	BS	A *2A -1A -4A -1A *1A	# 3.51
840	BS	A *2A -1A -4A -1A *2A	# 3.51
843	BS	A *2A -1A -4A -1A *2A	# 0.38
840	BS	A *2A -1A -4A -1A *4A	# 3.51
844	BS	A *2A -1A -4A -1A *4A	# 2.50

# Bond Sequences

Screen Number		Fragment Definition						Frequency Percent	
852	BS	A	*2A	-1A	-4A	-1A	-1A	#	9.56
855	BS	A	*2A	-1A	-4A	-1A	-2A	#	1.69
849	BS	A	*2A	-1A	-4A	-1A	-3A	#	1.26
855	BS	A	*2A	-1A	-4A	-1A	-4A	#	1.69
826	BS	A	*2A	-1A	-4A	-4A		#	3.47
836	BS	A	*2A	-1A	-4A	-4A	*1A	#	1.05
841	BS	A	*2A	-1A	-4A	-4A	*1A	#	0.60
841	BS	A	*2A	-1A	-4A	-4A	*4A	#	0.60
844	BS	A	*2A	-1A	-4A	-4A	*4A	#	2.50
851	BS	A	*2A	-1A	-4A	-4A	-1A	#	4.86
851	BS	A	*2A	-1A	-4A	-4A	-4A	#	4.86
729	BS	A	*4A	*1A	*1A				25.91
736	BS	A	*4A	*1A	*1A	*1A			15.85
750	BS	A	*4A	*1A	*1A	*1A	*2A	#	5.71
750	BS	A	*4A	*1A	*1A	*1A	*4A	#	5.71
754	BS	A	*4A	*1A	*1A	*1A	-1A	#	16.45
755	BS	A	*4A	*1A	*1A	*1A	-2A	#	7.52
755	BS	A	*4A	*1A	*1A	*1A	-4A	#	7.52
741	BS	A	*4A	*1A	*1A	*2A			10.64
757	BS	A	*4A	*1A	*1A	*2A	-1A	#	7.07
742	BS	A	*4A	*1A	*1A	*4A			5.18
757	BS	A	*4A	*1A	*1A	*4A	-1A	#	7.07
758	BS	A	*4A	*1A	*1A	*4A	-4A	#	0.97
768	BS	A	*4A	*1A	*1A	-1A		#	26.83
778	BS	A	*4A	*1A	*1A	-1A	-2A	#	2.25
778	BS	A	*4A	*1A	*1A	-1A	-4A	#	2.25
769	BS	A	*4A	*1A	*1A	-2A		#	10.73
769	BS	A	*4A	*1A	*1A	-4A		#	10.73
732	BS	A	*4A	*1A	*2A				12.99
752	BS	A	*4A	*1A	*2A	*1A	*2A	#	1.61
752	BS	A	*4A	*1A	*2A	*1A	*4A	#	1.61
759	BS	A	*4A	*1A	*2A	*1A	-1A	#	13.23
760	BS	A	*4A	*1A	*2A	*1A	-2A	#	4.14
760	BS	A	*4A	*1A	*2A	*1A	-4A	#	4.14
770	BS	A	*4A	*1A	*2A	-1A		#	17.24
779	BS	A	*4A	*1A	*2A	-1A	-2A	#	1.43
779	BS	A	*4A	*1A	*2A	-1A	-4A	#	1.43
733	BS	A	*4A	*1A	*4A				3.43
738	BS	A	*4A	*1A	*4A	*1A			3.11
752	BS	A	*4A	*1A	*4A	*1A	*2A	#	1.61
752	BS	A	*4A	*1A	*4A	*1A	*4A	#	1.61
759	BS	A	*4A	*1A	*4A	*1A	-1A	#	13.23
760	BS	A	*4A	*1A	*4A	*1A	-2A	#	4.14
760	BS	A	*4A	*1A	*4A	*1A	-4A	#	4.14
761	BS	A	*4A	*1A	*4A	*4A	-1A	#	3.88
762	BS	A	*4A	*1A	*4A	*4A	-4A	#	0.88
770	BS	A	*4A	*1A	*4A	-1A		#	17.24
780	BS	A	*4A	*1A	*4A	-1A	-2A	#	0.18
780	BS	A	*4A	*1A	*4A	-1A	-4A	#	0.18
771	BS	A	*4A	*1A	*4A	-4A		#	3.22
789	BS	A	*4A	*1A	-1A	-1A		#	15.32
790	BS	A	*4A	*1A	-1A	-2A		#	6.14
790	BS	A	*4A	*1A	-1A	-4A		#	6.14
791	BS	A	*4A	*1A	-2A	-1A		#	2.06
791	BS	A	*4A	*1A	-4A	-1A		#	2.06

# Bond Sequences

Screen Number		Fragment Definition	Frequency Percent
772	BS	A *4A *4A *1A -1A	12.57
773	BS	A *4A *4A *1A -2A	# 5.73
773	BS	A *4A *4A *1A -4A	# 5.73
743	BS	A *4A *4A *4A *4A	70.68
792	BS	A *4A *4A -1A -1A	50.44
793	BS	A *4A *4A -1A -2A	21.99
794	BS	A *4A *4A -1A -4A	14.39
798	BS	A *4A -1A *1A	17.07
801	BS	A *4A -1A *2A	6.81
802	BS	A *4A -1A *4A	4.33
814	BS	A *4A -1A -1A *1A	8.26
818	BS	A *4A -1A -1A *2A	1.80
819	BS	A *4A -1A -1A *4A	7.50
827	BS	A *4A -1A -1A -1A	32.93
834	BS	A *4A -1A -1A -1A *1A	# 9.08
837	BS	A *4A -1A -1A -1A *1A	# 7.61
834	BS	A *4A -1A -1A -1A *2A	# 9.08
844	BS	A *4A -1A -1A -1A *2A	# 2.50
834	BS	A *4A -1A -1A -1A *4A	# 9.08
845	BS	A *4A -1A -1A -1A *4A	# 7.44
858	BS	A *4A -1A -1A -1A -1A	19.79
859	BS	A *4A -1A -1A -1A -2A	# 10.42
849	BS	A *4A -1A -1A -1A -3A	# 1.26
859	BS	A *4A -1A -1A -1A -4A	# 10.42
828	BS	A *4A -1A -1A -2A	6.41
837	BS	A *4A -1A -1A -2A *1A	# 7.61
838	BS	A *4A -1A -1A -2A *1A	# 0.72
850	BS	A *4A -1A -1A -2A -1A	# 6.05
824	BS	A *4A -1A -1A -3A	# 1.16
829	BS	A *4A -1A -1A -4A	3.12
837	BS	A *4A -1A -1A -4A *1A	# 7.61
838	BS	A *4A -1A -1A -4A *1A	# 0.72
838	BS	A *4A -1A -1A -4A *4A	# 0.72
845	BS	A *4A -1A -1A -4A *4A	# 7.44
850	BS	A *4A -1A -1A -4A -1A	# 6.05
851	BS	A *4A -1A -1A -4A -4A	# 4.86
816	BS	A *4A -1A -2A *1A	# 2.34
830	BS	A *4A -1A -2A -1A	7.09
837	BS	A *4A -1A -2A -1A *1A	# 7.61
839	BS	A *4A -1A -2A -1A *1A	# 3.00
839	BS	A *4A -1A -2A -1A *2A	# 3.00
844	BS	A *4A -1A -2A -1A *2A	# 2.50
839	BS	A *4A -1A -2A -1A *4A	# 3.00
845	BS	A *4A -1A -2A -1A *4A	# 7.44
852	BS	A *4A -1A -2A -1A -1A	# 9.56
853	BS	A *4A -1A -2A -1A -2A	# 3.89
849	BS	A *4A -1A -2A -1A -3A	# 1.26
853	BS	A *4A -1A -2A -1A -4A	# 3.89
806	BS	A *4A -1A -3A	# 3.87
849	BS	A *4A -1A -3A -1A -3A	# 1.26
816	BS	A *4A -1A -4A *1A	# 2.34
815	BS	A *4A -1A -4A *4A	# 1.79
831	BS	A *4A -1A -4A -1A	9.50
837	BS	A *4A -1A -4A -1A *1A	# 7.61
840	BS	A *4A -1A -4A -1A *1A	# 3.51

# Bond Sequences

Screen Number		Fragment Definition					Frequency Percent
840	BS	A	*4A	-1A	-4A	-1A *2A	# 3.51
844	BS	A	*4A	-1A	-4A	-1A *2A	# 2.50
840	BS	A	*4A	-1A	-4A	-1A *4A	# 3.51
845	BS	A	*4A	-1A	-4A	-1A *4A	# 7.44
852	BS	A	*4A	-1A	-4A	-1A -1A	# 9.56
855	BS	A	*4A	-1A	-4A	-1A -2A	# 1.69
849	BS	A	*4A	-1A	-4A	-1A -3A	# 1.26
855	BS	A	*4A	-1A	-4A	-1A -4A	# 1.69
832	BS	A	*4A	-1A	-4A	-4A	# 8.33
837	BS	A	*4A	-1A	-4A	-4A *1A	# 7.61
841	BS	A	*4A	-1A	-4A	-4A *1A	# 0.60
841	BS	A	*4A	-1A	-4A	-4A *4A	# 0.60
845	BS	A	*4A	-1A	-4A	-4A *4A	# 7.44
851	BS	A	*4A	-1A	-4A	-4A -1A	# 4.86
851	BS	A	*4A	-1A	-4A	-4A	# 4.86
810	BS	A	*4A	-4A	-1A		# 2.32
815	BS	A	*4A	-4A	-1A	*1A	# 1.79
815	BS	A	*4A	-4A	-1A	*2A	# 1.79
815	BS	A	*4A	-4A	-1A	*4A	# 1.79
838	BS	A	*4A	-4A	-1A	-1A *1A	# 0.72
838	BS	A	*4A	-4A	-1A	-1A *2A	# 0.72
844	BS	A	*4A	-4A	-1A	-1A *2A	# 2.50
838	BS	A	*4A	-4A	-1A	-1A *4A	# 0.72
845	BS	A	*4A	-4A	-1A	-1A *4A	# 7.44
854	BS	A	*4A	-4A	-1A	-1A -1A	# 5.30
856	BS	A	*4A	-4A	-1A	-1A -2A	# 0.24
849	BS	A	*4A	-4A	-1A	-1A -3A	# 1.26
856	BS	A	*4A	-4A	-1A	-1A -4A	# 0.24
837	BS	A	*4A	-4A	-1A	-2A *1A	# 7.61
842	BS	A	*4A	-4A	-1A	-2A *1A	# 0.16
857	BS	A	*4A	-4A	-1A	-2A -1A	# 0.76
824	BS	A	*4A	-4A	-1A	-3A	# 1.16
837	BS	A	*4A	-4A	-1A	-4A *1A	# 7.61
842	BS	A	*4A	-4A	-1A	-4A *1A	# 0.16
842	BS	A	*4A	-4A	-1A	-4A *4A	# 0.16
845	BS	A	*4A	-4A	-1A	-4A *4A	# 7.44
857	BS	A	*4A	-4A	-1A	-4A -1A	# 0.76
851	BS	A	*4A	-4A	-1A	-4A -4A	# 4.86
807	BS	A	*4A	-4A	-4A		# 1.54
815	BS	A	*4A	-4A	-4A	*1A	# 1.79
815	BS	A	*4A	-4A	-4A	*4A	# 1.79
837	BS	A	*4A	-4A	-4A	-1A *1A	# 7.61
841	BS	A	*4A	-4A	-4A	-1A *1A	# 0.60
841	BS	A	*4A	-4A	-4A	-1A *2A	# 0.60
844	BS	A	*4A	-4A	-4A	-1A *2A	# 2.50
841	BS	A	*4A	-4A	-4A	-1A *4A	# 0.60
845	BS	A	*4A	-4A	-4A	-1A *4A	# 7.44
851	BS	A	*4A	-4A	-4A	-1A -1A	# 4.86
851	BS	A	*4A	-4A	-4A	-1A -2A	# 4.86
849	BS	A	*4A	-4A	-4A	-1A -3A	# 1.26
851	BS	A	*4A	-4A	-4A	-1A -4A	# 4.86
837	BS	A	*4A	-4A	-4A	-4A *1A	# 7.61
841	BS	A	*4A	-4A	-4A	-4A *1A	# 0.60
841	BS	A	*4A	-4A	-4A	-4A *4A	# 0.60
845	BS	A	*4A	-4A	-4A	-4A *4A	# 7.44

# Bond Sequences

Screen Number		Fragment Definition	Frequency Percent
851	BS	A *4A -4A -4A -4A -1A	# 4.86
851	BS	A *4A -4A -4A -4A -4A	# 4.86
860	BS	A - A * A * A * A - A	60.97
872	BS	A - A * A * A - A	53.81
803	BS	A - A * A * A - A * A	16.99
884	BS	A - A * A - A	52.87
804	BS	A - A * A - A * A	15.25
893	BS	A - A * A - A * A - A	2.80
820	BS	A - A * A - A - A * A	11.11
846	BS	A - A - A - A - A * A	49.89
926	BS	A - A - A - A - A - A	44.76
763	BS	A -1A *1A *1A *1A	43.32
754	BS	A -1A *1A *1A *1A *2A	# 16.45
754	BS	A -1A *1A *1A *1A *4A	# 16.45
861	BS	A -1A *1A *1A *1A -1A	18.92
862	BS	A -1A *1A *1A *1A -2A	7.82
863	BS	A -1A *1A *1A *1A -4A	0.85
768	BS	A -1A *1A *1A *2A	# 26.83
864	BS	A -1A *1A *1A *2A -1A	# 14.38
768	BS	A -1A *1A *1A *4A	# 26.83
865	BS	A -1A *1A *1A *4A -1A	# 5.70
866	BS	A -1A *1A *1A *4A -4A	# 3.89
873	BS	A -1A *1A *1A -1A	20.93
874	BS	A -1A *1A *1A -2A	# 12.22
875	BS	A -1A *1A *1A -4A	# 2.85
781	BS	A -1A *1A *2A	20.76
759	BS	A -1A *1A *2A *1A *2A	# 13.23
759	BS	A -1A *1A *2A *1A *4A	# 13.23
865	BS	A -1A *1A *2A *1A -1A	# 5.70
867	BS	A -1A *1A *2A *1A -2A	# 7.30
866	BS	A -1A *1A *2A *1A -4A	# 3.89
876	BS	A -1A *1A *2A -1A	# 10.85
766	BS	A -1A *1A *4A *1A	# 15.89
759	BS	A -1A *1A *4A *1A *2A	# 13.23
759	BS	A -1A *1A *4A *1A *4A	# 13.23
864	BS	A -1A *1A *4A *1A -1A	# 14.38
867	BS	A -1A *1A *4A *1A -2A	# 7.30
866	BS	A -1A *1A *4A *1A -4A	# 3.89
772	BS	A -1A *1A *4A *4A	12.57
864	BS	A -1A *1A *4A *4A -1A	# 14.38
866	BS	A -1A *1A *4A *4A -4A	# 3.89
876	BS	A -1A *1A *4A -1A	# 10.85
875	BS	A -1A *1A *4A -4A	# 2.85
885	BS	A -1A *1A -1A	23.45
886	BS	A -1A *1A -2A	14.04
887	BS	A -1A *1A -4A	2.47
765	BS	A -1A *2A *1A *1A	# 24.92
756	BS	A -1A *2A *1A *1A *2A	# 8.46
757	BS	A -1A *2A *1A *1A *4A	# 7.07
864	BS	A -1A *2A *1A *1A -1A	# 14.38
867	BS	A -1A *2A *1A *1A -2A	# 7.30
866	BS	A -1A *2A *1A *1A -4A	# 3.89
770	BS	A -1A *2A *1A *2A	# 17.24
864	BS	A -1A *2A *1A *2A -1A	# 14.38
770	BS	A -1A *2A *1A *4A	# 17.24



# Bond Sequences

Screen Number		Fragment Definition	Frequency Percent
864	BS	A -1A *2A *1A *4A -1A	# 14.38
866	BS	A -1A *2A *1A *4A -4A	# 3.89
876	BS	A -1A *2A *1A -1A	# 10.85
874	BS	A -1A *2A *1A -2A	# 12.22
875	BS	A -1A *2A *1A -4A	# 2.85
888	BS	A -1A *2A -1A	8.13
765	BS	A -1A *4A *1A *1A	# 24.92
757	BS	A -1A *4A *1A *1A *2A	# 7.07
757	BS	A -1A *4A *1A *1A *4A	# 7.07
865	BS	A -1A *4A *1A *1A -1A	# 5.70
867	BS	A -1A *4A *1A *1A -2A	# 7.30
866	BS	A -1A *4A *1A *1A -4A	# 3.89
770	BS	A -1A *4A *1A *2A	# 17.24
864	BS	A -1A *4A *1A *2A -1A	# 14.38
770	BS	A -1A *4A *1A *4A	# 17.24
864	BS	A -1A *4A *1A *4A -1A	# 14.38
866	BS	A -1A *4A *1A *4A -4A	# 3.89
876	BS	A -1A *4A *1A -1A	# 10.85
874	BS	A -1A *4A *1A -2A	# 12.22
875	BS	A -1A *4A *1A -4A	# 2.85
767	BS	A -1A *4A *4A *1A	# 14.13
761	BS	A -1A *4A *4A *1A *2A	# 3.88
761	BS	A -1A *4A *4A *1A *4A	# 3.88
864	BS	A -1A *4A *4A *1A -1A	# 14.38
867	BS	A -1A *4A *4A *1A -2A	# 7.30
866	BS	A -1A *4A *4A *1A -4A	# 3.89
753	BS	A -1A *4A *4A *4A *1A	# 11.30
868	BS	A -1A *4A *4A *4A -1A	35.57
869	BS	A -1A *4A *4A *4A -4A	0.88
877	BS	A -1A *4A *4A -1A	25.09
881	BS	A -1A *4A *4A -1A -1A	15.57
882	BS	A -1A *4A *4A -1A -2A	7.58
883	BS	A -1A *4A *4A -1A -4A	5.64
878	BS	A -1A *4A *4A -4A	2.01
889	BS	A -1A *4A -1A	24.67
894	BS	A -1A *4A -1A -1A	16.03
895	BS	A -1A *4A -1A -2A	7.01
896	BS	A -1A *4A -1A -4A	5.42
890	BS	A -1A *4A -4A	0.92
784	BS	A -1A -1A *1A *1A	38.04
774	BS	A -1A -1A *1A *1A *1A	31.09
789	BS	A -1A -1A *1A *2A	# 15.32
789	BS	A -1A -1A *1A *4A	# 15.32
808	BS	A -1A -1A *2A	# 14.59
787	BS	A -1A -1A *4A *1A	2.71
792	BS	A -1A -1A *4A *4A	50.44
881	BS	A -1A -1A *4A *4A -1A	15.57
894	BS	A -1A -1A *4A -1A	16.03
897	BS	A -1A -1A *4A -1A -1A	5.51
898	BS	A -1A -1A *4A -1A -2A	# 4.41
898	BS	A -1A -1A *4A -1A -4A	# 4.41
821	BS	A -1A -1A -1A *1A	# 29.59
821	BS	A -1A -1A -1A *2A	# 29.59
827	BS	A -1A -1A -1A *4A	32.93
915	BS	A -1A -1A -1A -1A	45.77

# Bond Sequences

Screen Number		Fragment Definition	Frequency Percent
847	BS	A -1A -1A -1A -1A *1A	# 19.15
847	BS	A -1A -1A -1A -1A *2A	# 19.15
858	BS	A -1A -1A -1A -1A *4A	19.79
927	BS	A -1A -1A -1A -1A -1A	30.55
928	BS	A -1A -1A -1A -1A -2A	# 24.95
928	BS	A -1A -1A -1A -1A -3A	# 24.95
928	BS	A -1A -1A -1A -1A -4A	# 24.95
916	BS	A -1A -1A -1A -2A	26.16
854	BS	A -1A -1A -1A -2A *1A	# 5.30
929	BS	A -1A -1A -1A -2A -1A	# 18.34
918	BS	A -1A -1A -1A -3A	2.42
929	BS	A -1A -1A -1A -3A -1A	# 18.34
917	BS	A -1A -1A -1A -4A	18.40
854	BS	A -1A -1A -1A -4A *1A	# 5.30
854	BS	A -1A -1A -1A -4A *4A	# 5.30
929	BS	A -1A -1A -1A -4A -1A	# 18.34
930	BS	A -1A -1A -1A -4A -4A	9.93
900	BS	A -1A -1A -2A	36.03
919	BS	A -1A -1A -2A -1A	# 23.74
852	BS	A -1A -1A -2A -1A *1A	# 9.56
852	BS	A -1A -1A -2A -1A *2A	# 9.56
852	BS	A -1A -1A -2A -1A *4A	# 9.56
931	BS	A -1A -1A -2A -1A -1A	# 10.49
902	BS	A -1A -1A -3A	4.52
919	BS	A -1A -1A -3A -1A	# 23.74
931	BS	A -1A -1A -3A -1A -1A	# 10.49
901	BS	A -1A -1A -4A	23.62
919	BS	A -1A -1A -4A -1A	# 23.74
854	BS	A -1A -1A -4A -1A *1A	# 5.30
852	BS	A -1A -1A -4A -1A *2A	# 9.56
852	BS	A -1A -1A -4A -1A *4A	# 9.56
931	BS	A -1A -1A -4A -1A -1A	# 10.49
920	BS	A -1A -1A -4A -4A	12.63
851	BS	A -1A -1A -4A -4A *1A	# 4.86
851	BS	A -1A -1A -4A -4A *4A	# 4.86
786	BS	A -1A -2A *1A *1A	# 4.41
791	BS	A -1A -2A *1A *2A	# 2.06
791	BS	A -1A -2A *1A *4A	# 2.06
903	BS	A -1A -2A -1A	13.44
825	BS	A -1A -2A -1A *1A	# 9.84
825	BS	A -1A -2A -1A *2A	# 9.84
830	BS	A -1A -2A -1A *4A	7.09
919	BS	A -1A -2A -1A -1A	# 23.74
850	BS	A -1A -2A -1A -1A *1A	# 6.05
850	BS	A -1A -2A -1A -1A *2A	# 6.05
850	BS	A -1A -2A -1A -1A *4A	# 6.05
929	BS	A -1A -2A -1A -1A -1A	# 18.34
921	BS	A -1A -2A -1A -2A	# 7.65
857	BS	A -1A -2A -1A -2A *1A	# 0.76
932	BS	A -1A -2A -1A -2A -1A	# 3.30
921	BS	A -1A -2A -1A -3A	# 7.65
932	BS	A -1A -2A -1A -3A -1A	# 3.30
921	BS	A -1A -2A -1A -4A	# 7.65
857	BS	A -1A -2A -1A -4A *1A	# 0.76
857	BS	A -1A -2A -1A -4A *4A	# 0.76

# Bond Sequences

Screen Number		Fragment Definition	Frequency Percent
932	BS	A -1A -2A -1A -4A -1A	# 3.30
904	BS	A -1A -2A -2A	1.23
907	BS	A -1A -3A -1A	1.31
919	BS	A -1A -3A -1A -1A	# 23.74
929	BS	A -1A -3A -1A -1A -1A	# 18.34
921	BS	A -1A -3A -1A -2A	# 7.65
932	BS	A -1A -3A -1A -2A -1A	# 3.30
921	BS	A -1A -3A -1A -3A	# 7.65
932	BS	A -1A -3A -1A -3A -1A	# 3.30
921	BS	A -1A -3A -1A -4A	# 7.65
932	BS	A -1A -3A -1A -4A -1A	# 3.30
786	BS	A -1A -4A *1A *1A	# 4.41
791	BS	A -1A -4A *1A *2A	# 2.06
791	BS	A -1A -4A *1A *4A	# 2.06
810	BS	A -1A -4A *4A	2.32
905	BS	A -1A -4A -1A	20.88
825	BS	A -1A -4A -1A *1A	# 9.84
825	BS	A -1A -4A -1A *2A	# 9.84
831	BS	A -1A -4A -1A *4A	9.50
919	BS	A -1A -4A -1A -1A	# 23.74
850	BS	A -1A -4A -1A -1A *1A	# 6.05
850	BS	A -1A -4A -1A -1A *2A	# 6.05
850	BS	A -1A -4A -1A -1A *4A	# 6.05
929	BS	A -1A -4A -1A -1A -1A	# 18.34
921	BS	A -1A -4A -1A -2A	# 7.65
857	BS	A -1A -4A -1A -2A *1A	# 0.76
932	BS	A -1A -4A -1A -2A -1A	# 3.30
921	BS	A -1A -4A -1A -3A	# 7.65
932	BS	A -1A -4A -1A -3A -1A	# 3.30
921	BS	A -1A -4A -1A -4A	# 7.65
857	BS	A -1A -4A -1A -4A *1A	# 0.76
857	BS	A -1A -4A -1A -4A *4A	# 0.76
932	BS	A -1A -4A -1A -4A -1A	# 3.30
906	BS	A -1A -4A -4A	23.99
922	BS	A -1A -4A -4A -1A	# 2.48
851	BS	A -1A -4A -4A -1A *1A	# 4.86
851	BS	A -1A -4A -4A -1A *2A	# 4.86
851	BS	A -1A -4A -4A -1A *4A	# 4.86
922	BS	A -1A -4A -4A -4A	# 2.48
851	BS	A -1A -4A -4A -4A *1A	# 4.86
851	BS	A -1A -4A -4A -4A *4A	# 4.86
764	BS	A -2A *1A *1A *1A	# 16.95
755	BS	A -2A *1A *1A *1A *2A	# 7.52
755	BS	A -2A *1A *1A *1A *4A	# 7.52
862	BS	A -2A *1A *1A *1A -1A	7.82
870	BS	A -2A *1A *1A *1A -2A	# 3.88
871	BS	A -2A *1A *1A *1A -4A	# 1.29
769	BS	A -2A *1A *1A *2A	# 10.73
867	BS	A -2A *1A *1A *2A -1A	# 7.30
769	BS	A -2A *1A *1A *4A	# 10.73
867	BS	A -2A *1A *1A *4A -1A	# 7.30
871	BS	A -2A *1A *1A *4A -4A	# 1.29
874	BS	A -2A *1A *1A -1A	# 12.22
879	BS	A -2A *1A *1A -2A	3.77
880	BS	A -2A *1A *1A -4A	# 2.69

# Bond Sequences

Screen Number		Fragment Definition	Frequency Percent
782	BS	A -2A *1A *2A	7.00
760	BS	A -2A *1A *2A *1A *2A	# 4.14
760	BS	A -2A *1A *2A *1A *4A	# 4.14
867	BS	A -2A *1A *2A *1A -1A	# 7.30
870	BS	A -2A *1A *2A *1A -2A	# 3.88
871	BS	A -2A *1A *2A *1A -4A	# 1.29
874	BS	A -2A *1A *2A -1A	# 12.22
766	BS	A -2A *1A *4A *1A	# 15.89
760	BS	A -2A *1A *4A *1A *2A	# 4.14
760	BS	A -2A *1A *4A *1A *4A	# 4.14
867	BS	A -2A *1A *4A *1A -1A	# 7.30
870	BS	A -2A *1A *4A *1A -2A	# 3.88
871	BS	A -2A *1A *4A *1A -4A	# 1.29
773	BS	A -2A *1A *4A *4A	# 5.73
867	BS	A -2A *1A *4A *4A -1A	# 7.30
871	BS	A -2A *1A *4A *4A -4A	# 1.29
874	BS	A -2A *1A *4A -1A	# 12.22
880	BS	A -2A *1A *4A -4A	# 2.69
886	BS	A -2A *1A -1A	14.04
891	BS	A -2A *1A -2A	1.95
892	BS	A -2A *1A -4A	# 0.54
785	BS	A -2A -1A *1A *1A	# 19.91
775	BS	A -2A -1A *1A *1A *1A	# 15.47
777	BS	A -2A -1A *1A *1A *2A	# 4.54
778	BS	A -2A -1A *1A *1A *4A	# 2.25
790	BS	A -2A -1A *1A *2A	# 6.14
790	BS	A -2A -1A *1A *4A	# 6.14
809	BS	A -2A -1A *2A	# 8.95
779	BS	A -2A -1A *2A *1A *4A	# 1.43
788	BS	A -2A -1A *4A *1A	# 0.92
780	BS	A -2A -1A *4A *1A *4A	# 0.18
793	BS	A -2A -1A *4A *4A	21.99
776	BS	A -2A -1A *4A *4A *1A	# 3.05
882	BS	A -2A -1A *4A *4A -1A	7.58
895	BS	A -2A -1A *4A -1A	7.01
898	BS	A -2A -1A *4A -1A -1A	# 4.41
899	BS	A -2A -1A *4A -1A -2A	# 1.55
899	BS	A -2A -1A *4A -1A -4A	# 1.55
900	BS	A -2A -1A -1A	36.03
822	BS	A -2A -1A -1A *1A	# 6.54
822	BS	A -2A -1A -1A *2A	# 6.54
828	BS	A -2A -1A -1A *4A	6.41
916	BS	A -2A -1A -1A -1A	26.16
848	BS	A -2A -1A -1A -1A *1A	# 7.95
848	BS	A -2A -1A -1A -1A *2A	# 7.95
859	BS	A -2A -1A -1A -1A *4A	# 10.42
928	BS	A -2A -1A -1A -1A -1A	# 24.95
933	BS	A -2A -1A -1A -1A -2A	# 6.75
933	BS	A -2A -1A -1A -1A -3A	# 6.75
933	BS	A -2A -1A -1A -1A -4A	# 6.75
923	BS	A -2A -1A -1A -2A	# 9.54
856	BS	A -2A -1A -1A -2A *1A	# 0.24
924	BS	A -2A -1A -1A -3A	# 1.72
923	BS	A -2A -1A -1A -4A	# 9.54
856	BS	A -2A -1A -1A -4A *1A	# 0.24

# Bond Sequences

Screen Number		Fragment Definition	Frequency Percent
856	BS	A -2A -1A -1A -4A *4A	# 0.24
908	BS	A -2A -1A -2A	5.38
921	BS	A -2A -1A -2A -1A	# 7.65
853	BS	A -2A -1A -2A -1A *1A	# 3.89
853	BS	A -2A -1A -2A -1A *2A	# 3.89
853	BS	A -2A -1A -2A -1A *4A	# 3.89
934	BS	A -2A -1A -2A -1A -2A	# 1.22
934	BS	A -2A -1A -2A -1A -3A	# 1.22
934	BS	A -2A -1A -2A -1A -4A	# 1.22
910	BS	A -2A -1A -3A	1.19
921	BS	A -2A -1A -3A -1A	# 7.65
934	BS	A -2A -1A -3A -1A -2A	# 1.22
934	BS	A -2A -1A -3A -1A -3A	# 1.22
934	BS	A -2A -1A -3A -1A -4A	# 1.22
909	BS	A -2A -1A -4A	4.21
921	BS	A -2A -1A -4A -1A	# 7.65
855	BS	A -2A -1A -4A -1A *1A	# 1.69
855	BS	A -2A -1A -4A -1A *2A	# 1.69
855	BS	A -2A -1A -4A -1A *4A	# 1.69
934	BS	A -2A -1A -4A -1A -2A	# 1.22
934	BS	A -2A -1A -4A -1A -3A	# 1.22
934	BS	A -2A -1A -4A -1A -4A	# 1.22
925	BS	A -2A -1A -4A -4A	# 3.29
851	BS	A -2A -1A -4A -4A *1A	# 4.86
851	BS	A -2A -1A -4A -4A *4A	# 4.86
904	BS	A -2A -2A -1A	1.23
806	BS	A -3A -1A *1A	# 3.87
806	BS	A -3A -1A *2A	# 3.87
806	BS	A -3A -1A *4A	# 3.87
902	BS	A -3A -1A -1A	4.52
824	BS	A -3A -1A -1A *1A	# 1.16
824	BS	A -3A -1A -1A *2A	# 1.16
824	BS	A -3A -1A -1A *4A	# 1.16
918	BS	A -3A -1A -1A -1A	2.42
849	BS	A -3A -1A -1A -1A *1A	# 1.26
849	BS	A -3A -1A -1A -1A *2A	# 1.26
849	BS	A -3A -1A -1A -1A *4A	# 1.26
928	BS	A -3A -1A -1A -1A -1A	# 24.95
933	BS	A -3A -1A -1A -1A -2A	# 6.75
933	BS	A -3A -1A -1A -1A -3A	# 6.75
933	BS	A -3A -1A -1A -1A -4A	# 6.75
924	BS	A -3A -1A -1A -2A	# 1.72
849	BS	A -3A -1A -1A -2A *1A	# 1.26
924	BS	A -3A -1A -1A -3A	# 1.72
924	BS	A -3A -1A -1A -4A	# 1.72
849	BS	A -3A -1A -1A -4A *1A	# 1.26
849	BS	A -3A -1A -1A -4A *4A	# 1.26
910	BS	A -3A -1A -2A	1.19
824	BS	A -3A -1A -2A *1A	# 1.16
921	BS	A -3A -1A -2A -1A	# 7.65
849	BS	A -3A -1A -2A -1A *1A	# 1.26
849	BS	A -3A -1A -2A -1A *2A	# 1.26
849	BS	A -3A -1A -2A -1A *4A	# 1.26
934	BS	A -3A -1A -2A -1A -2A	# 1.22
934	BS	A -3A -1A -2A -1A -3A	# 1.22

# Bond Sequences

Screen Number		Fragment Definition	Frequency Percent
934	BS	A -3A -1A -2A -1A -4A	# 1.22
914	BS	A -3A -1A -3A	0.09
921	BS	A -3A -1A -3A -1A	# 7.65
849	BS	A -3A -1A -3A -1A *1A	# 1.26
849	BS	A -3A -1A -3A -1A *2A	# 1.26
849	BS	A -3A -1A -3A -1A *4A	# 1.26
934	BS	A -3A -1A -3A -1A -2A	# 1.22
934	BS	A -3A -1A -3A -1A -3A	# 1.22
934	BS	A -3A -1A -3A -1A -4A	# 1.22
913	BS	A -3A -1A -4A	0.00
824	BS	A -3A -1A -4A *1A	# 1.16
824	BS	A -3A -1A -4A *4A	# 1.16
921	BS	A -3A -1A -4A -1A	# 7.65
849	BS	A -3A -1A -4A -1A *1A	# 1.26
849	BS	A -3A -1A -4A -1A *2A	# 1.26
849	BS	A -3A -1A -4A -1A *4A	# 1.26
934	BS	A -3A -1A -4A -1A -2A	# 1.22
934	BS	A -3A -1A -4A -1A -3A	# 1.22
934	BS	A -3A -1A -4A -1A -4A	# 1.22
925	BS	A -3A -1A -4A -4A	# 3.29
849	BS	A -3A -1A -4A -4A *1A	# 1.26
849	BS	A -3A -1A -4A -4A *4A	# 1.26
764	BS	A -4A *1A *1A *1A	# 16.95
755	BS	A -4A *1A *1A *1A *2A	# 7.52
755	BS	A -4A *1A *1A *1A *4A	# 7.52
863	BS	A -4A *1A *1A *1A -1A	0.85
871	BS	A -4A *1A *1A *1A -2A	# 1.29
871	BS	A -4A *1A *1A *1A -4A	# 1.29
769	BS	A -4A *1A *1A *2A	# 10.73
866	BS	A -4A *1A *1A *2A -1A	# 3.89
769	BS	A -4A *1A *1A *4A	# 10.73
866	BS	A -4A *1A *1A *4A -1A	# 3.89
871	BS	A -4A *1A *1A *4A -4A	# 1.29
875	BS	A -4A *1A *1A -1A	# 2.85
880	BS	A -4A *1A *1A -2A	# 2.69
880	BS	A -4A *1A *1A -4A	# 2.69
783	BS	A -4A *1A *2A	1.11
760	BS	A -4A *1A *2A *1A *2A	# 4.14
760	BS	A -4A *1A *2A *1A *4A	# 4.14
866	BS	A -4A *1A *2A *1A -1A	# 3.89
871	BS	A -4A *1A *2A *1A -2A	# 1.29
871	BS	A -4A *1A *2A *1A -4A	# 1.29
875	BS	A -4A *1A *2A -1A	# 2.85
766	BS	A -4A *1A *4A *1A	# 15.89
760	BS	A -4A *1A *4A *1A *2A	# 4.14
760	BS	A -4A *1A *4A *1A *4A	# 4.14
866	BS	A -4A *1A *4A *1A -1A	# 3.89
871	BS	A -4A *1A *4A *1A -2A	# 1.29
871	BS	A -4A *1A *4A *1A -4A	# 1.29
773	BS	A -4A *1A *4A *4A	# 5.73
866	BS	A -4A *1A *4A *4A -1A	# 3.89
871	BS	A -4A *1A *4A *4A -4A	# 1.29
875	BS	A -4A *1A *4A -1A	# 2.85
880	BS	A -4A *1A *4A -4A	# 2.69
887	BS	A -4A *1A -1A	2.47

# Bond Sequences

Screen Number		Fragment Definition	Frequency Percent
892	BS	A -4A *1A -2A	# 0.54
892	BS	A -4A *1A -4A	# 0.54
765	BS	A -4A *4A *1A	# 24.92
758	BS	A -4A *4A *1A *1A *2A	# 0.97
758	BS	A -4A *4A *1A *1A *4A	# 0.97
866	BS	A -4A *4A *1A *1A -1A	# 3.89
871	BS	A -4A *4A *1A *1A -2A	# 1.29
871	BS	A -4A *4A *1A *1A -4A	# 1.29
771	BS	A -4A *4A *1A *2A	# 3.22
866	BS	A -4A *4A *1A *2A -1A	# 3.89
771	BS	A -4A *4A *1A *4A	# 3.22
866	BS	A -4A *4A *1A *4A -1A	# 3.89
871	BS	A -4A *4A *1A *4A -4A	# 1.29
875	BS	A -4A *4A *1A -1A	# 2.85
880	BS	A -4A *4A *1A -2A	# 2.69
880	BS	A -4A *4A *1A -4A	# 2.69
767	BS	A -4A *4A *4A *1A	# 14.13
762	BS	A -4A *4A *4A *1A *2A	# 0.88
762	BS	A -4A *4A *4A *1A *4A	# 0.88
866	BS	A -4A *4A *4A *1A -1A	# 3.89
871	BS	A -4A *4A *4A *1A -2A	# 1.29
871	BS	A -4A *4A *4A *1A -4A	# 1.29
753	BS	A -4A *4A *4A *4A *1A	# 11.30
869	BS	A -4A *4A *4A *4A -1A	0.88
871	BS	A -4A *4A *4A *4A -4A	# 1.29
878	BS	A -4A *4A *4A -1A	2.01
880	BS	A -4A *4A *4A -4A	# 2.69
890	BS	A -4A *4A -1A	0.92
892	BS	A -4A *4A -4A	# 0.54
785	BS	A -4A -1A *1A *1A	# 19.91
775	BS	A -4A -1A *1A *1A *1A	# 15.47
777	BS	A -4A -1A *1A *1A *2A	# 4.54
778	BS	A -4A -1A *1A *1A *4A	# 2.25
790	BS	A -4A -1A *1A *2A	# 6.14
790	BS	A -4A -1A *1A *4A	# 6.14
809	BS	A -4A -1A *2A	# 8.95
779	BS	A -4A -1A *2A *1A *4A	# 1.43
788	BS	A -4A -1A *4A *1A	# 0.92
780	BS	A -4A -1A *4A *1A *4A	# 0.18
794	BS	A -4A -1A *4A *4A	14.39
776	BS	A -4A -1A *4A *4A *1A	# 3.05
883	BS	A -4A -1A *4A *4A -1A	5.64
896	BS	A -4A -1A *4A -1A	5.42
898	BS	A -4A -1A *4A -1A -1A	# 4.41
899	BS	A -4A -1A *4A -1A -2A	# 1.55
899	BS	A -4A -1A *4A -1A -4A	# 1.55
901	BS	A -4A -1A -1A	23.62
823	BS	A -4A -1A -1A *1A	# 3.08
823	BS	A -4A -1A -1A *2A	# 3.08
829	BS	A -4A -1A -1A *4A	3.12
917	BS	A -4A -1A -1A -1A	18.40
848	BS	A -4A -1A -1A -1A *1A	# 7.95
848	BS	A -4A -1A -1A -1A *2A	# 7.95
859	BS	A -4A -1A -1A -1A *4A	# 10.42
928	BS	A -4A -1A -1A -1A -1A	# 24.95

# Bond Sequences

Screen Number		Fragment Definition	Frequency Percent
933	BS	A -4A -1A -1A -1A -2A	# 6.75
933	BS	A -4A -1A -1A -1A -3A	# 6.75
933	BS	A -4A -1A -1A -1A -4A	# 6.75
923	BS	A -4A -1A -1A -2A	# 9.54
856	BS	A -4A -1A -1A -2A *1A	# 0.24
924	BS	A -4A -1A -1A -3A	# 1.72
923	BS	A -4A -1A -1A -4A	# 9.54
856	BS	A -4A -1A -1A -4A *1A	# 0.24
856	BS	A -4A -1A -1A -4A *4A	# 0.24
909	BS	A -4A -1A -2A	4.21
921	BS	A -4A -1A -2A -1A	# 7.65
853	BS	A -4A -1A -2A -1A *1A	# 3.89
853	BS	A -4A -1A -2A -1A *2A	# 3.89
853	BS	A -4A -1A -2A -1A *4A	# 3.89
934	BS	A -4A -1A -2A -1A -2A	# 1.22
934	BS	A -4A -1A -2A -1A -3A	# 1.22
934	BS	A -4A -1A -2A -1A -4A	# 1.22
913	BS	A -4A -1A -3A	0.00
921	BS	A -4A -1A -3A -1A	# 7.65
934	BS	A -4A -1A -3A -1A -2A	# 1.22
934	BS	A -4A -1A -3A -1A -3A	# 1.22
934	BS	A -4A -1A -3A -1A -4A	# 1.22
911	BS	A -4A -1A -4A	0.72
921	BS	A -4A -1A -4A -1A	# 7.65
855	BS	A -4A -1A -4A -1A *1A	# 1.69
855	BS	A -4A -1A -4A -1A *2A	# 1.69
855	BS	A -4A -1A -4A -1A *4A	# 1.69
934	BS	A -4A -1A -4A -1A -2A	# 1.22
934	BS	A -4A -1A -4A -1A -3A	# 1.22
934	BS	A -4A -1A -4A -1A -4A	# 1.22
925	BS	A -4A -1A -4A -4A	# 3.29
851	BS	A -4A -1A -4A -4A *1A	# 4.86
851	BS	A -4A -1A -4A -4A *4A	# 4.86
807	BS	A -4A -4A *1A	# 1.54
807	BS	A -4A -4A *4A	# 1.54
906	BS	A -4A -4A -1A	23.99
826	BS	A -4A -4A -1A *1A	# 3.47
826	BS	A -4A -4A -1A *2A	# 3.47
832	BS	A -4A -4A -1A *4A	8.33
920	BS	A -4A -4A -1A -1A	12.63
851	BS	A -4A -4A -1A -1A *1A	# 4.86
851	BS	A -4A -4A -1A -1A *2A	# 4.86
851	BS	A -4A -4A -1A -1A *4A	# 4.86
930	BS	A -4A -4A -1A -1A -1A	9.93
925	BS	A -4A -4A -1A -2A	# 3.29
851	BS	A -4A -4A -1A -2A *1A	# 4.86
925	BS	A -4A -4A -1A -3A	# 3.29
925	BS	A -4A -4A -1A -4A	# 3.29
851	BS	A -4A -4A -1A -4A *1A	# 4.86
851	BS	A -4A -4A -1A -4A *4A	# 4.86
912	BS	A -4A -4A -4A	2.45
922	BS	A -4A -4A -4A -1A	# 2.48
851	BS	A -4A -4A -4A -1A *1A	# 4.86
851	BS	A -4A -4A -4A -1A *2A	# 4.86
851	BS	A -4A -4A -4A -1A *4A	# 4.86



## Bond Sequences

Screen Number		Fragment Definition					Frequency Percent	
925	BS	A	-4A	-4A	-4A	-4A	#	3.29
851	BS	A	-4A	-4A	-4A	-4A *1A	#	4.86
851	BS	A	-4A	-4A	-4A	-4A *4A	#	4.86

## Connectivity Sequences

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### CS Screens

**Connectivity sequence (CS)** screens specify the connectivity values (the number of non-hydrogen attachments) of the atoms in the string and the types of bonds between them, as in:

CS   1   2   \*   2   \*   3   \*   3   -   1

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### CS Screen Definitions

These screens are descriptions of non-hydrogen connectivities for linear sequences of 4, 5, or 6 atoms, often including bond types but never bond values. *The connectivity values here are the exact number of non-hydrogen attachments, not the usual "or more" specification*, so that, for example, a "1" would always indicate a terminal atom and a "2" an atom with exactly two non-hydrogen attachments.

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# Connectivity Sequences

Screen Number		Fragment Definition	Frequency Percent
513	CS	1 - 2 - 2 - 2 - 2 - 1	0.16
514	CS	1 - 2 - 2 - 2 - 2 - 2	5.75
515	CS	1 - 2 - 2 - 2 - 2 - 3	3.74
516	CS	1 - 2 - 2 - 2 - 2 - 3	5.04
517	CS	1 2 2 2 4	0.88
518	CS	1 - 2 - 2 - 3 - 1	5.12
519	CS	1 - 2 - 2 - 3 * 2	3.51
520	CS	1 - 2 - 2 - 3 - 2	3.25
521	CS	1 - 2 - 2 - 3 * 3	2.60
522	CS	1 - 2 - 2 - 3 - 3	4.06
523	CS	1 2 2 3 4	0.61
524	CS	1 2 2 4 1	0.95
525	CS	1 2 2 4 2	1.19
526	CS	1 - 2 - 3 - 2 - 1	2.00
527	CS	1 - 2 - 3 - 2 - 2	3.69
528	CS	1 - 2 - 3 * 2 * 2 * 2	3.10
529	CS	1 - 2 - 3 * 2 * 2 * 3	7.71
530	CS	1 - 2 - 3 - 2 - 2 - 3	1.46
531	CS	1 - 2 - 3 * 2 * 3	9.36
532	CS	1 - 2 - 3 - 2 - 3	4.54
533	CS	1 - 2 - 3 * 3	12.00
534	CS	1 - 2 - 3 - 3	10.15
535	CS	1 - 2 - 3 - 3 - 1	4.42
536	CS	1 - 2 - 3 - 3 * 2	3.69
537	CS	1 - 2 - 3 - 3 - 2	4.54
538	CS	1 - 2 - 3 - 3 * 3	2.36
539	CS	1 - 2 - 3 - 3 - 3	3.11
540	CS	1 2 3 4	1.45
541	CS	1 2 4	3.93
518	CS	1 - 3 - 2 - 2 - 1	5.12
542	CS	1 - 3 - 2 - 2 - 2 - 2	8.38
543	CS	1 - 3 * 2 * 2 * 3 - 1	1.79
544	CS	1 - 3 - 2 - 2 - 3 - 1	5.14
545	CS	1 - 3 * 2 * 2 * 3 - 2	8.51
546	CS	1 - 3 - 2 - 2 - 3 - 2	5.61
547	CS	1 - 3 * 2 * 2 * 3 - 3	8.12
548	CS	1 - 3 * 2 * 2 * 3 - 4	# 3.16
549	CS	1 - 3 * 2 * 3 - 1	7.34
550	CS	1 - 3 - 2 - 3 - 1	4.92
551	CS	1 - 3 * 2 * 3 - 2	9.61
552	CS	1 - 3 - 2 - 3 * 2	16.48
553	CS	1 - 3 - 2 - 3 - 2	9.26
554	CS	1 - 3 - 2 - 3 - 2 - 2	5.66
555	CS	1 - 3 * 2 * 3 - 3	8.64
556	CS	1 - 3 - 2 - 3 * 3	10.21
557	CS	1 - 3 - 2 - 3 - 3	9.58
558	CS	1 - 3 * 2 * 3 * 3 - 1	5.64
559	CS	1 - 3 * 2 * 3 * 3 - 2	4.75
560	CS	1 - 3 * 2 * 3 * 3 - 3	3.92
548	CS	1 - 3 * 2 * 3 * 3 - 4	# 3.16
561	CS	1 3 2 3 4	4.25
562	CS	1 - 3 * 2 * 3 - 4	# 1.86
563	CS	1 3 2 4	6.81
564	CS	1 3 2 4 1	4.90
565	CS	1 - 3 * 3 - 1	9.71

# Connectivity Sequences

Screen Number		Fragment Definition	Frequency Percent
566	CS	1 - 3 - 3 - 1	9.12
567	CS	1 - 3 * 3 - 2	19.66
535	CS	1 - 3 - 3 - 2 - 1	4.42
568	CS	1 - 3 - 3 - 2 - 2	8.72
569	CS	1 - 3 - 3 * 2 * 2 * 2	11.24
570	CS	1 - 3 - 3 * 2 * 2 * 3	14.08
571	CS	1 - 3 - 3 * 2 * 3	14.13
572	CS	1 - 3 - 3 - 2 - 3	10.45
558	CS	1 - 3 * 3 * 2 * 3 - 1	5.64
573	CS	1 - 3 * 3 * 2 * 3 - 2	6.02
574	CS	1 - 3 * 3 * 2 * 3 - 3	5.24
548	CS	1 - 3 * 3 * 2 * 3 - 4	# 3.16
575	CS	1 - 3 * 3 - 3	15.42
576	CS	1 - 3 - 3 * 3	18.41
577	CS	1 - 3 - 3 - 3	9.33
578	CS	1 - 3 * 3 * 3 - 1	9.40
579	CS	1 - 3 - 3 - 3 - 1	4.71
580	CS	1 - 3 * 3 * 3 - 2	7.26
581	CS	1 - 3 - 3 - 3 - 2	4.79
582	CS	1 - 3 * 3 * 3 - 3	6.31
583	CS	1 - 3 * 3 * 3 * 3 - 1	5.57
584	CS	1 - 3 * 3 * 3 * 3 - 2	6.50
585	CS	1 - 3 * 3 * 3 * 3 - 3	4.88
548	CS	1 - 3 * 3 * 3 * 3 - 4	# 3.16
562	CS	1 - 3 * 3 * 3 - 4	# 1.86
586	CS	1 - 3 * 3 - 4	1.75
587	CS	1 3 4	8.58
588	CS	1 4 1	27.09
589	CS	1 - 4 * 2	7.98
524	CS	1 4 2 2 1	0.95
590	CS	1 4 2 2 2	4.04
564	CS	1 4 2 3 1	4.90
591	CS	1 - 4 * 3	7.10
592	CS	1 4 3 2 3 2	7.50
593	CS	2 - 2 - 2 - 2 - 2	8.75
514	CS	2 - 2 - 2 - 2 - 2 - 1	5.75
594	CS	2 * 2 * 2 * 2 * 2 * 2	1.48
595	CS	2 - 2 - 2 - 2 - 2 - 2	6.35
596	CS	2 * 2 * 2 * 2 * 2 * 3	29.58
597	CS	2 - 2 - 2 - 2 - 2 - 3	7.57
542	CS	2 - 2 - 2 - 2 - 3 - 1	8.38
598	CS	2 * 2 * 2 * 2 * 3 - 2	20.16
599	CS	2 - 2 - 2 - 2 - 3 * 2	5.76
600	CS	2 * 2 * 2 * 2 * 3 * 3	21.07
601	CS	2 * 2 * 2 * 2 * 3 - 3	18.36
602	CS	2 2 2 2 4	3.60
603	CS	2 - 2 - 2 - 3 * 2	11.91
604	CS	2 - 2 - 2 - 3 - 2	10.91
528	CS	2 * 2 * 2 * 3 - 2 - 1	3.10
605	CS	2 * 2 * 2 * 3 * 2 * 3	15.52
606	CS	2 - 2 - 2 - 3 * 3	7.09
607	CS	2 - 2 - 2 - 3 - 3	9.62
569	CS	2 * 2 * 2 * 3 - 3 - 1	11.24
608	CS	2 * 2 * 2 * 3 * 3 * 3	18.39
609	CS	2 2 2 3 4	9.00

# Connectivity Sequences

Screen Number		Fragment Definition							Frequency Percent
590	CS	2	2	2	4	1			4.04
610	CS	2	2	2	4	2	2		2.71
527	CS	2	-	2	-	3	-	2	3.69
611	CS	2	-	2	-	3	-	2	6.69
612	CS	2	*	2	*	3	*	2	30.31
613	CS	2	-	2	-	3	-	2	4.05
614	CS	2	-	2	-	3	-	3	11.92
554	CS	2	-	2	-	3	-	3	5.66
615	CS	2	-	2	-	3	-	3	4.78
616	CS	2	*	2	*	3	*	2	26.19
617	CS	2	2	3	2	3	4		5.82
568	CS	2	-	2	-	3	-	3	8.72
618	CS	2	-	2	-	3	-	3	9.84
619	CS	2	-	2	-	3	-	3	7.18
620	CS	2	-	2	-	3	-	3	5.14
621	CS	2	-	2	-	3	-	3	3.49
622	CS	2	*	2	*	3	*	3	18.21
610	CS	2	2	4	2	2	2		2.71
623	CS	2	2	4	2	3			4.49
519	CS	2	*	3	-	2	-	2	3.51
520	CS	2	-	3	-	2	-	2	3.25
603	CS	2	*	3	-	2	-	2	11.91
604	CS	2	-	3	-	2	-	2	10.91
599	CS	2	*	3	-	2	-	2	5.76
598	CS	2	-	3	*	2	*	2	20.16
624	CS	2	*	3	-	2	-	2	16.28
545	CS	2	-	3	*	2	*	2	8.51
546	CS	2	-	3	-	2	-	2	5.61
625	CS	2	*	3	-	2	-	2	# 7.26
626	CS	2	-	3	*	2	*	2	7.61
627	CS	2	-	3	-	2	-	2	1.66
625	CS	2	*	3	-	2	-	2	# 7.26
628	CS	2	-	3	*	2	*	2	12.20
629	CS	2	-	3	*	2	*	2	# 3.11
552	CS	2	*	3	-	2	-	2	16.48
551	CS	2	-	3	*	2	*	2	9.61
553	CS	2	-	3	-	2	-	2	9.26
630	CS	2	*	3	-	2	-	2	8.16
631	CS	2	*	3	-	2	-	2	12.19
632	CS	2	-	3	*	2	*	2	7.31
631	CS	2	-	3	-	2	-	2	12.19
633	CS	2	-	3	-	2	-	2	4.05
615	CS	2	*	3	-	2	-	2	4.78
634	CS	2	*	3	*	2	*	2	10.75
635	CS	2	*	3	-	2	-	2	8.27
636	CS	2	*	3	-	2	-	2	12.48
637	CS	2	-	3	*	2	*	2	9.61
638	CS	2	-	3	-	2	-	2	5.52
639	CS	2	-	3	-	2	-	2	7.60
573	CS	2	-	3	*	2	*	2	6.02
640	CS	2	*	3	-	2	-	2	# 2.57
641	CS	2	*	3	-	2	-	2	# 6.65
642	CS	2	-	3	*	2	*	2	6.04
643	CS	2	*	3	*	2	*	2	19.19
644	CS	2	*	3	-	2	-	2	# 1.81

# Connectivity Sequences

Screen Number		Fragment Definition	Frequency Percent
641	CS	2 * 3 - 2 - 3 - 3 * 3	# 6.65
645	CS	2 - 3 * 2 * 3 * 3 - 3	3.14
629	CS	2 - 3 * 2 * 3 * 3 - 4	# 3.11
646	CS	2 - 3 * 2 * 3 - 4	# 2.00
592	CS	2 3 2 3 4 1	7.50
647	CS	2 3 2 4	11.56
567	CS	2 - 3 * 3 - 1	19.66
648	CS	2 * 3 - 3 * 2	16.88
649	CS	2 - 3 * 3 - 2	10.47
650	CS	2 - 3 - 3 - 2	10.14
536	CS	2 * 3 - 3 - 2 - 1	3.69
537	CS	2 - 3 - 3 - 2 - 1	4.54
618	CS	2 * 3 - 3 - 2 - 2	9.84
619	CS	2 - 3 - 3 - 2 - 2	7.18
651	CS	2 * 3 - 3 - 2 - 3	10.75
652	CS	2 - 3 - 3 - 2 - 3	8.39
559	CS	2 - 3 * 3 * 2 * 3 - 1	4.75
641	CS	2 * 3 - 3 - 2 - 3 * 2	# 6.65
642	CS	2 - 3 * 3 * 2 * 3 - 2	6.04
640	CS	2 - 3 * 3 - 2 - 3 * 2	# 2.57
653	CS	2 * 3 * 3 * 2 * 3 * 3	15.08
641	CS	2 * 3 - 3 - 2 - 3 * 3	# 6.65
654	CS	2 - 3 * 3 * 2 * 3 - 3	5.08
640	CS	2 - 3 * 3 - 2 - 3 * 3	# 2.57
629	CS	2 - 3 * 3 * 2 * 3 - 4	# 3.11
655	CS	2 * 3 - 3 * 3	15.68
656	CS	2 * 3 - 3 - 3	11.02
657	CS	2 - 3 * 3 - 3	10.72
658	CS	2 - 3 - 3 * 3	11.95
659	CS	2 - 3 - 3 - 3	8.93
580	CS	2 - 3 * 3 * 3 - 1	7.26
581	CS	2 - 3 - 3 - 3 - 1	4.79
660	CS	2 * 3 - 3 * 3 - 2	4.50
661	CS	2 * 3 - 3 - 3 * 2	4.23
662	CS	2 - 3 * 3 * 3 - 2	4.50
660	CS	2 - 3 * 3 - 3 * 2	4.50
663	CS	2 - 3 - 3 - 3 - 2	2.35
664	CS	2 * 3 - 3 * 3 - 3	3.93
665	CS	2 * 3 - 3 - 3 * 3	2.75
666	CS	2 - 3 * 3 * 3 - 3	4.43
667	CS	2 - 3 * 3 - 3 * 3	1.37
584	CS	2 - 3 * 3 * 3 * 3 - 1	6.50
668	CS	2 * 3 - 3 - 3 * 3 - 2	# 0.60
669	CS	2 * 3 - 3 - 3 - 3 * 2	# 0.80
670	CS	2 - 3 * 3 * 3 * 3 - 2	2.95
668	CS	2 - 3 * 3 - 3 - 3 * 2	# 0.60
671	CS	2 * 3 * 3 * 3 * 3 * 3	15.97
672	CS	2 * 3 - 3 - 3 * 3 - 3	# 0.96
669	CS	2 * 3 - 3 - 3 - 3 * 3	# 0.80
673	CS	2 - 3 * 3 * 3 * 3 - 3	3.75
668	CS	2 - 3 * 3 - 3 - 3 * 3	# 0.60
629	CS	2 - 3 * 3 * 3 * 3 - 4	# 3.11
646	CS	2 - 3 * 3 * 3 - 4	# 2.00
674	CS	2 - 3 * 3 - 4	1.37
675	CS	2 * 3 * 4	7.98

# Connectivity Sequences

Screen Number	Fragment Definition	Frequency Percent
676	CS 2 * 3 - 4	14.83
677	CS 2 - 3 * 4	2.36
678	CS 2 - 3 - 4	4.44
589	CS 2 * 4 - 1	7.98
679	CS 2 * 4 - 2	3.49
679	CS 2 - 4 * 2	3.49
525	CS 2 4 2 2 1	1.19
680	CS 2 4 2 3	8.39
681	CS 2 * 4 * 3	7.86
682	CS 2 * 4 - 3	3.23
683	CS 2 - 4 * 3	2.54
684	CS 2 - 4 - 3	6.98
516	CS 3 - 2 - 2 - 2 - 1	5.04
515	CS 3 - 2 - 2 - 2 - 2 - 1	3.74
596	CS 3 * 2 * 2 * 2 * 2 * 2	29.58
597	CS 3 - 2 - 2 - 2 - 2 - 2	7.57
685	CS 3 - 2 - 2 - 2 - 2 - 3	4.23
686	CS 3 - 2 - 2 - 2 - 3	6.76
687	CS 3 2 2 2 4	2.05
624	CS 3 - 2 - 2 - 3 * 2	16.28
529	CS 3 * 2 * 2 * 3 - 2 - 1	7.71
530	CS 3 - 2 - 2 - 3 - 2 - 1	1.46
612	CS 3 * 2 * 2 * 3 * 2 * 2	30.31
613	CS 3 - 2 - 2 - 3 - 2 - 2	4.05
688	CS 3 - 2 - 2 - 3 - 2 - 3	6.96
689	CS 3 - 2 - 2 - 3 * 3	9.91
690	CS 3 - 2 - 2 - 3 - 3	9.42
570	CS 3 * 2 * 2 * 3 - 3 - 1	14.08
691	CS 3 2 2 3 4	10.08
692	CS 3 2 2 4	8.19
531	CS 3 * 2 * 3 - 2 - 1	9.36
532	CS 3 - 2 - 3 - 2 - 1	4.54
614	CS 3 - 2 - 3 - 2 - 2	11.92
605	CS 3 * 2 * 3 * 2 * 2 * 2	15.52
688	CS 3 - 2 - 3 - 2 - 2 - 3	6.96
693	CS 3 - 2 - 3 - 2 - 3	7.87
634	CS 3 * 2 * 3 * 2 * 3 * 2	10.75
694	CS 3 2 3 2 3 4	3.99
571	CS 3 * 2 * 3 - 3 - 1	14.13
572	CS 3 - 2 - 3 - 3 - 1	10.45
651	CS 3 - 2 - 3 - 3 * 2	10.75
652	CS 3 - 2 - 3 - 3 - 2	8.39
695	CS 3 - 2 - 3 - 3 - 3	5.68
680	CS 3 2 4 2	8.39
623	CS 3 2 4 2 2	4.49
533	CS 3 * 3 - 2 - 1	12.00
534	CS 3 - 3 - 2 - 1	10.15
521	CS 3 * 3 - 2 - 2 - 1	2.60
522	CS 3 - 3 - 2 - 2 - 1	4.06
606	CS 3 * 3 - 2 - 2 - 2	7.09
607	CS 3 - 3 - 2 - 2 - 2	9.62
600	CS 3 * 3 * 2 * 2 * 2 * 2	21.07
601	CS 3 - 3 * 2 * 2 * 2 * 2	18.36
689	CS 3 * 3 - 2 - 2 - 3	9.91
690	CS 3 - 3 - 2 - 2 - 3	9.42

# Connectivity Sequences

Screen Number		Fragment Definition	Frequency Percent
547	CS	3 - 3 * 2 * 2 * 3 - 1	8.12
625	CS	3 * 3 - 2 - 2 - 3 * 2	# 7.26
628	CS	3 - 3 * 2 * 2 * 3 - 2	12.20
625	CS	3 * 3 - 2 - 2 - 3 * 3	# 7.26
696	CS	3 - 3 * 2 * 2 * 3 - 3	4.81
697	CS	3 - 3 * 2 * 2 * 3 - 4	# 2.13
556	CS	3 * 3 - 2 - 3 - 1	10.21
555	CS	3 - 3 * 2 * 3 - 1	8.64
557	CS	3 - 3 - 2 - 3 - 1	9.58
635	CS	3 * 3 - 2 - 3 * 2	8.27
638	CS	3 * 3 - 2 - 3 - 2	5.52
637	CS	3 - 3 * 2 * 3 - 2	9.61
636	CS	3 - 3 - 2 - 3 * 2	12.48
639	CS	3 - 3 - 2 - 3 - 2	7.60
616	CS	3 * 3 * 2 * 3 * 2 * 2	26.19
698	CS	3 * 3 - 2 - 3 * 3	2.62
699	CS	3 * 3 - 2 - 3 - 3	5.51
700	CS	3 - 3 * 2 * 3 - 3	5.43
699	CS	3 - 3 - 2 - 3 * 3	5.51
701	CS	3 - 3 - 2 - 3 - 3	5.59
574	CS	3 - 3 * 2 * 3 * 3 - 1	5.24
653	CS	3 * 3 * 2 * 3 * 3 * 2	15.08
640	CS	3 * 3 - 2 - 3 * 3 - 2	# 2.57
641	CS	3 * 3 - 2 - 3 - 3 * 2	# 6.65
654	CS	3 - 3 * 2 * 3 * 3 - 2	5.08
644	CS	3 * 3 - 2 - 3 * 3 - 3	# 1.81
641	CS	3 * 3 - 2 - 3 - 3 * 3	# 6.65
702	CS	3 - 3 * 2 * 3 * 3 - 3	2.80
697	CS	3 - 3 * 2 * 3 * 3 - 4	# 2.13
703	CS	3 3 2 3 4	7.93
704	CS	3 - 3 * 2 * 3 - 4	# 1.89
705	CS	3 3 2 4	9.47
576	CS	3 * 3 - 3 - 1	18.41
575	CS	3 - 3 * 3 - 1	15.42
577	CS	3 - 3 - 3 - 1	9.33
655	CS	3 * 3 - 3 * 2	15.68
658	CS	3 * 3 - 3 - 2	11.95
657	CS	3 - 3 * 3 - 2	10.72
656	CS	3 - 3 - 3 * 2	11.02
659	CS	3 - 3 - 3 - 2	8.93
538	CS	3 * 3 - 3 - 2 - 1	2.36
539	CS	3 - 3 - 3 - 2 - 1	3.11
620	CS	3 * 3 - 3 - 2 - 2	5.14
621	CS	3 - 3 - 3 - 2 - 2	3.49
608	CS	3 * 3 * 3 * 2 * 2 * 2	18.39
695	CS	3 - 3 - 3 - 2 - 3	5.68
560	CS	3 - 3 * 3 * 2 * 3 - 1	3.92
643	CS	3 * 3 * 3 * 2 * 3 * 2	19.19
641	CS	3 * 3 - 3 - 2 - 3 * 2	# 6.65
645	CS	3 - 3 * 3 * 2 * 3 - 2	3.14
644	CS	3 - 3 * 3 - 2 - 3 * 2	# 1.81
641	CS	3 * 3 - 3 - 2 - 3 * 3	# 6.65
702	CS	3 - 3 * 3 * 2 * 3 - 3	2.80
644	CS	3 - 3 * 3 - 2 - 3 * 3	# 1.81
697	CS	3 - 3 * 3 * 2 * 3 - 4	# 2.13



# Connectivity Sequences

Screen Number		Fragment Definition	Frequency Percent
706	CS	3 * 3 - 3 * 3	3.65
707	CS	3 * 3 - 3 - 3	6.09
708	CS	3 - 3 * 3 - 3	7.00
707	CS	3 - 3 - 3 * 3	6.09
709	CS	3 - 3 - 3 - 3	2.79
582	CS	3 - 3 * 3 * 3 - 1	6.31
667	CS	3 * 3 - 3 * 3 - 2	1.37
665	CS	3 * 3 - 3 - 3 * 2	2.75
666	CS	3 - 3 * 3 * 3 - 2	4.43
664	CS	3 - 3 * 3 - 3 * 2	3.93
622	CS	3 * 3 * 3 * 3 * 2 * 2	18.21
710	CS	3 * 3 - 3 * 3 - 3	1.08
711	CS	3 * 3 - 3 - 3 * 3	0.75
712	CS	3 - 3 * 3 * 3 - 3	2.35
710	CS	3 - 3 * 3 - 3 * 3	1.08
585	CS	3 - 3 * 3 * 3 * 3 - 1	4.88
671	CS	3 * 3 * 3 * 3 * 3 * 2	15.97
668	CS	3 * 3 - 3 - 3 * 3 - 2	# 0.60
669	CS	3 * 3 - 3 - 3 - 3 * 2	# 0.80
673	CS	3 - 3 * 3 * 3 * 3 - 2	3.75
672	CS	3 - 3 * 3 - 3 - 3 * 2	# 0.96
713	CS	3 * 3 * 3 * 3 * 3 * 3	7.52
672	CS	3 * 3 - 3 - 3 * 3 - 3	# 0.96
669	CS	3 * 3 - 3 - 3 - 3 * 3	0.80
714	CS	3 - 3 * 3 * 3 * 3 - 3	1.64
672	CS	3 - 3 * 3 - 3 - 3 * 3	# 0.96
697	CS	3 - 3 * 3 * 3 * 3 - 4	# 2.13
704	CS	3 - 3 * 3 * 3 - 4	# 1.89
715	CS	3 3 3 4	10.43
716	CS	3 - 3 * 3 - 4	# 1.02
717	CS	3 3 4	15.49
591	CS	3 * 4 - 1	7.10
681	CS	3 * 4 * 2	7.86
683	CS	3 * 4 - 2	2.54
682	CS	3 - 4 * 2	3.23
684	CS	3 - 4 - 2	6.98
718	CS	3 4 3	13.57
719	CS	3 * 4 - 3	2.12
719	CS	3 - 4 * 3	2.12
541	CS	4 2 1	3.93
517	CS	4 2 2 2 1	0.88
602	CS	4 2 2 2 2	3.60
720	CS	4 2 2 2 2 4	# 3.12
687	CS	4 2 2 2 3	2.05
720	CS	4 2 2 2 3 4	# 3.12
721	CS	4 2 2 2 4	# 5.18
692	CS	4 2 2 3	8.19
720	CS	4 2 2 3 2 4	# 3.12
720	CS	4 2 2 3 3 4	# 3.12
721	CS	4 2 2 3 4	# 5.18
722	CS	4 2 2 4	# 3.29
563	CS	4 2 3 1	6.81
647	CS	4 2 3 2	11.56
720	CS	4 2 3 2 2 4	# 3.12
720	CS	4 2 3 2 3 4	# 3.12

# Connectivity Sequences

Screen Number		Fragment Definition							Frequency Percent
721	CS	4	2	3	2	4			# 5.18
705	CS	4	2	3	3				9.47
720	CS	4	2	3	3	2	4		# 3.12
720	CS	4	2	3	3	3	4		# 3.12
721	CS	4	2	3	3	4			# 5.18
722	CS	4	2	3	4				# 3.29
723	CS	4	2	4					2.20
587	CS	4	3	1					8.58
675	CS	4	*	3	*	2			7.98
677	CS	4	*	3	-	2			2.36
676	CS	4	-	3	*	2			14.83
678	CS	4	-	3	-	2			4.44
540	CS	4	3	2	1				1.45
523	CS	4	3	2	2	1			0.61
609	CS	4	3	2	2	2			9.00
720	CS	4	3	2	2	2	4		# 3.12
691	CS	4	3	2	2	3			10.08
548	CS	4	-	3	*	2	*	2	# 3.16
629	CS	4	-	3	*	2	*	2	# 3.11
697	CS	4	-	3	*	2	*	2	# 2.13
720	CS	4	3	2	2	3	4		# 3.12
724	CS	4	-	3	*	2	*	2	# 0.32
721	CS	4	3	2	2	4			# 5.18
561	CS	4	3	2	3	1			4.25
562	CS	4	-	3	*	2	*	3	# 1.86
646	CS	4	-	3	*	2	*	3	# 2.00
617	CS	4	3	2	3	2	2		5.82
694	CS	4	3	2	3	2	3		3.99
720	CS	4	3	2	3	2	4		# 3.12
703	CS	4	3	2	3	3			7.93
704	CS	4	-	3	*	2	*	3	# 1.89
548	CS	4	-	3	*	2	*	3	# 3.16
629	CS	4	-	3	*	2	*	3	# 3.11
697	CS	4	-	3	*	2	*	3	# 2.13
720	CS	4	3	2	3	3	4		# 3.12
724	CS	4	-	3	*	2	*	3	# 0.32
721	CS	4	3	2	3	4			# 5.18
725	CS	4	-	3	*	2	*	3	0.78
722	CS	4	3	2	4				# 3.29
717	CS	4	3	3					15.49
586	CS	4	-	3	*	3	-	1	1.75
674	CS	4	-	3	*	3	-	2	1.37
720	CS	4	3	3	2	2	4		# 3.12
548	CS	4	-	3	*	3	*	2	# 3.16
629	CS	4	-	3	*	3	*	2	# 3.11
697	CS	4	-	3	*	3	*	2	# 2.13
720	CS	4	3	3	2	3	4		# 3.12
724	CS	4	-	3	*	3	*	2	# 0.32
721	CS	4	3	3	2	4			# 5.18
715	CS	4	3	3	3				10.43
716	CS	4	-	3	*	3	-	3	# 1.02
562	CS	4	-	3	*	3	*	3	# 1.86
646	CS	4	-	3	*	3	*	3	# 2.00
720	CS	4	3	3	3	2	4		# 3.12
704	CS	4	-	3	*	3	*	3	# 1.89

### Connectivity Sequences

Screen Number		Fragment Definition	Frequency Percent
548	CS	4 - 3 * 3 * 3 * 3 - 1	# 3.16
629	CS	4 - 3 * 3 * 3 * 3 - 2	# 3.11
697	CS	4 - 3 * 3 * 3 * 3 - 3	# 2.13
720	CS	4 3 3 3 3 4	# 3.12
724	CS	4 - 3 * 3 * 3 * 3 - 4	# 0.32
721	CS	4 3 3 3 4	# 5.18
725	CS	4 - 3 * 3 * 3 - 4	0.78
722	CS	4 3 3 4	# 3.29
716	CS	4 - 3 * 3 - 4	# 1.02
726	CS	4 3 4	1.90
727	CS	4 4	5.62

## Atom Count

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**AC Screens**      The 19 **atom count (AC)** screens specify the number of atoms “or more” present.

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**AC Screen Definitions**      These screens specify the minimum number of atoms having at least a specified number of non-hydrogen atoms attached to them. AC screens are provided which specify non-hydrogen connectivities from three or more to six or more.

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Atom Count			Frequency Percent
Screen Number	Fragment Definition		
1899	AC	1	98.15
1900	AC	6	92.64
1901	AC	8	91.95
1902	AC	10	90.59
1903	AC	12	88.21
1904	AC	14	84.50
1905	AC	16	79.75
1906	AC	18	73.85
1907	AC	20	67.45
1908	AC	22	60.62
1909	AC	24	53.61
1910	AC	26	46.59
1911	AC	28	40.01
1912	AC	30	33.97
1913	AC	35	21.92
1914	AC	40	14.78
1915	AC	50	8.50
1916	AC	70	4.27
1917	AC	90	2.45

## Degree of Connectivity

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**DC Screens**      The 17 **degree of connectivity (DC)** screens specify the minimum number of atoms having at least a specified number of non-hydrogen atoms attached to them.

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**DC Screen Definitions**      The DC screens specify non-hydrogen connectivities from three or more to six or more.

The DC 6 3 screen, specifies the presence of six or more atoms having non-hydrogen connectivities of three or more atoms.

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Degree of Connectivity				
Screen Number	Fragment Definition			Frequency Percent
2111	DC		3	92.87
2112	DC	3	3	87.28
2113	DC	5	3	75.61
2114	DC	7	3	59.22
2115	DC	9	3	41.91
2116	DC	12	3	21.66
2117	DC	14	3	13.95
2118	DC	16	3	9.96
2119	DC	20	3	6.39
2120	DC		4	42.03
2121	DC	2	4	17.53
2122	DC	3	4	8.61
2123	DC	4	4	4.94
2124	DC	5	4	3.04
2125	DC	6	4	2.10
950	DC		5	5.63
2126	DC		6	4.73

# Ring Count

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**RC Screens**      The 10 **ring count (RC)** screens specify the minimum number “or more” of rings (not ring systems) present.

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**RC Screen Definitions**      These screens specify the minimum number of rings present in the structure. Technically speaking, this is a count of the ring closure pairs present in the structure record, which is equal to the minimum number of bonds that would have to be broken to open all rings.

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			Ring Count		
Screen Number	Fragment Definition			Frequency	Percent
1838	RC	1		86.17	
1839	RC	2		72.82	
1840	RC	3		53.05	
1841	RC	4		33.05	
1842	RC	5		17.59	
1843	RC	6		10.11	
1844	RC	7		6.54	
1845	RC	8		5.01	
1846	RC	10		3.12	
1847	RC	15		1.13	

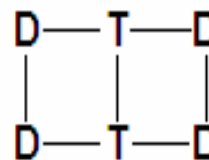
## Type of Rings

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<b>TR Screens</b>	The <b>type of ring (TR)</b> screens specify the rings that are present in terms of numbers of atoms and whether the atoms are part of a ring fusion site.
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<b>TR Screen Definitions</b>	<p>The TR screens describe the node sequences of rings of 3 to 7 atoms. The symbol "<b>D</b>" is used to indicate a non-fused ring atom (an atom attached to exactly two other ring atoms) and "<b>T</b>" to indicate a fusion point or bridgehead atom with three or more bonds to other ring atoms. The "smallest set of smallest rings" definition is used to define a "ring" here, so that the "envelope" rings circumscribing smaller rings are not considered; in the simple bridged ring shown here, there would be two DDTT rings but no DDTDDT ring -- the 6-membered envelope ring is not recognized by the TR screen generation procedure.</p>
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There is also a TR screen that simply provides an indicator that an 8-membered or larger ring is present.

**Example:** if a searcher were to specify that the two 6-membered rings were to be isolated (i.e., could not be part of larger ring systems) the TR 2 DDDDDD screen would be used to describe them.

Note that both D and T are exact node symbols -- if the searcher were to allow fusion to the benzene ring in a query for the example structure, then all fusion node possibilities would have to be specified or a loss of retrieval would occur.

---

# Type of Ring

Screen Number	Fragment Definition			Frequency Percent
1848	TR		DDD	2.06
1849	TR	2	DDD	0.21
1850	TR		DDT	0.26
1851	TR		DTT	# 2.46
1851	TR		TTT	# 2.46
1852	TR		DDDD	0.97
1853	TR		DDDT	# 2.17
1853	TR		DDTT	# 2.17
1854	TR	2	DDTT	0.04
1853	TR		DTDT	# 2.17
1853	TR		DTTT	# 2.17
1853	TR		TTTT	# 2.17
1855	TR		DDDDD	21.27
1856	TR	2	DDDDD	4.03
1857	TR	3	DDDDD	0.93
1858	TR		DDDDT	1.30
1859	TR		DDDDT	17.81
1860	TR	2	DDDDT	3.68
1861	TR	3	DDDDT	0.68
1862	TR		DDTDT	1.60
1863	TR		DDTTT	2.02
1864	TR		DTDTT	0.62
1865	TR		DTTTT	3.57
1866	TR		TTTTT	1.04
1867	TR		DDDDDD	64.12
1868	TR	2	DDDDDD	36.55
1869	TR	3	DDDDDD	15.00
1870	TR	4	DDDDDD	5.96
1871	TR	5	DDDDDD	2.30
1872	TR	6	DDDDDD	1.49
1873	TR		DDDDDT	1.07
1874	TR		DDDDTT	31.00
1875	TR	2	DDDDTT	16.61
1876	TR	3	DDDDTT	2.91
1877	TR	4	DDDDTT	1.76
1878	TR		DDDTDT	1.04
1879	TR	2	DDDTDT	0.34
1880	TR		DDDTTT	2.10
1881	TR	2	DDDTTT	1.32
1882	TR	3	DDDTTT	0.53
1883	TR		DDTDDT	0.66
1884	TR		DDTDTT	0.64
1885	TR		DDTTTT	4.57
1886	TR	2	DDTTTT	2.20
1887	TR		DTDTDT	0.53
1888	TR		DTDTTT	0.35
1889	TR		DTTDTT	3.09
1890	TR	2	DTTDTT	0.66
1891	TR		DTTTTT	1.26
1892	TR		TTTTTT	0.59
1893	TR		DDDDDDD	0.67
1894	TR	2	DDDDDDD	0.03
1895	TR		DDDDDDT	# 0.49
1896	TR		DDDDDTT	0.94
1895	TR		DDDDTDT	# 0.49



		Type of Ring			
Screen Number		Fragment Definition		Frequency Percent	
1895	TR	DDDDTTT	#	0.49	
1895	TR	DDDTDDT	#	0.49	
1895	TR	DDDTDTT	#	0.49	
1897	TR	DDDTTTT	#	0.64	
1895	TR	DDTDDTT	#	0.49	
1895	TR	DDTDTDT	#	0.49	
1895	TR	DDTDTTT	#	0.49	
1897	TR	DDTTDTT	#	0.64	
1895	TR	DDTTTTT	#	0.49	
1895	TR	DTDTDTT	#	0.49	
1895	TR	DTDTTTT	#	0.49	
1895	TR	DTTDTTT	#	0.49	
1895	TR	DTTTTTT	#	0.49	
1895	TR	TTTTTTT	#	0.49	
1898	TR	8-membered ring or larger		2.61	

# Element Count and Graph Modifier Fragments

**Introduction** As a result of extensive screen number sharing, most elements do not have specific screen numbers for element count (EC) and graph modifier (GM) fragments. Accordingly, three tables of fragments are provided instead of the screen dictionary listings:

- Table I --- Specific Element Count and Graph Modifier Fragments
  - Table II --- Generic Element Count and Graph Modifier Fragments
  - Table III --- Generic Element Count and Graph Modifier Fragments in Screen Number order
  - Special-purpose Graph Modifier Screens
  - Periodic Table of the Elements Showing Fragment Numbers
- 

**Table I** Table I lists EC and GM fragments in element order. These fragments fall into three classes:

- Element Count (EC) --- (CT Graph)
- Graph Modifier (GM) --- (Single Atom Fragment (SAF))
- EC or GM --- (SAF + CT Graph)

Most elements can be specified only as present in the structure as a whole, either in the connection table (CT) itself or in a single atom fragment (SAF).

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## **EC or GM (Common Elements)**

The more common elements, such as Al or Br, have a dedicated screen number to specify the presence of one or more atoms of the element in the CT and/or as a SAF.

The very common elements, such as Br, can be specified as present in the connection table or as present as an SAF. Here, the fragment for a count of one ("one or more") is always a composite CT + SAF fragment, while fragments for counts of two or higher, in the column headed "Element Count (CT Graph)", refer to atoms of the element present in the connection table graph itself. The nine elements that most frequently occur as SAFs have dedicated fragments specifying the presence of the element as an SAF. These fragments are in the column headed "Graph Modifier (SAF)", and are provided for Br, Ca, Cl, H, I, K, N, Na and O.

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**EC or GM  
(Less  
Common  
Elements)**

The less common elements, such as Ag, are specified by combining two generic fragments with AND logic, one fragment specifying the elements in a vertical group from the periodic table and the other those in a horizontal series. These fragments are listed in Tables II and III. Note that the frequency of occurrence cited for such an element is a maximum value, not an actual value, and is the lower of the frequencies for the two ANDed fragments. As a reminder, the frequency cited is followed by the abbreviation "**max.**"

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**EC or GM  
(Rarest  
Elements)**

The rarest elements, such as Ac, can be specified only via a generic fragment for a periodic series. Here again, the frequency of occurrence cited for such an element is a maximum value, not an actual value, and is simply the frequency of occurrence of structures containing one or more atoms of any element in the series. Again, the frequency cited is followed by the abbreviation "**max.**".

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**Note  
(Table I)**

Table I also provides fragments for the specification of "halogen" in the CT graph. These fragments, found under the generic halogen element symbol "X", specify the total "or more" count of halogen atoms present in the CT, whether F, Cl, Br or I.

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**Note  
(Table II)**

Table II lists the generic EC/GM fragments by category. These fragments simply record the presence of one or more atoms of any of the cited elements, whether in CT or SAF. Two special generic fragments should be mentioned:

- 1918 "metals" specifies the presence of any metal atom
  - 2029 "SAFs" specifies the presence as a single atom fragment of any element except Br, Ca, Cl, H, I, K, N, Na and O, the nine elements with specific SAF screens
- 

**Note  
(Table III)**

Table III lists the generic EC/GM fragments in screen number order, and is provided for the convenience of the searcher.

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**Table I -- Specific Element Count and Graph Modifier Fragments  
- Element Order**

"Or-more" Count		Element Count (CT Graph)		Graph Modifier (SAF)	EC or GM (CT + SAF)		
Ac	1				1919	0.19% max.	
Ag	1				1920 AND 1921	2.20% max.	
Al	1				1922	1.27%	
Am	1				1919	0.19% max.	
Ar	1				1924	0.03% max.	
As	1				1927	0.28%	
	2	1928	0.08%				
At	1				1929 AND 1930	0.76% max.	
Au	1				1920 AND 1931	1.90% max.	
B	1				1932	1.36%	
	2	1933	0.26%				
	3	1934	0.17%				
Ba	1				1935 AND 1936	1.24% max.	
Be	1				1937	0.05%	
Bi	1				1925 AND 1930	0.76% max.	
Bk	1				1919	0.19% max.	
Br	1			2030	0.55%	1938	5.30%
	2	1939	1.12%				
	3	1940	0.30%				
	4	1941	0.18%				
C	1				2110	93.59%	
	4	1942	91.88%				
	6	1943	90.62%				
	8	1944	87.91%				
	10	1945	83.53%				
	12	1946	77.56%				
	14	1947	70.23%				
	16	1948	61.95%				
	18	1949	53.38%				
	20	1950	44.93%				
	25	1951	26.45%				
	30	1952	15.81%				
	35	1953	10.30%				
	40	1954	7.56%				

"Or-more" Count		Element Count (CT Graph)		Graph Modifier (SAF)		EC or GM (CT + SAF)	
Ca	1			2031	0.06%	1955	0.34%
Cd	1					1935 AND 1956	1.03% max.
Ce	1					1957	1.31% max.
Cf	1					1919	0.19% max.
Cl	1			2032	2.95%	1958	18.33%
	2	1959	6.14%				
	3	1960	2.93%				
	4	1961	0.93%				
	5	1962	0.39%				
Cm	1					1919	0.19% max.
Co	1					1963	1.32%
Cr	1					1964 AND 1966	2.44% max.
Cs	1					1935 AND 1967	1.75% max.
Cu	1					1920 AND 1964	2.10% max.
Dy	1					1957	1.31% max.
Er	1					1957	1.31% max.
Es	1					1919	0.19% max.
Eu	1					1957	1.31% max.
F	1					1968	10.62%
	2	1969	6.99%				
	3	1970	5.71%				
	4	1971	2.67%				
	5	1972	1.96%				
	6	1973	1.70%				
	7	1974	0.85%				
Fe	1					1975	2.96%
Fm	1					1919	0.19% max.
Fr	1					1930 AND 1967	0.76% max.
Ga	1					1923 AND 1926	2.27% max.
Gd	1					1957	1.31% max.

"Or-more" Count		Element Count (CT Graph)		Graph Modifier (SAF)		EC or GM (CT + SAF)	
Ge	1					1926 AND 1983	2.27% max.
H	1			2033	3.85%		
He	1					1924	0.03% max.
Hf	1					1931 AND 1984	1.39% max.
Hg	1					1930 AND 1956	0.76% max.
Ho	1					1957	1.31% max.
I	1			2034	0.45%	1985	1.71%
	2	1986	0.33%				
In	1					1923 AND 1935	1.75% max.
Ir	1					1931 AND 1965	1.90% max.
K	1			2035	0.30%	1987	0.42%
Kr	1					1924 AND 1926	0.03% max.
La	1					1957 AND 1988	0.53% max.
Li	1					1989	0.40%
Lu	1					1957	1.31% max.
Lr	1					1919	0.19% max.
Md	1					1919	0.19% max.
Mg	1					1990	0.52%
Mn	1					1964 AND 1991	1.96% max.
Mo	1					1921 AND 1966	2.44% max.
N	1			2036	0.15%	1992	71.10%
	2	1993	53.96%				
	3	1994	35.41%				
	4	1995	23.08%				
	6	1996	9.30%				
	8	1997	5.03%				
	10	1998	3.47%				
	14	1999	2.13%				
Na	1			2037	0.95%	2000	1.11%

"Or-more" Count		Element Count (CT Graph)		Graph Modifier (SAF)		EC or GM (CT + SAF)	
Nb	1					1921 AND 2001	1.12% max.
Nd	1					1957	1.31% max.
Ne	1					1924	0.03% max.
Ni	1					2002	1.81%
No	1					1919	0.19% max.
Np	1					1919	0.19% max.
O	1			2038	0.50%	2004	83.63%
	2	2005	70.64%				
	3	2006	53.74%				
	4	2007	39.45%				
	5	2008	25.77%				
	6	2009	18.58%				
	7	2010	12.97%				
	8	2011	10.08%				
	10	2012	6.70%				
	12	2013	5.07%				
	15	2014	3.37%				
	18	2015	2.40%				
Os	1					1931 AND 1965	1.90% max.
P	1					2016	5.44%
	2	2017	1.90%				
	3	2018	0.76%				
Pa	1					1919	0.19% max.
Pb	1					1930 AND 1983	0.76% max.
Pd	1					1921 AND 1965	3.35% max.
Pm	1					1957	1.31% max.
Po	1					1930 AND 2019	0.66% max.
Pr	1					1957	1.31% max.
Pt	1					2020	0.50%
Pu	1					1919	0.19% max.
Ra	1					1930 AND 1936	0.76% max.
Rb	1					1926 AND 1967	2.00% max.

"Or-more" Count		Element Count (CT Graph)		Graph Modifier (SAF)	EC or GM (CT + SAF)	
Re	1				1931 AND 1991	1.90% max.
Rh	1				1921 AND 1965	3.35% max.
Rn	1				1924 AND 1930	0.03% max.
Ru	1				1921 AND 1965	3.35% max.
S	1				2021	26.05%
	2	2022	7.69%			
	3	2023	2.16%			
	4	2024	1.14%			
	5	2025	0.44%			
Sb	1				1925 AND 1935	1.75%
Sc	1				1988	0.53% max.
Se	1				1926 AND 2019	0.66% max.
Si	1				2026	4.55%
	2	2027	0.86%			
	3	2028	0.39%			
Sm	1				1957	1.31% max.
Sn	1				1935 AND 1983	1.75% max.
Sr	1				1926 AND 1936	1.24% max.
Ta	1				1931 AND 2001	1.12% max.
Tb	1				1957	1.31% max.
Tc	1				1921 AND 1991	1.96% max.
Te	1				1935 AND 2019	0.66% max.
Th	1				1919	0.19% max.
Ti	1				1964 AND 1984	1.39% max.
Tl	1				1923 AND 1930	0.76% max.
Tm	1				1957	1.31% max.
U	1				1919	0.19% max.
V	1				1964 AND 2001	1.12% max.



"Or-more" Count		Element Count (CT Graph)		Graph Modifier (SAF)	EC or GM (CT + SAF)	
W	1				1931 AND 1966	1.90% max.
X	2	1976	15.15%			
	3	1977	8.64%			
	4	1978	4.76%			
	5	1979	2.84%			
	6	1980	2.22%			
	8	1981	0.95%			
	10	1982	0.64%			
Xe	1				1924 AND 1935	0.03% max.
Y	1				1926 AND 1988	0.53% max.
Yb	1				1957	1.31% max.
Zn	1				1926 AND 1956	1.03% max.
Zr	1				1921 AND 1984	1.35% max.

**Table II -- Generic Element Count and Graph Modifier Screens**

Screen	Freq.	Description	Elements
1918	14.51%	"metals"	all <u>except</u> Ar As At B Br C Cl F H He I Kr N Ne O P Rn S Se Si Te Xe
1967	2.00%	group Ia	Cs Fr K Li Na Rb
1936	1.24%	group IIa	Ba Be Ca Mg Ra Sr
1988	0.53%	group IIIa	La Sc Y
1984	1.39%	group IVa	Hf Ti Zr
2001	1.12%	group Va	Nb Ta V
1966	2.44%	group VIa	Cr Mo W
1991	1.96%	group VIIa	Mn Re Tc
1965	6.72%	group VIII	Co Fe Ir Ni Os Pd Pt Rh Ru
1920	2.10%	group Ib	Ag Au Cu
1956	1.03%	group IIb	Cd Hg Zn
1923	2.93%	group IIIb	Al B Ga In Tl
1983	5.61%	group IVb	Ge Pb Si Sn
1925	6.12%	group Vb	As Bi P Sb
2003	86.62%		O S
2019	0.66%		Po Se Te
1929	31.99%	group VIIb	At Br Cl F I
1924	0.03%	group 0	Ar He Kr Ne Rn Xe
1964	7.39%	transition series I	Co Cr Cu Fe Mn Ni Ti V
1926	2.27%		As Ga Ge Kr Rb Se Sr Y Zn
1921	3.35%	transition series II	Ag Mo Nb Pd Rh Ru Tc Zr
1935	1.75%		Ba Cd Cs In Sb Sn Te Xe
1957	1.31%	lanthanide series	Ce Dy Er Eu Gd Ho La Lu Nd Pm Pr Sm Tb Tm Yb
1931	1.90%	transition series III	Au Hf Ir Os Pt Re Ta W
1930	0.76%		At Bi Fr Hg Pb Po Ra Rn Tl
1919	0.19%	actinide series	Ac Am Bk Cf Cm Es Fm Lr Md No Np Pa Pu Th U
2029	0.61%	"SAFs"	all except Br Ca Cl H I K N Na O

**Table III -- Generic Element Count and Graph Modifier Screens in Screen Number Order**

Screen	Freq.	Description	Elements
1918	14.84%	"metals"	all <u>except</u> Ar As At B Br C Cl F H He I Kr N Ne O P Rn S Se Si Te Xe
1919	0.19%	actinide series	Ac Am Bk Cf Cm Es Fm Lr Md No Np Pa Pu Th U
1920	1.10%	group Ib	Ag Au Cu
1921	3.35%	transition series II	Ag Mo Nb Pd Rh Ru Tc Zr
1923	2.93%	group IIIb	Al B Ga In Tl
1924	0.03%	group 0	Ar He Kr Ne Rn Xe
1925	6.12%	group Vb	As Bi P Sb
1926	2.27%		As Ga Ge Kr Rb Se Sr Y Zn
1929	31.99%	group VIIb	At Br Cl F I
1930	0.76%		At Bi Fr Hg Pb Po Ra Rn Tl
1931	1.90%	transition series III	Au Hf Ir Os Pt Re Ta W
1935	1.75%		Ba Cd Cs In Sb Sn Te Xe
1936	1.24%	group IIa	Ba Be Ca Mg Ra Sr
1956	1.03%	group IIb	Cd Hg Zn
1957	1.31%	lanthanide series	Ce Dy Er Eu Gd Ho La Lu Nd Pm Pr Sm Tb Tm Yb
1964	7.39%	transition series I	Co Cr Cu Fe Mn Ni Ti V
1965	6.72%	group VIII	Co Fe Ir Ni Os Pd Pt Rh Ru
1966	2.44%	group VIa	Cr Mo W
1967	2.00%	group Ia	Cs Fr K Li Na Rb
1983	5.61%	group IVb	Ge Pb Si Sn
1984	1.39%	group IVa	Hf Ti Zr
1988	0.53%	group IIIa	La Sc Y
1991	1.96%	group VIIa	Mn Re Tc
2001	1.12%	group Va	Nb Ta V
2003	86.62%		O S
2019	0.66%		Po Se Te
2029	0.61%	"SAFs"	all <u>except</u> Br Ca Cl H I K N Na O

# Periodic Table of the Elements Showing Fragment Numbers

1. line = Element Number 2. line = Vertical Group Number 3. line = Horizontal Group Number 1918 = Common Metal

Ia	Ila	Illa I	IVa	Va	Via	VIIa	VIII	Ib	Ilb	IIlb	IVb	Vb	Vlb	VIlb	0
														>= 2X 1976-1982	He = 1924
Li 1989 1967 - 1918	Be 1937 1936 - 1918														Ne - 1924
Na 2000 1967 - 1918	Mg 1990 1936 - 1918													F 1968-1974 1929	Ar - 1924
K 1987 1967 - 1918	Ca 1955 1936 - 1918	Sc - 1988 - 1918	Ti - 1984 1964 1918	V - 2001 1918	Cr - 1966 1964 1918	Mn - 1991 1964 1918	Fe 1975 1965 1964 1918	Co 1963 1965 1964 1918	Ni 1975 1965 1964 1918	Cu - 1920 1964 1918	Zn - 1956 1926 1918				Kr - 1924 1926
Rb - 1967 1926 1918	Sr - 1936 1926 1918	Y - 1988 1926 1918	Zr - 1984 1921 1918	Nb - 2001 1921 1918	Mo - 1966 1921 1918	Tc - 1991 1921 1918	Ru - 1965 1921 1918	Rh - 1965 1921 1918	Pd - 1965 1921 1918	Ag - 1920 1921 1918	Cd - 1956 1935 1918			I 1985-1986 1929	Xe - 1924 1935
Cs - 1967 1935 1918	Ba - 1936 1935 1918	La* - 1988 1957 1918	Hf - 1984 1931 1918	Ta - 2001 1931 1918	W - 1966 1931 1918	Re - 1991 1931 1918	Os - 1965 1931 1918	Ir - 1965 1931 1918	Pt 2020 1965 1931 1918	Au - 1920 1931 1918	Hg - 1956 1930 1918			At 1985-1986 1929	Rn - 1924 1930
Fr - 1967 1930 1918	Ra - 1936 1930 1918	Ac** - 1919 1918	Rf - 1918	Db - 1918	Sg - 1918	Bh - 1918	Hs - 1918	Mt - 1918	Ds - 1918	Uuu - 1918	Uub - 1918				-
*Lanthanide Series		Ce - 1957 1918	Pr - 1957 1918	Nd - 1957 1918	Pm - 1957 1918	Sm - 1957 1918	Eu - 1957 1918	Gd - 1957 1918	Tb - 1957 1918	Dy - 1957 1918	Ho - 1957 1918	Er - 1957 1918	Tm - 1957 1918	Yb - 1957 1918	Lu - 1957 1918
**Actinide Series		Th - 1919 1918	Pa - 1919 1918	U - 1919 1918	Np - 1919 1918	Pu - 1919 1918	Am - 1919 1918	Cm - 1919 1918	Bk - 1919 1918	Cf - 1919 1918	Es - 1919 1918	Fm - 1919 1918	Md - 1919 1918	No - 1919 1918	Lr - 1919 1918

## Special-purpose Graph Modifier Screens

Screen	Description	Freq.
<b><u>Structural feature screens</u></b>		
2039	abnormal mass -- all isotopic specifications	0.97%
2045	deuterium isotope	0.49%
2046	tritium and higher H isotopes (e.g., <sup>4</sup> H, <sup>5</sup> H, etc.)	0.06%
2047	isotope at unknown location (IUL)	0.05%
2041	abnormal valence	32.34%
2040	charge -- all charges: fixed, tautomeric or delocalized	12.50%
2042	delocalized charge only	0.10%
2076	tautomer	39.88%
<b><u>Multi-component substance screens</u></b>		
2127	2 or more components	18.61%
2077	3 or more components	7.24%
2078	4 or more components	4.55%
2079	single atom fragment (SAF)	6.69%
<b><u>Chemical substance class identifier screens</u></b>		
Note that these screens are not mutually exclusive -- a substance may belong to as many classes as are appropriate		
2050	alloy	3.22%
2082	CASREACT compound	14.04%
2049	coordination compound	8.16%
2048	incompletely defined (ID) substance	1.43%
2071	ID - unknown structure (ID molform)	0.21%
2072	ID - unknown point of attachment	0.99%
2073	ID - ester	0.14%
2074	ID - hydrogen (bond)	0.10%
2053	manual registration	221.62% <sup>1</sup>
2052	mineral	0.05%
2051	mixture (substance named as "mixt. with" in CA)	0.29%
2043	polymer (general category)	4.18%
2067	homopolymers and copolymers [ (A) <sub>x</sub> , (A.B) <sub>x</sub> , etc.]	3.20%
2068	polymers defined as structural repeating units (SRUs)	1.48%
2069	SRU with end groups [ X-(Y)-Z ]	0.52%
2070	SRU without end groups [ -(Y)- ]	1.00%
2054	radical ion	0.23%

<sup>1</sup> The high percentage of manual registrations is due to the many sequence registrations (peptides and nucleotides)

		Screen Number Order		Fragment Definition	Frequency Percent
Screen Number					
1	AS			C * C - C * C	13.51
2	AS			C * C - C - C	34.96
	AS			C - C - C * C	
3	AS			C - C * C - C	14.19
4	AS			C - C - C - C	32.65
5	AS			C * C * C * C * C	78.62
6	AS			Br- C * C - C * C	7.08
	AS			C * C - C * C - Br	
	AS			C * C - C * C - C	
	AS			C - C * C - C * C	
	AS			C * C - C * C - Cl	
	AS			C * C - C * C - F	
	AS			C * C - C * C - I	
	AS			C * C - C * C - N	
	AS			C * C - C * C - O	
	AS			C * C - C * C - S	
	AS			Cl- C * C - C * C	
	AS			F - C * C - C * C	
	AS			I - C * C - C * C	
	AS			N - C * C - C * C	
	AS			O - C * C - C * C	
	AS			S - C * C - C * C	
7	AS			C * C - C * C - C	6.85
	AS			C - C * C - C * C	
	AS			C * C - C - C * C - C	
	AS			C - C * C - C - C * C	
	AS			C - C * C - N - C * C	
	AS			C - C * C - O - C * C	
	AS			C - C * C - S - C * C	
	AS			C * C - N - C * C - C	
	AS			C * C - O - C * C - C	
	AS			C * C - S - C * C - C	
8	AS			C * C - C - C * C	6.91
9	AS			C * C - C - C - C	17.57
	AS			C - C - C - C * C	
10	AS			C - C * C * C - C	12.64
11	AS			C - C * C - C - C	6.14
	AS			C - C - C * C - C	
12	AS			C - C - C - C - C	19.16
13	AS			C * C * C * C * C * C	74.51

		Screen Number Order										
Screen Number		Fragment Definition										Frequency Percent
14	AS	Br-	C *	C -	C -	C *	C					3.46
	AS	C *	C -	C -	C *	C -	Br					
	AS	C *	C -	C -	C *	C -	C					
	AS	C -	C *	C -	C -	C *	C					
	AS	C *	C -	C -	C *	C -	Cl					
	AS	C *	C -	C -	C *	C -	F					
	AS	C *	C -	C -	C *	C -	I					
	AS	C *	C -	C -	C *	C -	N					
	AS	C *	C -	C -	C *	C -	O					
	AS	C *	C -	C -	C *	C -	S					
	AS	Cl-	C *	C -	C -	C *	C					
	AS	F -	C *	C -	C -	C *	C					
	AS	I -	C *	C -	C -	C *	C					
	AS	N -	C *	C -	C -	C *	C					
	AS	O -	C *	C -	C -	C *	C					
	AS	S -	C *	C -	C -	C *	C					
15	AS	C *	C -	C -	C -	C *	C				1.98	
16	AS	C *	C -	C -	C -	C -	C				6.81	
	AS	C -	C -	C -	C -	C *	C					
17	AS	C -	C *	C *	C *	C *	C -	C			11.88	
18	AS	C -	C *	C *	C -	C -	C				4.49	
	AS	C -	C -	C *	C *	C -	C					
19	AS	C -	C -	C *	C -	C -	C				1.06	
20	AS	C -	C -	C -	C -	C -	C				12.15	
21	AS	Br-	C *	C -	C *	C					1.70	
	AS	Br-	C *	C -	C -	C *	C					
	AS	Br-	C *	C -	N -	C *	C					
	AS	Br-	C *	C -	O -	C *	C					
	AS	Br-	C *	C -	S -	C *	C					
	AS	C *	C -	C *	C -	Br						
	AS	C *	C -	C -	C *	C -	Br					
	AS	C *	C -	C -	C *	C -	Cl					
	AS	C *	C -	C -	C *	C -	F					
	AS	C *	C -	C -	C *	C -	I					
	AS	C *	C -	C *	C -	Cl						
	AS	C *	C -	C *	C -	F						
	AS	C *	C -	C *	C -	I						
	AS	C *	C -	N -	C *	C -	Br					
	AS	C *	C -	N -	C *	C -	Cl					
	AS	C *	C -	N -	C *	C -	F					
	AS	C *	C -	N -	C *	C -	I					
	AS	C *	C -	O -	C *	C -	Br					
	AS	C *	C -	O -	C *	C -	Cl					
	AS	C *	C -	O -	C *	C -	F					
	AS	C *	C -	O -	C *	C -	I					
	AS	C *	C -	S -	C *	C -	Br					
	AS	C *	C -	S -	C *	C -	Cl					
	AS	C *	C -	S -	C *	C -	F					

Screen Number Order			
Screen Number		Fragment Definition	Frequency Percent
21	AS	C * C - S - C * C - I	1.70 (continued)
	AS	Cl- C * C - C * C	
	AS	Cl- C * C - C - C * C	
	AS	Cl- C * C - N - C * C	
	AS	Cl- C * C - O - C * C	
	AS	Cl- C * C - S - C * C	
	AS	F - C * C - C * C	
	AS	F - C * C - C - C * C	
	AS	F - C * C - N - C * C	
	AS	F - C * C - O - C * C	
	AS	F - C * C - S - C * C	
	AS	I - C * C - C * C	
	AS	I - C * C - C - C * C	
	AS	I - C * C - N - C * C	
	AS	I - C * C - O - C * C	
	AS	I - C * C - S - C * C	
22	AS	Br- C * C * C * C - C	5.91
	AS	C - C * C * C * C - Br	
	AS	C - C * C * C * C - Cl	
	AS	C - C * C * C * C - F	
	AS	C - C * C * C * C - I	
	AS	Cl- C * C * C * C - C	
	AS	F - C * C * C * C - C	
	AS	I - C * C * C * C - C	
23	AS	Br- C - C - C - C - C	0.96
	AS	C - C - C - C - C - Br	
	AS	C - C - C - C - C - Cl	
	AS	C - C - C - C - C - F	
	AS	C - C - C - C - C - I	
	AS	Cl- C - C - C - C - C	
	AS	F - C - C - C - C - C	
	AS	I - C - C - C - C - C	
24	AS	C * C * C * C * C * N	27.22
	AS	N * C * C * C * C * C	
25	AS	C * C - C * C * C * N	4.17
	AS	N * C * C * C - C * C	
26	AS	C * C - C - C * C - N	1.63
	AS	C * C - C * C - N	
	AS	C * C - N - C * C - N	
	AS	C * C - O - C * C - N	
	AS	C * C - S - C * C - N	
	AS	N - C * C - C * C	
	AS	N - C * C - C - C * C	
	AS	N - C * C - N - C * C	
	AS	N - C * C - O - C * C	
	AS	N - C * C - S - C * C	
27	AS	C * C - C - C - C - N	5.29
	AS	N - C - C - C - C * C	



		Screen Number Order											
Screen Number		Fragment Definition											Frequency Percent
28	AS	C	-	C	*	C	*	C	*	C	*	N	11.69
	AS	N	*	C	*	C	*	C	*	C	-	C	
29	AS	C	-	C	*	C	*	C	*	C	-	N	8.40
	AS	N	-	C	*	C	*	C	*	C	-	C	
30	AS	C	-	C	*	C	*	C	-	C	-	N	2.36
	AS	N	-	C	-	C	*	C	*	C	-	C	
31	AS	C	-	C	*	C	-	C	-	C	-	N	0.41
	AS	N	-	C	-	C	-	C	*	C	-	C	
32	AS	C	-	C	-	C	*	C	*	C	-	N	0.92
	AS	N	-	C	*	C	*	C	-	C	-	C	
33	AS	C	-	C	-	C	*	C	-	C	-	N	0.34
	AS	N	-	C	-	C	*	C	-	C	-	C	
34	AS	C	-	C	-	C	-	C	-	C	-	N	7.98
	AS	N	-	C	-	C	-	C	-	C	-	C	
35	AS	C	*	C	*	C	*	C	*	C	*	O	14.10
	AS	C	*	C	*	C	*	C	*	C	*	S	
	AS	O	*	C	*	C	*	C	*	C	*	C	
	AS	S	*	C	*	C	*	C	*	C	*	C	
36	AS	C	*	C	-	C	*	C	*	C	*	O	1.56
	AS	C	*	C	-	C	*	C	*	C	*	S	
	AS	O	*	C	*	C	*	C	-	C	*	C	
	AS	S	*	C	*	C	*	C	-	C	*	C	
37	AS	C	*	C	-	C	*	C	*	C	-	O	2.60
	AS	C	*	C	-	C	*	C	*	C	-	S	
	AS	O	-	C	*	C	*	C	-	C	*	C	
	AS	S	-	C	*	C	*	C	-	C	*	C	
38	AS	C	*	C	-	C	-	C	*	C	-	O	5.99
	AS	C	*	C	-	C	-	C	*	C	-	S	
	AS	C	*	C	-	C	*	C	-	O			
	AS	C	*	C	-	C	*	C	-	S			
	AS	C	*	C	-	N	-	C	*	C	-	O	
	AS	C	*	C	-	N	-	C	*	C	-	S	
	AS	C	*	C	-	O	-	C	*	C	-	O	
	AS	C	*	C	-	O	-	C	*	C	-	S	
	AS	C	*	C	-	S	-	C	*	C	-	O	
	AS	C	*	C	-	S	-	C	*	C	-	S	
	AS	O	-	C	*	C	-	C	*	C			
	AS	O	-	C	*	C	-	C	-	C	*	C	
	AS	O	-	C	*	C	-	N	-	C	*	C	
	AS	O	-	C	*	C	-	O	-	C	*	C	
	AS	O	-	C	*	C	-	S	-	C	*	C	
	AS	S	-	C	*	C	-	C	*	C			
	AS	S	-	C	*	C	-	C	-	C	*	C	
	AS	S	-	C	*	C	-	N	-	C	*	C	
	AS	S	-	C	*	C	-	O	-	C	*	C	
	AS	S	-	C	*	C	-	S	-	C	*	C	

		Screen Number Order											
Screen Number		Fragment Definition							Frequency Percent				
39	AS	C	*	C	-	C	-	C	-	O	7.78		
	AS	C	*	C	-	C	-	C	-	S			
	AS	O	-	C	-	C	-	C	*	C			
	AS	S	-	C	-	C	-	C	-	C			
40	AS	C	-	C	*	C	*	C	*	C	*	O	9.53
	AS	C	-	C	*	C	*	C	*	C	*	S	
	AS	O	*	C	*	C	*	C	*	C	-	C	
	AS	S	*	C	*	C	*	C	*	C	-	C	
41	AS	C	-	C	*	C	*	C	*	C	-	O	19.86
	AS	C	-	C	*	C	*	C	*	C	-	S	
	AS	O	-	C	*	C	*	C	*	C	-	C	
	AS	S	-	C	*	C	*	C	*	C	-	C	
42	AS	C	-	C	*	C	*	C	-	C	-	O	4.15
	AS	C	-	C	*	C	*	C	-	C	-	S	
	AS	O	-	C	-	C	*	C	*	C	-	C	
	AS	S	-	C	-	C	*	C	*	C	-	C	
43	AS	C	-	C	*	C	-	C	-	C	-	O	1.01
	AS	C	-	C	*	C	-	C	-	C	-	S	
	AS	O	-	C	-	C	-	C	*	C	-	C	
	AS	S	-	C	-	C	-	C	*	C	-	C	
44	AS	C	-	C	-	C	*	C	*	C	-	O	4.16
	AS	C	-	C	-	C	*	C	*	C	-	S	
	AS	O	-	C	*	C	*	C	-	C	-	C	
	AS	S	-	C	*	C	*	C	-	C	-	C	
45	AS	C	-	C	-	C	*	C	-	C	-	O	1.26
	AS	C	-	C	-	C	*	C	-	C	-	S	
	AS	O	-	C	-	C	*	C	-	C	-	C	
	AS	S	-	C	-	C	*	C	-	C	-	C	
46	AS	C	-	C	-	C	-	C	-	C	-	O	12.64
	AS	C	-	C	-	C	-	C	-	C	-	S	
	AS	O	-	C	-	C	-	C	-	C	-	C	
	AS	S	-	C	-	C	-	C	-	C	-	C	
47	AS	As	C		C		C		C		C		3.83
	AS	B		C		C		C		C		C	
	AS	C		C		C		C		C		As	
	AS	C		C		C		C		C		B	
	AS	C		C		C		C		C		P	
	AS	C		C		C		C		C		Se	
	AS	C		C		C		C		C		Si	
	AS	C		C		C		C		C		Te	
	AS	P		C		C		C		C		C	
	AS	Se		C		C		C		C		C	
	AS	Si		C		C		C		C		C	
	AS	Te		C		C		C		C		C	

		Screen Number Order		Frequency Percent
Screen Number		Fragment Definition		
48	AS	Br- C - C - C * C		0.77
	AS	C * C - C - C - Br		
	AS	C * C - C - C - Cl		
	AS	C * C - C - C - F		
	AS	C * C - C - C - I		
	AS	Cl- C - C - C * C		
	AS	F - C - C - C * C		
	AS	I - C - C - C * C		
49	AS	Br- C * C * C - C		4.52
	AS	C - C * C * C - Br		
	AS	C - C * C * C - Cl		
	AS	C - C * C * C - F		
	AS	C - C * C * C - I		
	AS	Cl- C * C * C - C		
	AS	F - C * C * C - C		
	AS	I - C * C * C - C		
50	AS	Br- C * C - C - C		1.14
	AS	C - C - C * C - Br		
	AS	C - C - C * C - Cl		
	AS	C - C - C * C - F		
	AS	C - C - C * C - I		
	AS	Cl- C * C - C - C		
	AS	F - C * C - C - C		
	AS	I - C * C - C - C		
51	AS	Br- C - C - C - C		1.49
	AS	C - C - C - C - Br		
	AS	C - C - C - C - Cl		
	AS	C - C - C - C - F		
	AS	C - C - C - C - I		
	AS	Cl- C - C - C - C		
	AS	F - C - C - C - C		
	AS	I - C - C - C - C		
52	AS	C * C * C * C * N		31.81
	AS	N * C * C * C * C		
53	AS	C * C - C * C * N		2.97
	AS	N * C * C - C * C		
54	AS	C * C - C - C * N		1.62
	AS	N * C - C - C * C		
55	AS	C * C - C - C - N		8.56
	AS	N - C - C - C * C		
56	AS	C - C * C * C * N		13.91
	AS	N * C * C * C - C		
57	AS	C - C * C * C - N		6.09
	AS	N - C * C * C - C		

		Screen Number Order											
Screen Number		Fragment Definition					Frequency Percent						
58	AS	C	-	C	*	C	-	C	-	N	2.87		
	AS	N	-	C	-	C	*	C	-	C			
59	AS	C	-	C	-	C	*	C	*	N	7.01		
	AS	N	*	C	*	C	-	C	-	C			
60	AS	C	-	C	-	C	*	C	-	N	1.24		
	AS	N	-	C	*	C	-	C	-	C			
61	AS	C	-	C	-	C	-	C	-	N	14.08		
	AS	N	-	C	-	C	-	C	-	C			
62	AS	C	*	C	-	C	-	C	-	N	*	C	1.14
	AS	C	*	N	-	C	-	C	-	C	*	C	
63	AS	C	*	C	-	C	-	C	-	N	-	C	5.95
	AS	C	-	N	-	C	-	C	-	C	*	C	
64	AS	C	-	C	*	C	*	C	*	N	-	C	5.71
	AS	C	-	N	*	C	*	C	*	C	-	C	
65	AS	C	-	C	*	C	*	C	-	N	-	C	2.97
	AS	C	-	N	-	C	*	C	*	C	-	C	
66	AS	C	-	C	*	C	-	C	-	N	-	C	1.27
	AS	C	-	N	-	C	-	C	*	C	-	C	
67	AS	C	*	C	*	C	*	C	*	N	*	N	2.26
	AS	N	*	N	*	C	*	C	*	C	*	C	
68	AS	C	*	C	-	C	-	C	-	N	-	N	0.23
	AS	N	-	N	-	C	-	C	-	C	*	C	
69	AS	C	-	C	*	C	*	C	-	N	-	N	0.49
	AS	N	-	N	-	C	*	C	*	C	-	C	
70	AS	C	*	C	-	C	-	C	-	N	-	O	0.32
	AS	C	*	C	-	C	-	C	-	N	-	S	
	AS	O	-	N	-	C	-	C	-	C	*	C	
	AS	S	-	N	-	C	-	C	-	C	*	C	
71	AS	C	-	C	*	C	*	C	-	N	-	O	1.36
	AS	C	-	C	*	C	*	C	-	N	-	S	
	AS	O	-	N	-	C	*	C	*	C	-	C	
	AS	S	-	N	-	C	*	C	*	C	-	C	
72	AS	C	*	C	*	C	*	C	*	O	19.48		
	AS	C	*	C	*	C	*	C	*	S			
	AS	O	*	C	*	C	*	C	*	C			
	AS	S	*	C	*	C	*	C	*	C			
73	AS	C	*	C	-	C	*	C	*	O	2.01		
	AS	C	*	C	-	C	*	C	*	S			
	AS	O	*	C	*	C	-	C	*	C			
	AS	S	*	C	*	C	-	C	*	C			

		Screen Number Order											
Screen Number		Fragment Definition							Frequency Percent				
74	AS	C	*	C	-	C	-	C	*	O	1.34		
	AS	C	*	C	-	C	-	C	*	S			
	AS	O	*	C	-	C	-	C	*	C			
	AS	S	*	C	-	C	-	C	*	C			
75	AS	C	*	C	-	C	-	C	-	O	6.25		
	AS	C	*	C	-	C	-	C	-	S			
	AS	O	-	C	-	C	-	C	*	C			
	AS	S	-	C	-	C	-	C	*	C			
76	AS	C	-	C	*	C	*	C	*	O	7.10		
	AS	C	-	C	*	C	*	C	*	S			
	AS	O	*	C	*	C	*	C	-	C			
	AS	S	*	C	*	C	*	C	-	C			
77	AS	C	-	C	*	C	*	C	-	O	14.59		
	AS	C	-	C	*	C	*	C	-	S			
	AS	O	-	C	*	C	*	C	-	C			
	AS	S	-	C	*	C	*	C	-	C			
78	AS	C	-	C	*	C	-	C	-	O	6.22		
	AS	C	-	C	*	C	-	C	-	S			
	AS	O	-	C	-	C	*	C	-	C			
	AS	S	-	C	-	C	*	C	-	C			
79	AS	C	-	C	-	C	*	C	-	O	6.96		
	AS	C	-	C	-	C	*	C	-	S			
	AS	O	-	C	*	C	-	C	-	C			
	AS	S	-	C	*	C	-	C	-	C			
80	AS	C	-	C	-	C	-	C	-	O	21.57		
	AS	C	-	C	-	C	-	C	-	S			
	AS	O	-	C	-	C	-	C	-	C			
	AS	S	-	C	-	C	-	C	-	C			
81	AS	C	*	C	-	C	-	C	-	O	-	C	2.56
	AS	C	*	C	-	C	-	C	-	S	-	C	
	AS	C	-	O	-	C	-	C	-	C	*	C	
	AS	C	-	S	-	C	-	C	-	C	*	C	
82	AS	C	-	C	*	C	*	C	-	O	-	C	7.34
	AS	C	-	C	*	C	*	C	-	S	-	C	
	AS	C	-	O	-	C	*	C	*	C	-	C	
	AS	C	-	S	-	C	*	C	*	C	-	C	
83	AS	C	-	C	*	C	-	C	-	O	-	C	2.79
	AS	C	-	C	*	C	-	C	-	S	-	C	
	AS	C	-	O	-	C	-	C	*	C	-	C	
	AS	C	-	S	-	C	-	C	*	C	-	C	
84	AS	C	-	C	-	C	*	C	-	O	-	C	1.91
	AS	C	-	C	-	C	*	C	-	S	-	C	
	AS	C	-	O	-	C	*	C	-	C	-	C	
	AS	C	-	S	-	C	*	C	-	C	-	C	

		Screen Number Order		Frequency Percent
Screen Number		Fragment Definition		
85	AS	C - C * C * C - O - N		0.42
	AS	C - C * C * C - S - N		
	AS	N - O - C * C * C - C		
	AS	N - S - C * C * C - C		
86	AS	C - C * C * C - O - O		0.75
	AS	C - C * C * C - O - S		
	AS	C - C * C * C - S - O		
	AS	C - C * C * C - S - S		
	AS	O - O - C * C * C - C		
	AS	O - S - C * C * C - C		
	AS	S - O - C * C * C - C		
	AS	S - S - C * C * C - C		
87	AS	Br- C - C * C		3.30
	AS	C * C - C - Br		
	AS	C * C - C - Cl		
	AS	C * C - C - F		
	AS	C * C - C - I		
	AS	Cl- C - C * C		
	AS	F - C - C * C		
	AS	I - C - C * C		
88	AS	Br- C * C - C		4.80
	AS	C - C * C - Br		
	AS	C - C * C - Cl		
	AS	C - C * C - F		
	AS	C - C * C - I		
	AS	Cl- C * C - C		
	AS	F - C * C - C		
	AS	I - C * C - C		
89	AS	Br- C - C - C		2.86
	AS	C - C - C - Br		
	AS	C - C - C - Cl		
	AS	C - C - C - F		
	AS	C - C - C - I		
	AS	Cl- C - C - C		
	AS	F - C - C - C		
	AS	I - C - C - C		
90	AS	C * C - C * N		8.61
	AS	N * C - C * C		
91	AS	C * C - C - N		22.25
	AS	N - C - C * C		22.25
92	AS	C - C * C * N		16.85
	AS	N * C * C - C		16.85
93	AS	C - C * C - N		6.37
	AS	N - C * C - C		
94	AS	C - C - C * N		6.85
	AS	N * C - C - C		

		Screen Number Order		Fragment Definition	Frequency Percent
Screen Number					
95	AS		C - C - C - N		24.66
	AS		N - C - C - C		
96	AS		C * C - C - N * C		4.61
	AS		C * N - C - C * C		
97	AS		C * C - C - N - C		12.91
	AS		C - N - C - C * C		
98	AS		C - C * C * N - C		5.92
	AS		C - N * C * C - C		
99	AS		C - C * C - N - C		1.84
	AS		C - N - C * C - C		
100	AS		C - C - C - N * C		7.00
	AS		C * N - C - C - C		
101	AS		C * C - C - N - C * C		4.57
	AS		C * C - N - C - C * C		
102	AS		Br- C * C - N - C * C		0.92
	AS		C - C * C - N - C * C		
	AS		C * C - N - C * C - Br		
	AS		C * C - N - C * C - C		
	AS		C * C - N - C * C - Cl		
	AS		C * C - N - C * C - F		
	AS		C * C - N - C * C - I		
	AS		C * C - N - C * C - N		
	AS		C * C - N - C * C - O		
	AS		C * C - N - C * C - S		
	AS		Cl- C * C - N - C * C		
	AS		F - C * C - N - C * C		
	AS		I - C * C - N - C * C		
	AS		N - C * C - N - C * C		
	AS		O - C * C - N - C * C		
	AS		S - C * C - N - C * C		
103	AS		C * C * C * N * C * N		9.30
	AS		N * C * N * C * C * C		
104	AS		C * C - C - N - C - N		0.88
	AS		N - C - N - C - C * C		
105	AS		C - C * C - N - C - N		0.37
	AS		N - C - N - C * C - C		
106	AS		C * C * C * N * C * O		2.79
	AS		C * C * C * N * C * S		
	AS		O * C * N * C * C * C		
	AS		S * C * N * C * C * C		
107	AS		C * C - C - N * C - O		1.02
	AS		C * C - C - N * C - S		
	AS		O - C * N - C - C * C		
	AS		S - C * N - C - C * C		

		Screen Number Order											
Screen Number		Fragment Definition							Frequency Percent				
108	AS	C	*	C	-	C	-	N	-	C	-	O	3.00
	AS	C	*	C	-	C	-	N	-	C	-	S	
	AS	O	-	C	-	N	-	C	-	C	*	C	
	AS	S	-	C	-	N	-	C	-	C	*	C	
109	AS	C	-	C	*	C	-	N	-	C	-	O	2.05
	AS	C	-	C	*	C	-	N	-	C	-	S	
	AS	O	-	C	-	N	-	C	*	C	-	C	
	AS	S	-	C	-	N	-	C	*	C	-	C	
110	AS	C	*	C	*	C	*	N	*	N			4.61
	AS	N	*	N	*	C	*	C	*	C			
111	AS	C	*	C	-	C	-	N	-	N			2.65
	AS	N	-	N	-	C	-	C	*	C			
112	AS	C	-	C	*	C	-	N	-	N			0.55
	AS	N	-	N	-	C	*	C	-	C			
113	AS	C	-	C	-	C	-	N	-	N			1.14
	AS	N	-	N	-	C	-	C	-	C			
114	AS	C	*	C	-	C	-	N	-	O			1.22
	AS	C	*	C	-	C	-	N	-	S			
	AS	O	-	N	-	C	-	C	*	C			
	AS	S	-	N	-	C	-	C	*	C			
115	AS	C	-	C	*	C	-	N	-	O			0.94
	AS	C	-	C	*	C	-	N	-	S			
	AS	O	-	N	-	C	*	C	-	C			
	AS	S	-	N	-	C	*	C	-	C			
116	AS	C	*	C	-	C	*	O					4.30
	AS	C	*	C	-	C	*	S					
	AS	O	*	C	-	C	*	C					
	AS	S	*	C	-	C	*	C					
117	AS	C	*	C	-	C	-	O					33.04
	AS	C	*	C	-	C	-	S					
	AS	O	-	C	-	C	*	C					
	AS	S	-	C	-	C	*	C					
118	AS	C	-	C	*	C	*	O					9.42
	AS	C	-	C	*	C	*	S					
	AS	O	*	C	*	C	-	C					
	AS	S	*	C	*	C	-	C					
119	AS	C	-	C	*	C	-	O					18.18
	AS	C	-	C	*	C	-	S					
	AS	O	-	C	*	C	-	C					
	AS	S	-	C	*	C	-	C					
120	AS	C	-	C	-	C	*	O					5.21
	AS	C	-	C	-	C	*	S					
	AS	O	*	C	-	C	-	C					
	AS	S	*	C	-	C	-	C					



		Screen Number Order		Frequency Percent
Screen Number		Fragment Definition		
121	AS	C - C - C - O		32.90
	AS	C - C - C - S		
	AS	O - C - C - C		
	AS	S - C - C - C		
122	AS	C * C - C - O - C		13.92
	AS	C * C - C - S - C		
	AS	C - O - C - C * C		
	AS	C - S - C - C * C		
123	AS	C - C * C - O - C		6.93
	AS	C - C * C - S - C		
	AS	C - O - C * C - C		
	AS	C - S - C * C - C		
124	AS	C - C - C - O - C		16.58
	AS	C - C - C - S - C		
	AS	C - O - C - C - C		
	AS	C - S - C - C - C		
125	AS	C * C - C - O - C * C		4.07
	AS	C * C - C - S - C * C		
	AS	C * C - O - C - C * C		
	AS	C * C - S - C - C * C		
126	AS	Br- C * C - O - C * C		2.20
	AS	Br- C * C - S - C * C		
	AS	C - C * C - O - C * C		
	AS	C - C * C - S - C * C		
	AS	C * C - O - C * C - Br		
	AS	C * C - O - C * C - C		
	AS	C * C - O - C * C - Cl		
	AS	C * C - O - C * C - F		
	AS	C * C - O - C * C - I		
	AS	C * C - O - C * C - N		
	AS	C * C - O - C * C - O		
	AS	C * C - O - C * C - S		
	AS	C * C - S - C * C - Br		
	AS	C * C - S - C * C - C		
	AS	C * C - S - C * C - Cl		
	AS	C * C - S - C * C - F		
	AS	C * C - S - C * C - I		
	AS	C * C - S - C * C - N		
	AS	C * C - S - C * C - O		
	AS	C * C - S - C * C - S		
	AS	Cl- C * C - O - C * C		
	AS	Cl- C * C - S - C * C		
	AS	F - C * C - O - C * C		
	AS	F - C * C - S - C * C		
	AS	I - C * C - O - C * C		
	AS	I - C * C - S - C * C		
	AS	N - C * C - O - C * C		
	AS	N - C * C - S - C * C		
	AS	O - C * C - O - C * C		
	AS	O - C * C - S - C * C		
	AS	S - C * C - O - C * C		
	AS	S - C * C - S - C * C		

		Screen Number Order											
Screen Number		Fragment Definition										Frequency Percent	
127	AS	C	-	C	-	C	-	O	-	C	*	C	5.20
	AS	C	-	C	-	C	-	S	-	C	*	C	
	AS	C	*	C	-	O	-	C	-	C	-	C	
	AS	C	*	C	-	S	-	C	-	C	-	C	
128	AS	C	*	C	-	C	-	O	-	C	-	O	3.28
	AS	C	*	C	-	C	-	O	-	C	-	S	
	AS	C	*	C	-	C	-	S	-	C	-	O	
	AS	C	*	C	-	C	-	S	-	C	-	S	
	AS	O	-	C	-	O	-	C	-	C	*	C	
	AS	O	-	C	-	S	-	C	-	C	*	C	
	AS	S	-	C	-	O	-	C	-	C	*	C	
	AS	S	-	C	-	S	-	C	-	C	*	C	
129	AS	C	*	C	-	C	-	O	-	N		0.35	
	AS	C	*	C	-	C	-	S	-	N			
	AS	N	-	O	-	C	-	C	*	C			
	AS	N	-	S	-	C	-	C	*	C			
130	AS	C	-	C	*	C	-	O	-	N		0.32	
	AS	C	-	C	*	C	-	S	-	N			
	AS	N	-	O	-	C	*	C	-	C			
	AS	N	-	S	-	C	*	C	-	C			
131	AS	C	*	C	-	C	-	O	-	O		0.48	
	AS	C	*	C	-	C	-	O	-	S			
	AS	C	*	C	-	C	-	S	-	O			
	AS	C	*	C	-	C	-	S	-	S			
	AS	O	-	O	-	C	-	C	*	C			
	AS	O	-	S	-	C	-	C	*	C			
	AS	S	-	O	-	C	-	C	*	C			
	AS	S	-	S	-	C	-	C	*	C			
132	AS	C	-	C	*	C	-	O	-	O		0.71	
	AS	C	-	C	*	C	-	O	-	S			
	AS	C	-	C	*	C	-	S	-	O			
	AS	C	-	C	*	C	-	S	-	S			
	AS	O	-	O	-	C	*	C	-	C			
	AS	O	-	S	-	C	*	C	-	C			
	AS	S	-	O	-	C	*	C	-	C			
	AS	S	-	S	-	C	*	C	-	C			
133	AS	C	-	C	-	C	-	O	-	O		1.20	
	AS	C	-	C	-	C	-	O	-	S			
	AS	C	-	C	-	C	-	S	-	O			
	AS	C	-	C	-	C	-	S	-	S			
	AS	O	-	O	-	C	-	C	-	C			
	AS	O	-	S	-	C	-	C	-	C			
	AS	S	-	O	-	C	-	C	-	C			
	AS	S	-	S	-	C	-	C	-	C			

		Screen Number Order				
Screen Number		Fragment Definition				Frequency Percent
134	AS	As	C	C	C	4.57
	AS	B	C	C	C	
	AS	C	C	C	As	
	AS	C	C	C	B	
	AS	C	C	C	P	
	AS	C	C	C	Se	
	AS	C	C	C	Si	
	AS	C	C	C	Te	
	AS	P	C	C	C	
	AS	Se	C	C	C	
	AS	Si	C	C	C	
	AS	Te	C	C	C	
135	AS	C * C - N * C				8.07
	AS	C * N - C * C				
136	AS	C * C - N - C				18.27
	AS	C - N - C * C				
137	AS	C - C * N - C				8.60
	AS	C - N * C - C				
138	AS	C - C - N * C				14.80
	AS	C * N - C - C				
139	AS	C - C - N - C				29.65
	AS	C - N - C - C				
140	AS	C * C * N * C * C				30.93
141	AS	C * C - N * C - C				1.71
	AS	C - C * N - C * C				
142	AS	C * C - N - C * C				1.80
143	AS	C * C - N - C - C				12.19
	AS	C - C - N - C * C				
144	AS	C - C * N * C - C				3.03
145	AS	C - C - N - C - C				15.23
146	AS	C * C * N * C * C * N				6.79
	AS	N * C * C * N * C * C				
147	AS	C * C - N - C - C - N				1.84
	AS	N - C - C - N - C * C				
148	AS	C * C * N * C * C * O				3.85
	AS	C * C * N * C * C * S				
	AS	O * C * C * N * C * C				
	AS	S * C * C * N * C * C				

		Screen Number Order											
Screen Number		Fragment Definition							Frequency Percent				
149	AS	C	*	C	-	N	-	C	-	C	-	O	2.49
	AS	C	*	C	-	N	-	C	-	C	-	S	
	AS	O	-	C	-	C	-	N	-	C	*	C	
	AS	S	-	C	-	C	-	N	-	C	*	C	
150	AS	C	*	C	*	N	*	C	*	N		12.29	
	AS	N	*	C	*	N	*	C	*	C			
151	AS	C	*	C	-	N	-	C	*	N		1.72	
	AS	N	*	C	-	N	-	C	*	C			
152	AS	C	*	C	-	N	-	C	-	N		2.36	
	AS	N	-	C	-	N	-	C	*	C			
153	AS	C	-	C	*	N	*	C	*	N		5.44	
	AS	N	*	C	*	N	*	C	-	C			
154	AS	C	-	C	*	N	*	C	-	N		2.20	
	AS	N	-	C	*	N	*	C	-	C			
155	AS	C	-	C	-	N	-	C	-	N		3.79	
	AS	N	-	C	-	N	-	C	-	C			
156	AS	C	*	C	-	N	-	C	-	N	-	C	1.65
	AS	C	-	N	-	C	-	N	-	C	*	C	
157	AS	C	*	C	*	N	*	C	*	O		6.29	
	AS	C	*	C	*	N	*	C	*	S			
	AS	O	*	C	*	N	*	C	*	C			
	AS	S	*	C	*	N	*	C	*	C			
158	AS	C	*	C	-	N	*	C	-	O		3.59	
	AS	C	*	C	-	N	*	C	-	S			
	AS	O	-	C	*	N	-	C	*	C			
	AS	S	-	C	*	N	-	C	*	C			
159	AS	C	*	C	-	N	-	C	*	O		0.71	
	AS	C	*	C	-	N	-	C	*	S			
	AS	O	*	C	-	N	-	C	*	C			
	AS	S	*	C	-	N	-	C	*	C			
160	AS	C	*	C	-	N	-	C	-	O		11.07	
	AS	C	*	C	-	N	-	C	-	S			
	AS	O	-	C	-	N	-	C	*	C			
	AS	S	-	C	-	N	-	C	*	C			
161	AS	C	-	C	*	N	*	C	*	O		3.21	
	AS	C	-	C	*	N	*	C	*	S			
	AS	O	*	C	*	N	*	C	-	C			
	AS	S	*	C	*	N	*	C	-	C			
162	AS	C	-	C	*	N	*	C	-	O		4.84	
	AS	C	-	C	*	N	*	C	-	S			
	AS	O	-	C	*	N	*	C	-	C			
	AS	S	-	C	*	N	*	C	-	C			

Screen Number Order			
Screen Number		Fragment Definition	Frequency Percent
163	AS	C - C * N - C - O	2.74
	AS	C - C * N - C - S	
	AS	O - C - N * C - C	
	AS	S - C - N * C - C	
164	AS	C - C - N - C - O	13.37
	AS	C - C - N - C - S	
	AS	O - C - N - C - C	
	AS	S - C - N - C - C	
165	AS	C * C - N - C - O - C	0.83
	AS	C * C - N - C - S - C	
	AS	C - O - C - N - C * C	
	AS	C - S - C - N - C * C	
166	AS	C * C - N * N	1.79
	AS	N * N - C * C	
167	AS	C * C - N - N	2.67
	AS	N - N - C * C	
168	AS	C - C * N * N	4.81
	AS	N * N * C - C	
169	AS	C - C - N - N	3.78
	AS	N - N - C - C	
170	AS	C - C * N * N - C	1.83
	AS	C - N * N * C - C	
171	AS	C - C - N - N - C	2.85
	AS	C - N - N - C - C	
172	AS	C * C - N - N - C * C	1.18
173	AS	C * C * N * O	1.32
	AS	C * C * N * S	
	AS	O * N * C * C	
	AS	S * N * C * C	
174	AS	C * C - N - O	6.36
	AS	C * C - N - S	
	AS	O - N - C * C	
	AS	S - N - C * C	
175	AS	C - C * N - O	0.56
	AS	C - C * N - S	
	AS	O - N * C - C	
	AS	S - N * C - C	
176	AS	C - C - N - O	3.06
	AS	C - C - N - S	
	AS	O - N - C - C	
	AS	S - N - C - C	

		Screen Number Order									
Screen Number		Fragment Definition						Frequency Percent			
177	AS	C	*	C	-	N	-	O	-	C	1.40
	AS	C	*	C	-	N	-	S	-	C	
	AS	C	-	O	-	N	-	C	*	C	
	AS	C	-	S	-	N	-	C	*	C	
178	AS	C	-	C	-	N	-	O	-	C	2.11
	AS	C	-	C	-	N	-	S	-	C	
	AS	C	-	O	-	N	-	C	-	C	
	AS	C	-	S	-	N	-	C	-	C	
179	AS	C	*	C	-	N	-	O	-	O	1.31
	AS	C	*	C	-	N	-	O	-	S	
	AS	C	*	C	-	N	-	S	-	O	
	AS	C	*	C	-	N	-	S	-	S	
	AS	O	-	O	-	N	-	C	*	C	
	AS	O	-	S	-	N	-	C	*	C	
	AS	S	-	O	-	N	-	C	*	C	
	AS	S	-	S	-	N	-	C	*	C	
180	AS	C	*	C	-	O	-	C			26.47
	AS	C	*	C	-	S	-	C			
	AS	C	-	O	-	C	*	C			
	AS	C	-	S	-	C	*	C			
181	AS	C	*	C	*	O	*	C	*	C	17.85
	AS	C	*	C	*	S	*	C	*	C	
182	AS	C	*	C	-	O	-	C	*	C	3.48
	AS	C	*	C	-	S	-	C	*	C	
183	AS	C	*	C	-	O	-	C	-	C	14.37
	AS	C	-	C	-	O	-	C	*	C	
	AS	C	*	C	-	S	-	C	-	C	
	AS	C	-	C	-	S	-	C	*	C	
184	AS	C	-	C	*	O	*	C	-	C	2.61
	AS	C	-	C	*	S	*	C	-	C	
185	AS	C	-	C	-	O	-	C	-	C	13.52
	AS	C	-	C	-	S	-	C	-	C	
186	AS	Br	C		C	O		C		C	2.66
	AS	Br	C		C	S		C		C	
	AS	C		C	O	C		C		Br	
	AS	C		C	O	C		C		Cl	
	AS	C		C	O	C		C		F	
	AS	C		C	O	C		C		I	
	AS	C		C	S	C		C		Br	
	AS	C		C	S	C		C		Cl	
	AS	C		C	S	C		C		F	
	AS	C		C	S	C		C		I	
	AS	Cl	C		C	O		C		C	
	AS	Cl	C		C	S		C		C	
	AS	F	C		C	O		C		C	
	AS	F	C		C	S		C		C	
	AS	I	C		C	O		C		C	
	AS	I	C		C	S		C		C	

		Screen Number Order											
Screen Number		Fragment Definition							Frequency Percent				
187	AS	C	*	C	-	O	-	C	-	C	-	O	3.29
	AS	C	*	C	-	O	-	C	-	C	-	S	
	AS	C	*	C	-	S	-	C	-	C	-	O	
	AS	C	*	C	-	S	-	C	-	C	-	S	
	AS	O	-	C	-	C	-	O	-	C	*	C	
	AS	O	-	C	-	C	-	S	-	C	*	C	
	AS	S	-	C	-	C	-	O	-	C	*	C	
	AS	S	-	C	-	C	-	S	-	C	*	C	
188	AS	C	*	C	-	O	-	C	*	N	0.61		
	AS	C	*	C	-	S	-	C	*	N			
	AS	N	*	C	-	O	-	C	*	C			
	AS	N	*	C	-	S	-	C	*	C			
189	AS	C	*	C	-	O	-	C	-	N	0.58		
	AS	C	*	C	-	S	-	C	-	N			
	AS	N	-	C	-	O	-	C	*	C			
	AS	N	-	C	-	S	-	C	*	C			
190	AS	C	-	C	*	O	*	C	*	N	2.79		
	AS	C	-	C	*	S	*	C	*	N			
	AS	N	*	C	*	O	*	C	-	C			
	AS	N	*	C	*	S	*	C	-	C			
191	AS	C	-	C	*	O	*	C	-	N	2.04		
	AS	C	-	C	*	S	*	C	-	N			
	AS	N	-	C	*	O	*	C	-	C			
	AS	N	-	C	*	S	*	C	-	C			
192	AS	C	*	C	-	O	-	C	*	O	1.20		
	AS	C	*	C	-	O	-	C	*	S			
	AS	C	*	C	-	S	-	C	*	O			
	AS	C	*	C	-	S	-	C	*	S			
	AS	O	*	C	-	O	-	C	*	C			
	AS	O	*	C	-	S	-	C	*	C			
	AS	S	*	C	-	O	-	C	*	C			
	AS	S	*	C	-	S	-	C	*	C			
193	AS	C	*	C	-	O	-	C	-	O	4.71		
	AS	C	*	C	-	O	-	C	-	S			
	AS	C	*	C	-	S	-	C	-	O			
	AS	C	*	C	-	S	-	C	-	S			
	AS	O	-	C	-	O	-	C	*	C			
	AS	O	-	C	-	S	-	C	*	C			
	AS	S	-	C	-	O	-	C	*	C			
	AS	S	-	C	-	S	-	C	*	C			
194	AS	C	-	C	*	O	*	C	-	O	3.38		
	AS	C	-	C	*	O	*	C	-	S			
	AS	C	-	C	*	S	*	C	-	O			
	AS	C	-	C	*	S	*	C	-	S			
	AS	O	-	C	*	O	*	C	-	C			
	AS	O	-	C	*	S	*	C	-	C			
	AS	S	-	C	*	O	*	C	-	C			
	AS	S	-	C	*	S	*	C	-	C			

		Screen Number Order									
Screen Number		Fragment Definition								Frequency Percent	
195	AS	C	-	C	-	O	-	C	-	O	13.48
	AS	C	-	C	-	O	-	C	-	S	
	AS	C	-	C	-	S	-	C	-	O	
	AS	C	-	C	-	S	-	C	-	S	
	AS	O	-	C	-	O	-	C	-	C	
	AS	O	-	C	-	S	-	C	-	C	
	AS	S	-	C	-	O	-	C	-	C	
	AS	S	-	C	-	S	-	C	-	C	
196	AS	Br		O		C		C			0.10
	AS	Br		S		C		C			
	AS	C		C		O		Br			
	AS	C		C		O		Cl			
	AS	C		C		O		F			
	AS	C		C		O		I			
	AS	C		C		S		Br			
	AS	C		C		S		Cl			
	AS	C		C		S		F			
	AS	C		C		S		I			
	AS	Cl		O		C		C			
	AS	Cl		S		C		C			
	AS	F		O		C		C			
	AS	F		S		C		C			
	AS	I		O		C		C			
	AS	I		S		C		C			
197	AS	C	*	C	-	O	-	N			3.51
	AS	C	*	C	-	S	-	N			
	AS	N	-	O	-	C	*	C			
	AS	N	-	S	-	C	*	C			
198	AS	C	-	C	*	O	*	N			0.77
	AS	C	-	C	*	S	*	N			
	AS	N	*	O	*	C	-	C			
	AS	N	*	S	*	C	-	C			
199	AS	C	-	C	-	O	-	N			1.12
	AS	C	-	C	-	S	-	N			
	AS	N	-	O	-	C	-	C			
	AS	N	-	S	-	C	-	C			
200	AS	C	*	C	-	O	-	N	-	C	2.34
	AS	C	*	C	-	S	-	N	-	C	
	AS	C	-	N	-	O	-	C	*	C	
	AS	C	-	N	-	S	-	C	*	C	
201	AS	C	*	C	-	O	-	O			6.11
	AS	C	*	C	-	O	-	S			
	AS	C	*	C	-	S	-	O			
	AS	C	*	C	-	S	-	S			
	AS	O	-	O	-	C	*	C			
	AS	O	-	S	-	C	*	C			
	AS	S	-	O	-	C	*	C			
	AS	S	-	S	-	C	*	C			



		Screen Number Order											
Screen Number		Fragment Definition							Frequency Percent				
202	AS	C	-	C	-	O	-	O	2.21				
	AS	C	-	C	-	O	-	S					
	AS	C	-	C	-	S	-	O					
	AS	C	-	C	-	S	-	S					
	AS	O	-	O	-	C	-	C					
	AS	O	-	S	-	C	-	C					
	AS	S	-	O	-	C	-	C					
	AS	S	-	S	-	C	-	C					
203	AS	C	*	C	-	O	-	O	-	C	*	C	0.20
	AS	C	*	C	-	O	-	S	-	C	*	C	
	AS	C	*	C	-	S	-	O	-	C	*	C	
	AS	C	*	C	-	S	-	S	-	C	*	C	
204	AS	C	*	N	-	C	*	C	*	C	*	N	0.75
	AS	N	*	C	*	C	*	C	-	N	*	C	
205	AS	C	*	N	-	C	-	C	-	C	-	N	0.86
	AS	N	-	C	-	C	-	C	-	N	*	C	
206	AS	C	-	N	*	C	*	C	-	C	-	N	1.01
	AS	N	-	C	-	C	*	C	*	N	-	C	
207	AS	C	-	N	-	C	*	C	*	C	-	N	0.82
	AS	N	-	C	*	C	*	C	-	N	-	C	
208	AS	C	-	N	*	C	*	C	*	C	-	O	3.76
	AS	C	-	N	*	C	*	C	*	C	-	S	
	AS	O	-	C	*	C	*	C	*	N	-	C	
	AS	S	-	C	*	C	*	C	*	N	-	C	
209	AS	C	-	N	-	C	*	C	*	C	-	O	2.16
	AS	C	-	N	-	C	*	C	*	C	-	S	
	AS	O	-	C	*	C	*	C	-	N	-	C	
	AS	S	-	C	*	C	*	C	-	N	-	C	
210	AS	C	-	N	-	C	*	C	-	C	-	O	1.11
	AS	C	-	N	-	C	*	C	-	C	-	S	
	AS	O	-	C	-	C	*	C	-	N	-	C	
	AS	S	-	C	-	C	*	C	-	N	-	C	
211	AS	C	-	N	-	C	-	C	*	C	-	O	1.57
	AS	C	-	N	-	C	-	C	*	C	-	S	
	AS	O	-	C	*	C	-	C	-	N	-	C	
	AS	S	-	C	*	C	-	C	-	N	-	C	
212	AS	Br	C	C	N	C							4.26
	AS	C	N	C	C	Br							
	AS	C	N	C	C	Cl							
	AS	C	N	C	C	F							
	AS	C	N	C	C	I							
	AS	Cl	C	C	N	C							
	AS	F	C	C	N	C							
	AS	I	C	C	N	C							

Screen Number		Screen Number Order						Fragment Definition		Frequency Percent	
213	AS	C * N - C * C * N								0.36	
	AS	N * C * C - N * C									
214	AS	C * N - C - C - N								3.24	
	AS	N - C - C - N * C									
215	AS	C - N * C * C * N								6.81	
	AS	N * C * C * N - C									
216	AS	C - N * C * C - N								1.18	
	AS	N - C * C * N - C									
217	AS	C - N * C - C - N								2.43	
	AS	N - C - C * N - C									
218	AS	C - N - C * C - N								0.85	
	AS	N - C * C - N - C									
219	AS	C - N - C - C - N								7.91	
	AS	N - C - C - N - C									
220	AS	C - N * C * C * N - C								2.77	
221	AS	C N C C N N								2.85	
	AS	N N C C N C									
222	AS	C - N - C * C - N - O								0.32	
	AS	C - N - C * C - N - S									
	AS	O - N - C * C - N - C									
	AS	S - N - C * C - N - C									
223	AS	C * N - C * C - O								0.96	
	AS	C * N - C * C - S									
	AS	O - C * C - N * C									
	AS	S - C * C - N * C									
224	AS	C * N - C - C - O								2.89	
	AS	C * N - C - C - S									
	AS	O - C - C - N * C									
	AS	S - C - C - N * C									
225	AS	C - N * C * C * O								3.33	
	AS	C - N * C * C * S									
	AS	O * C * C * N - C									
	AS	S * C * C * N - C									
226	AS	C - N * C * C - O								1.88	
	AS	C - N * C * C - S									
	AS	O - C * C * N - C									
	AS	S - C * C * N - C									
227	AS	C - N * C - C - O								2.68	
	AS	C - N * C - C - S									
	AS	O - C - C * N - C									
	AS	S - C - C * N - C									

Screen Number		Screen Number Order		Fragment Definition	Frequency Percent
228	AS			C - N - C * C - O	3.06
	AS			C - N - C * C - S	
	AS			O - C * C - N - C	
	AS			S - C * C - N - C	
229	AS			C - N - C - C - O	12.06
	AS			C - N - C - C - S	
	AS			O - C - C - N - C	
	AS			S - C - C - N - C	
230	AS			C - N - C * C - O - C	1.28
	AS			C - N - C * C - S - C	
	AS			C - O - C * C - N - C	
	AS			C - S - C * C - N - C	
231	AS			C * N - C * N	1.29
	AS			N * C - N * C	
232	AS			C * N - C - N	0.93
	AS			N - C - N * C	
233	AS			C - N * C * N	7.12
	AS			N * C * N - C	
234	AS			C - N - C * N	4.77
	AS			N * C - N - C	
235	AS			C - N - C - N	5.46
	AS			N - C - N - C	
236	AS			C - N * C * N - C	1.19
237	AS			C - N - C - N - C	2.24
238	AS			C * N * C * N * C * N	2.92
	AS			N * C * N * C * N * C	
239	AS			C * N - C * O	1.30
	AS			C * N - C * S	
	AS			O * C - N * C	
	AS			S * C - N * C	
240	AS			C * N - C - O	5.80
	AS			C * N - C - S	
	AS			O - C - N * C	
	AS			S - C - N * C	
241	AS			C - N * C * O	1.96
	AS			C - N * C * S	
	AS			O * C * N - C	
	AS			S * C * N - C	
242	AS			C - N * C - O	8.74
	AS			C - N * C - S	
	AS			O - C * N - C	
	AS			S - C * N - C	

		Screen Number Order									
Screen Number		Fragment Definition				Frequency Percent					
243	AS	C	-	N	-	C	-	O	23.15		
	AS	C	-	N	-	C	-	S			
	AS	O	-	C	-	N	-	C			
	AS	S	-	C	-	N	-	C			
244	AS	C	*	N	-	C	-	O	-	C	1.06
	AS	C	*	N	-	C	-	S	-	C	
	AS	C	-	O	-	C	-	N	*	C	
	AS	C	-	S	-	C	-	N	*	C	
245	AS	C	-	N	*	C	-	O	-	C	1.08
	AS	C	-	N	*	C	-	S	-	C	
	AS	C	-	O	-	C	*	N	-	C	
	AS	C	-	S	-	C	*	N	-	C	
246	AS	C	-	N	-	C	-	O	-	C	3.12
	AS	C	-	N	-	C	-	S	-	C	
	AS	C	-	O	-	C	-	N	-	C	
	AS	C	-	S	-	C	-	N	-	C	
247	AS	C	-	N	*	N	-	C			0.23
248	AS	C	-	N	-	N	-	C			4.27
249	AS	C	-	N	*	N	*	C	-	O	0.35
	AS	C	-	N	*	N	*	C	-	S	
	AS	O	-	C	*	N	*	N	-	C	
	AS	S	-	C	*	N	*	N	-	C	
250	AS	C		N		N		N			1.47
	AS	N		N		N		C			
251	AS	C	*	N	-	O	-	C			1.09
	AS	C	*	N	-	S	-	C			
	AS	C	-	O	-	N	*	C			
	AS	C	-	S	-	N	*	C			
252	AS	C	-	N	-	O	-	C			3.76
	AS	C	-	N	-	S	-	C			
	AS	C	-	O	-	N	-	C			
	AS	C	-	S	-	N	-	C			
253	AS	C	*	N	-	O	-	O			0.97
	AS	C	*	N	-	O	-	S			
	AS	C	*	N	-	S	-	O			
	AS	C	*	N	-	S	-	S			
	AS	O	-	O	-	N	*	C			
	AS	O	-	S	-	N	*	C			
	AS	S	-	O	-	N	*	C			
	AS	S	-	S	-	N	*	C			

		Screen Number Order							
Screen Number		Fragment Definition							Frequency Percent
254	AS	C - N - O * O							0.00
	AS	C - N - O * S							
	AS	C - N - S * O							
	AS	C - N - S * S							
	AS	O * O - N - C							
	AS	O * S - N - C							
	AS	S * O - N - C							
	AS	S * S - N - C							
255	AS	C - N - O - O							2.96
	AS	C - N - O - S							
	AS	C - N - S - O							
	AS	C - N - S - S							
	AS	O - O - N - C							
	AS	O - S - N - C							
	AS	S - O - N - C							
	AS	S - S - N - C							
256	AS	Br	C	C	C	O	C	3.02	
	AS	Br	C	C	C	S	C		
	AS	C	O	C	C	C	Br		
	AS	C	O	C	C	C	Cl		
	AS	C	O	C	C	C	F		
	AS	C	O	C	C	C	I		
	AS	C	S	C	C	C	Br		
	AS	C	S	C	C	C	Cl		
	AS	C	S	C	C	C	F		
	AS	C	S	C	C	C	I		
	AS	Cl	C	C	C	O	C		
	AS	Cl	C	C	C	S	C		
	AS	F	C	C	C	O	C		
	AS	F	C	C	C	S	C		
	AS	I	C	C	C	O	C		
	AS	I	C	C	C	S	C		
257	AS	C - O - C * C * C - N							1.86
	AS	C - S - C * C * C - N							
	AS	N - C * C * C - O - C							
	AS	N - C * C * C - S - C							
258	AS	C - O - C * C - C - N							1.12
	AS	C - S - C * C - C - N							
	AS	N - C - C * C - O - C							
	AS	N - C - C * C - S - C							
259	AS	C - O - C - C * C - N							0.72
	AS	C - S - C - C * C - N							
	AS	N - C * C - C - O - C							
	AS	N - C * C - C - S - C							
260	AS	C - O - C - C - C - N							2.88
	AS	C - S - C - C - C - N							
	AS	N - C - C - C - O - C							
	AS	N - C - C - C - S - C							

Screen Number Order			
Screen Number		Fragment Definition	Frequency Percent
261	AS	C - O - C * C * C - O	4.46
	AS	C - O - C * C * C - S	
	AS	C - S - C * C * C - O	
	AS	C - S - C * C * C - S	
	AS	O - C * C * C - O - C	
	AS	O - C * C * C - S - C	
	AS	S - C * C * C - O - C	
	AS	S - C * C * C - S - C	
262	AS	C - O - C * C - C - O	2.33
	AS	C - O - C * C - C - S	
	AS	C - S - C * C - C - O	
	AS	C - S - C * C - C - S	
	AS	O - C - C * C - O - C	
	AS	O - C - C * C - S - C	
	AS	S - C - C * C - O - C	
	AS	S - C - C * C - S - C	
263	AS	C - O - C - C * C - O	2.05
	AS	C - O - C - C * C - S	
	AS	C - S - C - C * C - O	
	AS	C - S - C - C * C - S	
	AS	O - C * C - C - O - C	
	AS	O - C * C - C - S - C	
	AS	S - C * C - C - O - C	
	AS	S - C * C - C - S - C	
264	AS	C - O - C - C - C - O	3.09
	AS	C - O - C - C - C - S	
	AS	C - S - C - C - C - O	
	AS	C - S - C - C - C - S	
	AS	O - C - C - C - O - C	
	AS	O - C - C - C - S - C	
	AS	S - C - C - C - O - C	
	AS	S - C - C - C - S - C	
265	AS	Br- C * C - O - C	1.77
	AS	Br- C * C - S - C	
	AS	C - O - C * C - Br	
	AS	C - O - C * C - Cl	
	AS	C - O - C * C - F	
	AS	C - O - C * C - I	
	AS	C - S - C * C - Br	
	AS	C - S - C * C - Cl	
	AS	C - S - C * C - F	
	AS	C - S - C * C - I	
	AS	Cl- C * C - O - C	
	AS	Cl- C * C - S - C	
	AS	F - C * C - O - C	
	AS	F - C * C - S - C	
	AS	I - C * C - O - C	
	AS	I - C * C - S - C	

		Screen Number Order											
Screen Number		Fragment Definition						Frequency Percent					
266	AS	C	-	O	-	C	*	C	*	N	1.56		
	AS	C	-	S	-	C	*	C	*	N			
	AS	N	*	C	*	C	-	O	-	C			
	AS	N	*	C	*	C	-	S	-	C			
267	AS	C	-	O	-	C	*	C	-	N	2.37		
	AS	C	-	S	-	C	*	C	-	N			
	AS	N	-	C	*	C	-	O	-	C			
	AS	N	-	C	*	C	-	S	-	C			
268	AS	C	-	O	-	C	-	C	*	N	1.79		
	AS	C	-	S	-	C	-	C	*	N			
	AS	N	*	C	-	C	-	O	-	C			
	AS	N	*	C	-	C	-	S	-	C			
269	AS	C	-	O	-	C	-	C	-	N	6.99		
	AS	C	-	S	-	C	-	C	-	N			
	AS	N	-	C	-	C	-	O	-	C			
	AS	N	-	C	-	C	-	S	-	C			
270	AS	C		O		C		C		N	N	2.19	
	AS	C		S		C		C		N	N		
	AS	N		N		C		C		O	C		
	AS	N		N		C		C		S	C		
271	AS	C	-	O	-	C	*	C	-	N	-	O	0.42
	AS	C	-	O	-	C	*	C	-	N	-	S	
	AS	C	-	S	-	C	*	C	-	N	-	O	
	AS	C	-	S	-	C	*	C	-	N	-	S	
	AS	O	-	N	-	C	*	C	-	O	-	C	
	AS	O	-	N	-	C	*	C	-	S	-	C	
	AS	S	-	N	-	C	*	C	-	O	-	C	
	AS	S	-	N	-	C	*	C	-	S	-	C	
272	AS	C	-	O	-	C	*	C	-	O			6.16
	AS	C	-	O	-	C	*	C	-	S			
	AS	C	-	S	-	C	*	C	-	O			
	AS	C	-	S	-	C	*	C	-	S			
	AS	O	-	C	*	C	-	O	-	C			
	AS	O	-	C	*	C	-	S	-	C			
	AS	S	-	C	*	C	-	O	-	C			
	AS	S	-	C	*	C	-	S	-	C			
273	AS	C	-	O	-	C	-	C	-	O			8.01
	AS	C	-	O	-	C	-	C	-	S			
	AS	C	-	S	-	C	-	C	-	O			
	AS	C	-	S	-	C	-	C	-	S			
	AS	O	-	C	-	C	-	O	-	C			
	AS	O	-	C	-	C	-	S	-	C			
	AS	S	-	C	-	C	-	O	-	C			
	AS	S	-	C	-	C	-	S	-	C			
274	AS	C	-	O	-	C	*	N					3.68
	AS	C	-	S	-	C	*	N					
	AS	N	*	C	-	O	-	C					
	AS	N	*	C	-	S	-	C					

		Screen Number Order									
Screen Number		Fragment Definition						Frequency Percent			
275	AS	C	-	O	-	C	-	N	4.54		
	AS	C	-	S	-	C	-	N			
	AS	N	-	C	-	O	-	C			
	AS	N	-	C	-	S	-	C			
276	AS	C	-	O	-	C	*	N	*	N	1.23
	AS	C	-	S	-	C	*	N	*	N	
	AS	N	*	N	*	C	-	O	-	C	
	AS	N	*	N	*	C	-	S	-	C	
277	AS	C	-	O	-	C	*	O	2.86		
	AS	C	-	O	-	C	*	S			
	AS	C	-	S	-	C	*	O			
	AS	C	-	S	-	C	*	S			
	AS	O	*	C	-	O	-	C			
	AS	O	*	C	-	S	-	C			
	AS	S	*	C	-	O	-	C			
	AS	S	*	C	-	S	-	C			
278	AS	C	-	O	-	C	-	O	-	C	1.42
	AS	C	-	O	-	C	-	S	-	C	
	AS	C	-	S	-	C	-	O	-	C	
	AS	C	-	S	-	C	-	S	-	C	
279	AS	C		O		N		O	0.17		
	AS	C		O		N		S			
	AS	C		S		N		O			
	AS	C		S		N		S			
	AS	O		N		O		C			
	AS	O		N		S		C			
	AS	S		N		O		C			
	AS	S		N		S		C			
280	AS	C	-	O	-	O	-	C	0.81		
	AS	C	-	O	-	S	-	C			
	AS	C	-	S	-	O	-	C			
	AS	C	-	S	-	S	-	C			
281	AS	C		O		O		N	0.09		
	AS	C		O		S		N			
	AS	C		S		O		N			
	AS	C		S		S		N			
	AS	N		O		O		C			
	AS	N		O		S		C			
	AS	N		S		O		C			
	AS	N		S		S		C			
282	AS	C		O		O		O	1.03		
	AS	C		O		O		S			
	AS	C		O		S		O			
	AS	C		O		S		S			
	AS	C		S		O		O			
	AS	C		S		O		S			
	AS	C		S		S		O			
	AS	C		S		S		S			



		Screen Number Order					
Screen Number		Fragment Definition				Frequency Percent	
282	AS	O	O	O	C	1.03	(continued)
	AS	O	O	S	C		
	AS	O	S	O	C		
	AS	O	S	S	C		
	AS	S	O	O	C		
	AS	S	O	S	C		
	AS	S	S	O	C		
	AS	S	S	S	C		
283	AS	Br-	C *	C *	C *	1.11	
	AS	Br-	C *	C *	C *		
	AS	Br-	C *	C *	C *		
	AS	Br-	C *	C *	C *		
	AS	Cl-	C *	C *	C *		
	AS	Cl-	C *	C *	C *		
	AS	Cl-	C *	C *	C *		
	AS	Cl-	C *	C *	C *		
	AS	F -	C *	C *	C *		
	AS	F -	C *	C *	C *		
	AS	F -	C *	C *	C *		
	AS	F -	C *	C *	C *		
	AS	I -	C *	C *	C *		
	AS	I -	C *	C *	C *		
	AS	I -	C *	C *	C *		
	AS	I -	C *	C *	C *		
284	AS	Br-	C -	C -	C -	0.36	
	AS	Br-	C -	C -	C -		
	AS	Br-	C -	C -	C -		
	AS	Br-	C -	C -	C -		
	AS	Cl-	C -	C -	C -		
	AS	Cl-	C -	C -	C -		
	AS	Cl-	C -	C -	C -		
	AS	Cl-	C -	C -	C -		
	AS	F -	C -	C -	C -		
	AS	F -	C -	C -	C -		
	AS	F -	C -	C -	C -		
	AS	F -	C -	C -	C -		
	AS	I -	C -	C -	C -		
	AS	I -	C -	C -	C -		
	AS	I -	C -	C -	C -		
	AS	I -	C -	C -	C -		
285	AS	Br	C	C	C	7.02	
	AS	Cl	C	C	C		
	AS	F	C	C	C		
	AS	I	C	C	C		
	AS	N	C	C	C		
	AS	N	C	C	C		
	AS	N	C	C	C		
	AS	N	C	C	C		

# Screen Number Order

Screen Number	Fragment Definition	Frequency Percent
286	AS Br- C * C * C * C - N	2.55
	AS Cl- C * C * C * C - N	
	AS F - C * C * C * C - N	
	AS I - C * C * C * C - N	
	AS N - C * C * C * C - Br	
	AS N - C * C * C * C - Cl	
	AS N - C * C * C * C - F	
	AS N - C * C * C * C - I	
287	AS Br- C * C * C - C - N	1.22
	AS Cl- C * C * C - C - N	
	AS F - C * C * C - C - N	
	AS I - C * C * C - C - N	
	AS N - C - C * C * C - Br	
	AS N - C - C * C * C - Cl	
	AS N - C - C * C * C - F	
	AS N - C - C * C * C - I	
288	AS Br C C C C O	6.39
	AS Br C C C C S	
	AS Cl C C C C O	
	AS Cl C C C C S	
	AS F C C C C O	
	AS F C C C C S	
	AS I C C C C O	
	AS I C C C C S	
	AS O C C C C Br	
	AS O C C C C Cl	
	AS O C C C C F	
	AS O C C C C I	
	AS S C C C C Br	
	AS S C C C C Cl	
	AS S C C C C F	
	AS S C C C C I	
289	AS Br- C * C * C * C - O	3.00
	AS Br- C * C * C * C - S	
	AS Cl- C * C * C * C - O	
	AS Cl- C * C * C * C - S	
	AS F - C * C * C * C - O	
	AS F - C * C * C * C - S	
	AS I - C * C * C * C - O	
	AS I - C * C * C * C - S	
	AS O - C * C * C * C - Br	
	AS O - C * C * C * C - Cl	
	AS O - C * C * C * C - F	
	AS O - C * C * C * C - I	
	AS S - C * C * C * C - Br	
	AS S - C * C * C * C - Cl	
	AS S - C * C * C * C - F	
	AS S - C * C * C * C - I	

# Screen Number Order

Screen Number	Fragment Definition	Frequency Percent
290	AS Br- C * C * C - C - O	1.30
	AS Br- C * C * C - C - S	
	AS Cl- C * C * C - C - O	
	AS Cl- C * C * C - C - S	
	AS F - C * C * C - C - O	
	AS F - C * C * C - C - S	
	AS I - C * C * C - C - O	
	AS I - C * C * C - C - S	
	AS O - C - C * C * C - Br	
	AS O - C - C * C * C - Cl	
	AS O - C - C * C * C - F	
	AS O - C - C * C * C - I	
	AS S - C - C * C * C - Br	
	AS S - C - C * C * C - Cl	
	AS S - C - C * C * C - F	
	AS S - C - C * C * C - I	
291	AS As C C C C As	0.79
	AS As C C C C B	
	AS As C C C C Br	
	AS As C C C C Cl	
	AS As C C C C F	
	AS As C C C C I	
	AS As C C C C N	
	AS As C C C C O	
	AS As C C C C P	
	AS As C C C C S	
	AS As C C C C Se	
	AS As C C C C Si	
	AS As C C C C Te	
	AS B C C C C As	
	AS B C C C C B	
	AS B C C C C Br	
	AS B C C C C Cl	
	AS B C C C C F	
	AS B C C C C I	
	AS B C C C C N	
	AS B C C C C O	
	AS B C C C C P	
	AS B C C C C S	
	AS B C C C C Se	
	AS B C C C C Si	
	AS B C C C C Te	
	AS Br C C C C As	
	AS Br C C C C B	
	AS Br C C C C P	
	AS Br C C C C Se	
	AS Br C C C C Si	
	AS Br C C C C Te	
	AS Cl C C C C As	
	AS Cl C C C C B	
	AS Cl C C C C P	
	AS Cl C C C C Se	
	AS Cl C C C C Si	
	AS Cl C C C C Te	

# Screen Number Order

Screen Number	Fragment Definition						Frequency Percent
291	AS	F	C	C	C	C	As
	AS	F	C	C	C	C	B
	AS	F	C	C	C	C	P
	AS	F	C	C	C	C	Se
	AS	F	C	C	C	C	Si
	AS	F	C	C	C	C	Te
	AS	I	C	C	C	C	As
	AS	I	C	C	C	C	B
	AS	I	C	C	C	C	P
	AS	I	C	C	C	C	Se
	AS	I	C	C	C	C	Si
	AS	I	C	C	C	C	Te
	AS	N	C	C	C	C	As
	AS	N	C	C	C	C	B
	AS	N	C	C	C	C	P
	AS	N	C	C	C	C	Se
	AS	N	C	C	C	C	Si
	AS	N	C	C	C	C	Te
	AS	O	C	C	C	C	As
	AS	O	C	C	C	C	B
	AS	O	C	C	C	C	P
	AS	O	C	C	C	C	Se
	AS	O	C	C	C	C	Si
	AS	O	C	C	C	C	Te
	AS	P	C	C	C	C	As
	AS	P	C	C	C	C	B
	AS	P	C	C	C	C	Br
	AS	P	C	C	C	C	Cl
	AS	P	C	C	C	C	F
	AS	P	C	C	C	C	I
	AS	P	C	C	C	C	N
	AS	P	C	C	C	C	O
	AS	P	C	C	C	C	P
	AS	P	C	C	C	C	S
	AS	P	C	C	C	C	Se
	AS	P	C	C	C	C	Si
	AS	P	C	C	C	C	Te
	AS	S	C	C	C	C	As
	AS	S	C	C	C	C	B
	AS	S	C	C	C	C	P
	AS	S	C	C	C	C	Se
	AS	S	C	C	C	C	Si
	AS	S	C	C	C	C	Te
	AS	Se	C	C	C	C	As
	AS	Se	C	C	C	C	B
	AS	Se	C	C	C	C	Br
	AS	Se	C	C	C	C	Cl
	AS	Se	C	C	C	C	F
	AS	Se	C	C	C	C	I
	AS	Se	C	C	C	C	N
	AS	Se	C	C	C	C	O
	AS	Se	C	C	C	C	P
	AS	Se	C	C	C	C	S
	AS	Se	C	C	C	C	Se
	AS	Se	C	C	C	C	Si

0.79 (continued)

# Screen Number Order

Screen Number	Fragment Definition	Frequency Percent
291	AS Se C C C C Te	0.79 (continued)
	AS Si C C C C As	
	AS Si C C C C B	
	AS Si C C C C Br	
	AS Si C C C C Cl	
	AS Si C C C C F	
	AS Si C C C C I	
	AS Si C C C C N	
	AS Si C C C C O	
	AS Si C C C C P	
	AS Si C C C C S	
	AS Si C C C C Se	
	AS Si C C C C Si	
	AS Si C C C C Te	
	AS Te C C C C As	
	AS Te C C C C B	
	AS Te C C C C Br	
	AS Te C C C C Cl	
	AS Te C C C C F	
	AS Te C C C C I	
	AS Te C C C C N	
	AS Te C C C C O	
	AS Te C C C C P	
	AS Te C C C C S	
	AS Te C C C C Se	
	AS Te C C C C Si	
	AS Te C C C C Te	
292	AS Br- C * C * C - Br	3.37
	AS Br- C * C * C - Cl	
	AS Br- C * C * C - F	
	AS Br- C * C * C - I	
	AS Cl- C * C * C - Br	
	AS Cl- C * C * C - Cl	
	AS Cl- C * C * C - F	
	AS Cl- C * C * C - I	
	AS F - C * C * C - Br	
	AS F - C * C * C - Cl	
	AS F - C * C * C - F	
	AS F - C * C * C - I	
	AS I - C * C * C - Br	
	AS I - C * C * C - Cl	
	AS I - C * C * C - F	
	AS I - C * C * C - I	
293	AS Br- C * C - C - Br	0.20
	AS Br- C - C * C - Br	
	AS Br- C * C - C - Cl	
	AS Br- C - C * C - Cl	
	AS Br- C * C - C - F	
	AS Br- C - C * C - F	
	AS Br- C * C - C - I	
	AS Br- C - C * C - I	
	AS Cl- C * C - C - Br	
	AS Cl- C - C * C - Br	

# Screen Number Order

Screen Number	Fragment Definition	Frequency Percent
293	AS Cl- C * C - C - Cl	0.20 (continued)
	AS Cl- C - C * C - Cl	
	AS Cl- C * C - C - F	
	AS Cl- C - C * C - F	
	AS Cl- C * C - C - I	
	AS Cl- C - C * C - I	
	AS F - C * C - C - Br	
	AS F - C - C * C - Br	
	AS F - C * C - C - Cl	
	AS F - C - C * C - Cl	
	AS F - C * C - C - F	
	AS F - C - C * C - F	
	AS F - C * C - C - I	
	AS F - C - C * C - I	
	AS I - C * C - C - Br	
	AS I - C - C * C - Br	
	AS I - C * C - C - Cl	
	AS I - C - C * C - Cl	
	AS I - C * C - C - F	
	AS I - C - C * C - F	
	AS I - C * C - C - I	
	AS I - C - C * C - I	
294	AS Br- C - C - C - Br	0.74
	AS Br- C - C - C - Cl	
	AS Br- C - C - C - F	
	AS Br- C - C - C - I	
	AS Cl- C - C - C - Br	
	AS Cl- C - C - C - Cl	
	AS Cl- C - C - C - F	
	AS Cl- C - C - C - I	
	AS F - C - C - C - Br	
	AS F - C - C - C - Cl	
	AS F - C - C - C - F	
	AS F - C - C - C - I	
	AS I - C - C - C - Br	
	AS I - C - C - C - Cl	
	AS I - C - C - C - F	
	AS I - C - C - C - I	
295	AS Br C C C N	5.58
	AS Cl C C C N	
	AS F C C C N	
	AS I C C C N	
	AS N C C C Br	
	AS N C C C Cl	
	AS N C C C F	
	AS N C C C I	

Screen Number Order							
Screen Number				Fragment Definition			Frequency Percent
296	AS	Br-	C *	C *	C *	N	1.36
	AS	Cl-	C *	C *	C *	N	
	AS	F -	C *	C *	C *	N	
	AS	I -	C *	C *	C *	N	
	AS	N *	C *	C *	C -	Br	
	AS	N *	C *	C *	C -	Cl	
	AS	N *	C *	C *	C -	F	
	AS	N *	C *	C *	C -	I	
297	AS	Br-	C *	C *	C -	N	1.96
	AS	Cl-	C *	C *	C -	N	
	AS	F -	C *	C *	C -	N	
	AS	I -	C *	C *	C -	N	
	AS	N -	C *	C *	C -	Br	
	AS	N -	C *	C *	C -	Cl	
	AS	N -	C *	C *	C -	F	
	AS	N -	C *	C *	C -	I	
298	AS	Br-	C *	C -	C -	N	1.26
	AS	Cl-	C *	C -	C -	N	
	AS	F -	C *	C -	C -	N	
	AS	I -	C *	C -	C -	N	
	AS	N -	C -	C *	C -	Br	
	AS	N -	C -	C *	C -	Cl	
	AS	N -	C -	C *	C -	F	
	AS	N -	C -	C *	C -	I	
299	AS	Br-	C -	C -	C -	N	0.37
	AS	Cl-	C -	C -	C -	N	
	AS	F -	C -	C -	C -	N	
	AS	I -	C -	C -	C -	N	
	AS	N -	C -	C -	C -	Br	
	AS	N -	C -	C -	C -	Cl	
	AS	N -	C -	C -	C -	F	
	AS	N -	C -	C -	C -	I	
300	AS	Br	C	C	C	N N	0.84
	AS	Cl	C	C	C	N N	
	AS	F	C	C	C	N N	
	AS	I	C	C	C	N N	
	AS	N	N	C	C	C Br	
	AS	N	N	C	C	C Cl	
	AS	N	N	C	C	C F	
	AS	N	N	C	C	C I	
301	AS	Br	C	C	C	N O	0.55
	AS	Br	C	C	C	N S	
	AS	Cl	C	C	C	N O	
	AS	Cl	C	C	C	N S	
	AS	F	C	C	C	N O	
	AS	F	C	C	C	N S	
	AS	I	C	C	C	N O	
	AS	I	C	C	C	N S	
	AS	O	N	C	C	C Br	
	AS	O	N	C	C	C Cl	

# Screen Number Order

Screen Number	Fragment Definition							Frequency Percent
301	AS	O	N	C	C	C	F	0.55 (continued)
	AS	O	N	C	C	C	I	
	AS	S	N	C	C	C	Br	
	AS	S	N	C	C	C	Cl	
	AS	S	N	C	C	C	F	
	AS	S	N	C	C	C	I	
302	AS	As	C	C	C	N	As	0.44
	AS	As	C	C	C	N	B	
	AS	As	C	C	C	N	P	
	AS	As	C	C	C	N	Se	
	AS	As	C	C	C	N	Si	
	AS	As	C	C	C	N	Te	
	AS	As	C	C	N	As		
	AS	As	C	C	N	B		
	AS	As	C	C	N	P		
	AS	As	C	C	N	Se		
	AS	As	C	C	N	Si		
	AS	As	C	C	N	Te		
	AS	As	N	C	C	As		
	AS	As	N	C	C	B		
	AS	As	N	C	C	Br		
	AS	As	N	C	C	C	As	
	AS	As	N	C	C	C	B	
	AS	As	N	C	C	C	Br	
	AS	As	N	C	C	C	Cl	
	AS	As	N	C	C	C	F	
	AS	As	N	C	C	C	I	
	AS	As	N	C	C	C	N	
	AS	As	N	C	C	C	O	
	AS	As	N	C	C	C	P	
	AS	As	N	C	C	C	S	
	AS	As	N	C	C	C	Se	
	AS	As	N	C	C	C	Si	
	AS	As	N	C	C	C	Te	
	AS	As	N	C	C	Cl		
	AS	As	N	C	C	F		
	AS	As	N	C	C	I		
	AS	As	N	C	C	N		
	AS	As	N	C	C	O		
	AS	As	N	C	C	P		
	AS	As	N	C	C	S		
	AS	As	N	C	C	Se		
	AS	As	N	C	C	Si		
	AS	As	N	C	C	Te		
	AS	B	C	C	C	N	As	
	AS	B	C	C	C	N	B	
	AS	B	C	C	C	N	P	
	AS	B	C	C	C	N	Se	
	AS	B	C	C	C	N	Si	
	AS	B	C	C	C	N	Te	
	AS	B	C	C	N	As		
	AS	B	C	C	N	B		
	AS	B	C	C	N	P		
	AS	B	C	C	N	Se		



# Screen Number Order

Screen Number	Fragment Definition						Frequency Percent
302	AS	B	C	C	N	Si	0.44 (continued)
	AS	B	C	C	N	Te	
	AS	B	N	C	C	As	
	AS	B	N	C	C	B	
	AS	B	N	C	C	Br	
	AS	B	N	C	C	C	As
	AS	B	N	C	C	C	B
	AS	B	N	C	C	C	Br
	AS	B	N	C	C	C	Cl
	AS	B	N	C	C	C	F
	AS	B	N	C	C	C	I
	AS	B	N	C	C	C	N
	AS	B	N	C	C	C	O
	AS	B	N	C	C	C	P
	AS	B	N	C	C	C	S
	AS	B	N	C	C	C	Se
	AS	B	N	C	C	C	Si
	AS	B	N	C	C	C	Te
	AS	B	N	C	C	Cl	
	AS	B	N	C	C	F	
	AS	B	N	C	C	I	
	AS	B	N	C	C	N	
	AS	B	N	C	C	O	
	AS	B	N	C	C	P	
	AS	B	N	C	C	S	
	AS	B	N	C	C	Se	
	AS	B	N	C	C	Si	
	AS	B	N	C	C	Te	
	AS	Br	C	C	C	N	As
	AS	Br	C	C	C	N	B
	AS	Br	C	C	C	N	P
	AS	Br	C	C	C	N	Se
	AS	Br	C	C	C	N	Si
	AS	Br	C	C	C	N	Te
	AS	Br	C	C	N	As	
	AS	Br	C	C	N	B	
	AS	Br	C	C	N	P	
	AS	Br	C	C	N	Se	
	AS	Br	C	C	N	Si	
	AS	Br	C	C	N	Te	
	AS	Cl	C	C	C	N	As
	AS	Cl	C	C	C	N	B
	AS	Cl	C	C	C	N	P
	AS	Cl	C	C	C	N	Se
	AS	Cl	C	C	C	N	Si
	AS	Cl	C	C	C	N	Te
	AS	Cl	C	C	N	As	
	AS	Cl	C	C	N	B	
	AS	Cl	C	C	N	P	
	AS	Cl	C	C	N	Se	
	AS	Cl	C	C	N	Si	
	AS	Cl	C	C	N	Te	
	AS	F	C	C	C	N	As
	AS	F	C	C	C	N	B
	AS	F	C	C	C	N	P

# Screen Number Order

Screen Number	Fragment Definition							Frequency Percent
302	AS	F	C	C	C	N	Se	0.44 (continued)
	AS	F	C	C	C	N	Si	
	AS	F	C	C	C	N	Te	
	AS	F	C	C	N	As		
	AS	F	C	C	N	B		
	AS	F	C	C	N	P		
	AS	F	C	C	N	Se		
	AS	F	C	C	N	Si		
	AS	F	C	C	N	Te		
	AS	I	C	C	C	N	As	
	AS	I	C	C	C	N	B	
	AS	I	C	C	C	N	P	
	AS	I	C	C	C	N	Se	
	AS	I	C	C	C	N	Si	
	AS	I	C	C	C	N	Te	
	AS	I	C	C	N	As		
	AS	I	C	C	N	B		
	AS	I	C	C	N	P		
	AS	I	C	C	N	Se		
	AS	I	C	C	N	Si		
	AS	I	C	C	N	Te		
	AS	N	C	C	C	N	As	
	AS	N	C	C	C	N	B	
	AS	N	C	C	C	N	P	
	AS	N	C	C	C	N	Se	
	AS	N	C	C	C	N	Si	
	AS	N	C	C	C	N	Te	
	AS	N	C	C	N	As		
	AS	N	C	C	N	B		
	AS	N	C	C	N	P		
	AS	N	C	C	N	Se		
	AS	N	C	C	N	Si		
	AS	N	C	C	N	Te		
	AS	O	C	C	C	N	As	
	AS	O	C	C	C	N	B	
	AS	O	C	C	C	N	P	
	AS	O	C	C	C	N	Se	
	AS	O	C	C	C	N	Si	
	AS	O	C	C	C	N	Te	
	AS	O	C	C	N	As		
	AS	O	C	C	N	B		
	AS	O	C	C	N	P		
	AS	O	C	C	N	Se		
	AS	O	C	C	N	Si		
	AS	O	C	C	N	Te		
	AS	P	C	C	C	N	As	
	AS	P	C	C	C	N	B	
	AS	P	C	C	C	N	P	
	AS	P	C	C	C	N	Se	
	AS	P	C	C	C	N	Si	
	AS	P	C	C	C	N	Te	
	AS	P	C	C	N	As		
	AS	P	C	C	N	B		
	AS	P	C	C	N	P		
	AS	P	C	C	N	Se		

# Screen Number Order

Screen Number	Fragment Definition						Frequency Percent
302	AS	P	C	C	N	Si	0.44 (continued)
	AS	P	C	C	N	Te	
	AS	P	N	C	C	As	
	AS	P	N	C	C	B	
	AS	P	N	C	C	Br	
	AS	P	N	C	C	C	As
	AS	P	N	C	C	C	B
	AS	P	N	C	C	C	Br
	AS	P	N	C	C	C	Cl
	AS	P	N	C	C	C	F
	AS	P	N	C	C	C	I
	AS	P	N	C	C	C	N
	AS	P	N	C	C	C	O
	AS	P	N	C	C	C	P
	AS	P	N	C	C	C	S
	AS	P	N	C	C	C	Se
	AS	P	N	C	C	C	Si
	AS	P	N	C	C	C	Te
	AS	P	N	C	C	Cl	
	AS	P	N	C	C	F	
	AS	P	N	C	C	I	
	AS	P	N	C	C	N	
	AS	P	N	C	C	O	
	AS	P	N	C	C	P	
	AS	P	N	C	C	S	
	AS	P	N	C	C	Se	
	AS	P	N	C	C	Si	
	AS	P	N	C	C	Te	
	AS	S	C	C	C	N	As
	AS	S	C	C	C	N	B
	AS	S	C	C	C	N	P
	AS	S	C	C	C	N	Se
	AS	S	C	C	C	N	Si
	AS	S	C	C	C	N	Te
	AS	S	C	C	N	As	
	AS	S	C	C	N	B	
	AS	S	C	C	N	P	
	AS	S	C	C	N	Se	
	AS	S	C	C	N	Si	
	AS	S	C	C	N	Te	
	AS	Se	C	C	C	N	As
	AS	Se	C	C	C	N	B
	AS	Se	C	C	C	N	P
	AS	Se	C	C	C	N	Se
	AS	Se	C	C	C	N	Si
	AS	Se	C	C	C	N	Te
	AS	Se	C	C	N	As	
	AS	Se	C	C	N	B	
	AS	Se	C	C	N	P	
	AS	Se	C	C	N	Se	
	AS	Se	C	C	N	Si	
	AS	Se	C	C	N	Te	
	AS	Se	N	C	C	As	
	AS	Se	N	C	C	B	
	AS	Se	N	C	C	Br	

# Screen Number Order

Screen Number	Fragment Definition							Frequency Percent
302	AS	Se	N	C	C	C	As	0.44 (continued)
	AS	Se	N	C	C	C	B	
	AS	Se	N	C	C	C	Br	
	AS	Se	N	C	C	C	Cl	
	AS	Se	N	C	C	C	F	
	AS	Se	N	C	C	C	I	
	AS	Se	N	C	C	C	N	
	AS	Se	N	C	C	C	O	
	AS	Se	N	C	C	C	P	
	AS	Se	N	C	C	C	S	
	AS	Se	N	C	C	C	Se	
	AS	Se	N	C	C	C	Si	
	AS	Se	N	C	C	C	Te	
	AS	Se	N	C	C	C	Cl	
	AS	Se	N	C	C	C	F	
	AS	Se	N	C	C	C	I	
	AS	Se	N	C	C	C	N	
	AS	Se	N	C	C	C	O	
	AS	Se	N	C	C	C	P	
	AS	Se	N	C	C	C	S	
	AS	Se	N	C	C	C	Se	
	AS	Se	N	C	C	C	Si	
	AS	Se	N	C	C	C	Te	
	AS	Si	C	C	C	N	As	
	AS	Si	C	C	C	N	B	
	AS	Si	C	C	C	N	P	
	AS	Si	C	C	C	N	Se	
	AS	Si	C	C	C	N	Si	
	AS	Si	C	C	C	N	Te	
	AS	Si	C	C	C	N	As	
	AS	Si	C	C	C	N	B	
	AS	Si	C	C	C	N	P	
	AS	Si	C	C	C	N	Se	
	AS	Si	C	C	C	N	Si	
	AS	Si	C	C	C	N	Te	
	AS	Si	N	C	C	C	As	
	AS	Si	N	C	C	C	B	
	AS	Si	N	C	C	C	Br	
	AS	Si	N	C	C	C	C	As
	AS	Si	N	C	C	C	C	B
	AS	Si	N	C	C	C	C	Br
	AS	Si	N	C	C	C	C	Cl
	AS	Si	N	C	C	C	C	F
	AS	Si	N	C	C	C	C	I
	AS	Si	N	C	C	C	C	N
	AS	Si	N	C	C	C	C	O
	AS	Si	N	C	C	C	C	P
	AS	Si	N	C	C	C	C	S
	AS	Si	N	C	C	C	C	Se
	AS	Si	N	C	C	C	C	Si
	AS	Si	N	C	C	C	C	Te
	AS	Si	N	C	C	C	C	Cl
	AS	Si	N	C	C	C	C	F
	AS	Si	N	C	C	C	C	I
	AS	Si	N	C	C	C	C	N

# Screen Number Order

Screen Number	Fragment Definition						Frequency Percent
302	AS	Si	N	C	C	O	0.44 (continued)
	AS	Si	N	C	C	P	
	AS	Si	N	C	C	S	
	AS	Si	N	C	C	Se	
	AS	Si	N	C	C	Si	
	AS	Si	N	C	C	Te	
	AS	Te	C	C	C	N As	
	AS	Te	C	C	C	N B	
	AS	Te	C	C	C	N P	
	AS	Te	C	C	C	N Se	
	AS	Te	C	C	C	N Si	
	AS	Te	C	C	C	N Te	
	AS	Te	C	C	N	As	
	AS	Te	C	C	N	B	
	AS	Te	C	C	N	P	
	AS	Te	C	C	N	Se	
	AS	Te	C	C	N	Si	
	AS	Te	C	C	N	Te	
	AS	Te	N	C	C	As	
	AS	Te	N	C	C	B	
	AS	Te	N	C	C	Br	
	AS	Te	N	C	C	C As	
	AS	Te	N	C	C	C B	
	AS	Te	N	C	C	C Br	
	AS	Te	N	C	C	C Cl	
	AS	Te	N	C	C	C F	
	AS	Te	N	C	C	C I	
	AS	Te	N	C	C	C N	
	AS	Te	N	C	C	C O	
	AS	Te	N	C	C	C P	
	AS	Te	N	C	C	C S	
	AS	Te	N	C	C	C Se	
	AS	Te	N	C	C	C Si	
	AS	Te	N	C	C	C Te	
	AS	Te	N	C	C	Cl	
	AS	Te	N	C	C	F	
	AS	Te	N	C	C	I	
	AS	Te	N	C	C	N	
	AS	Te	N	C	C	O	
	AS	Te	N	C	C	P	
	AS	Te	N	C	C	S	
	AS	Te	N	C	C	Se	
	AS	Te	N	C	C	Si	
	AS	Te	N	C	C	Te	
303	AS	Br	C	C	C	O	5.10
	AS	Br	C	C	C	S	
	AS	Cl	C	C	C	O	
	AS	Cl	C	C	C	S	
	AS	F	C	C	C	O	
	AS	F	C	C	C	S	
	AS	I	C	C	C	O	
	AS	I	C	C	C	S	
	AS	O	C	C	C	Br	
	AS	O	C	C	C	Cl	

		Screen Number Order						
Screen Number		Fragment Definition					Frequency Percent	
303	AS	O	C	C	C	F	5.10	(continued)
	AS	O	C	C	C	I		
	AS	S	C	C	C	Br		
	AS	S	C	C	C	Cl		
	AS	S	C	C	C	F		
	AS	S	C	C	C	I		
304	AS	Br-	C	*	C	*	O	0.64
	AS	Br-	C	*	C	*	S	
	AS	Cl-	C	*	C	*	O	
	AS	Cl-	C	*	C	*	S	
	AS	F	-	C	*	C	O	
	AS	F	-	C	*	C	S	
	AS	I	-	C	*	C	O	
	AS	I	-	C	*	C	S	
	AS	O	*	C	*	C	- Br	
	AS	O	*	C	*	C	- Cl	
	AS	O	*	C	*	C	- F	
	AS	O	*	C	*	C	- I	
	AS	S	*	C	*	C	- Br	
	AS	S	*	C	*	C	- Cl	
	AS	S	*	C	*	C	- F	
	AS	S	*	C	*	C	- I	
305	AS	Br-	C	*	C	*	O	1.72
	AS	Br-	C	*	C	*	S	
	AS	Cl-	C	*	C	*	O	
	AS	Cl-	C	*	C	*	S	
	AS	F	-	C	*	C	O	
	AS	F	-	C	*	C	S	
	AS	I	-	C	*	C	O	
	AS	I	-	C	*	C	S	
	AS	O	-	C	*	C	- Br	
	AS	O	-	C	*	C	- Cl	
	AS	O	-	C	*	C	- F	
	AS	O	-	C	*	C	- I	
	AS	S	-	C	*	C	- Br	
	AS	S	-	C	*	C	- Cl	
	AS	S	-	C	*	C	- F	
	AS	S	-	C	*	C	- I	
306	AS	Br-	C	*	C	-	O	1.61
	AS	Br-	C	*	C	-	S	
	AS	Cl-	C	*	C	-	O	
	AS	Cl-	C	*	C	-	S	
	AS	F	-	C	*	C	O	
	AS	F	-	C	*	C	S	
	AS	I	-	C	*	C	O	
	AS	I	-	C	*	C	S	
	AS	O	-	C	-	C	- Br	
	AS	O	-	C	-	C	- Cl	
	AS	O	-	C	-	C	- F	

# Screen Number Order

Screen Number	Fragment Definition	Frequency Percent
306	AS O - C - C * C - I	1.61 (continued)
	AS S - C - C * C - Br	
	AS S - C - C * C - Cl	
	AS S - C - C * C - F	
	AS S - C - C * C - I	
307	AS Br- C - C - C - O	0.86
	AS Br- C - C - C - S	
	AS Cl- C - C - C - O	
	AS Cl- C - C - C - S	
	AS F - C - C - C - O	
	AS F - C - C - C - S	
	AS I - C - C - C - O	
	AS I - C - C - C - S	
	AS O - C - C - C - Br	
	AS O - C - C - C - Cl	
	AS O - C - C - C - F	
	AS O - C - C - C - I	
	AS S - C - C - C - Br	
	AS S - C - C - C - Cl	
	AS S - C - C - C - F	
	AS S - C - C - C - I	
308	AS Br C C C O N	0.26
	AS Br C C C S N	
	AS Cl C C C O N	
	AS Cl C C C S N	
	AS F C C C O N	
	AS F C C C S N	
	AS I C C C O N	
	AS I C C C S N	
	AS N O C C C Br	
	AS N O C C C Cl	
	AS N O C C C F	
	AS N O C C C I	
	AS N S C C C Br	
	AS N S C C C Cl	
	AS N S C C C F	
	AS N S C C C I	
309	AS Br C C C O O	0.37
	AS Br C C C O S	
	AS Br C C C S O	
	AS Br C C C S S	
	AS Cl C C C O O	
	AS Cl C C C O S	
	AS Cl C C C S O	
	AS Cl C C C S S	
	AS F C C C O O	
	AS F C C C O S	
	AS F C C C S O	
	AS F C C C S S	
	AS I C C C O O	
	AS I C C C O S	
	AS I C C C S O	

Screen Number Order							
Screen Number	Fragment Definition						
309	AS	I	C	C	C	S	S
	AS	O	O	C	C	C	Br
	AS	O	O	C	C	C	Cl
	AS	O	O	C	C	C	F
	AS	O	O	C	C	C	I
	AS	O	S	C	C	C	Br
	AS	O	S	C	C	C	Cl
	AS	O	S	C	C	C	F
	AS	O	S	C	C	C	I
	AS	S	O	C	C	C	Br
	AS	S	O	C	C	C	Cl
	AS	S	O	C	C	C	F
	AS	S	O	C	C	C	I
	AS	S	S	C	C	C	Br
	AS	S	S	C	C	C	Cl
	AS	S	S	C	C	C	F
	AS	S	S	C	C	C	I
310	AS	As	C	C	C	O	As
	AS	As	C	C	C	O	B
	AS	As	C	C	C	O	P
	AS	As	C	C	C	O	Se
	AS	As	C	C	C	O	Si
	AS	As	C	C	C	O	Te
	AS	As	C	C	C	S	As
	AS	As	C	C	C	S	B
	AS	As	C	C	C	S	P
	AS	As	C	C	C	S	Se
	AS	As	C	C	C	S	Si
	AS	As	C	C	C	S	Te
	AS	As	C	C	O	As	
	AS	As	C	C	O	B	
	AS	As	C	C	O	P	
	AS	As	C	C	O	Se	
	AS	As	C	C	O	Si	
	AS	As	C	C	O	Te	
	AS	As	C	C	S	As	
	AS	As	C	C	S	B	
	AS	As	C	C	S	P	
	AS	As	C	C	S	Se	
	AS	As	C	C	S	Si	
	AS	As	C	C	S	Te	
	AS	As	O	C	C	As	
	AS	As	O	C	C	B	
	AS	As	O	C	C	Br	
	AS	As	O	C	C	C	As
	AS	As	O	C	C	C	B
	AS	As	O	C	C	C	Br
	AS	As	O	C	C	C	Cl
	AS	As	O	C	C	C	F
	AS	As	O	C	C	C	I
	AS	As	O	C	C	C	N
	AS	As	O	C	C	C	O
	AS	As	O	C	C	C	P
	AS	As	O	C	C	C	S



# Screen Number Order

Screen Number	Fragment Definition							Frequency Percent	
310	AS	As	O	C	C	C	Se	2.38	(continued)
	AS	As	O	C	C	C	Si		
	AS	As	O	C	C	C	Te		
	AS	As	O	C	C	Cl			
	AS	As	O	C	C	F			
	AS	As	O	C	C	I			
	AS	As	O	C	C	N			
	AS	As	O	C	C	O			
	AS	As	O	C	C	P			
	AS	As	O	C	C	S			
	AS	As	O	C	C	Se			
	AS	As	O	C	C	Si			
	AS	As	O	C	C	Te			
	AS	As	S	C	C	As			
	AS	As	S	C	C	B			
	AS	As	S	C	C	Br			
	AS	As	S	C	C	C	As		
	AS	As	S	C	C	C	B		
	AS	As	S	C	C	C	Br		
	AS	As	S	C	C	C	Cl		
	AS	As	S	C	C	C	F		
	AS	As	S	C	C	C	I		
	AS	As	S	C	C	C	N		
	AS	As	S	C	C	C	O		
	AS	As	S	C	C	C	P		
	AS	As	S	C	C	C	S		
	AS	As	S	C	C	C	Se		
	AS	As	S	C	C	C	Si		
	AS	As	S	C	C	C	Te		
	AS	As	S	C	C	Cl			
	AS	As	S	C	C	F			
	AS	As	S	C	C	I			
	AS	As	S	C	C	N			
	AS	As	S	C	C	O			
	AS	As	S	C	C	P			
	AS	As	S	C	C	S			
	AS	As	S	C	C	Se			
	AS	As	S	C	C	Si			
	AS	As	S	C	C	Te			
	AS	B	C	C	C	O	As		
	AS	B	C	C	C	O	B		
	AS	B	C	C	C	O	P		
	AS	B	C	C	C	O	Se		
	AS	B	C	C	C	O	Si		
	AS	B	C	C	C	O	Te		
	AS	B	C	C	C	S	As		
	AS	B	C	C	C	S	B		
	AS	B	C	C	C	S	P		
	AS	B	C	C	C	S	Se		
	AS	B	C	C	C	S	Si		
	AS	B	C	C	C	S	Te		
	AS	B	C	C	O	As			
	AS	B	C	C	O	B			
	AS	B	C	C	O	P			
	AS	B	C	C	O	Se			

# Screen Number Order

Screen Number	Fragment Definition						Frequency Percent
310	AS	B	C	C	O	Si	2.38 (continued)
	AS	B	C	C	O	Te	
	AS	B	C	C	S	As	
	AS	B	C	C	S	B	
	AS	B	C	C	S	P	
	AS	B	C	C	S	Se	
	AS	B	C	C	S	Si	
	AS	B	C	C	S	Te	
	AS	B	O	C	C	As	
	AS	B	O	C	C	B	
	AS	B	O	C	C	Br	
	AS	B	O	C	C	C	As
	AS	B	O	C	C	C	B
	AS	B	O	C	C	C	Br
	AS	B	O	C	C	C	Cl
	AS	B	O	C	C	C	F
	AS	B	O	C	C	C	I
	AS	B	O	C	C	C	N
	AS	B	O	C	C	C	O
	AS	B	O	C	C	C	P
	AS	B	O	C	C	C	S
	AS	B	O	C	C	C	Se
	AS	B	O	C	C	C	Si
	AS	B	O	C	C	C	Te
	AS	B	O	C	C	Cl	
	AS	B	O	C	C	F	
	AS	B	O	C	C	I	
	AS	B	O	C	C	N	
	AS	B	O	C	C	O	
	AS	B	O	C	C	P	
	AS	B	O	C	C	S	
	AS	B	O	C	C	Se	
	AS	B	O	C	C	Si	
	AS	B	O	C	C	Te	
	AS	B	S	C	C	As	
	AS	B	S	C	C	B	
	AS	B	S	C	C	Br	
	AS	B	S	C	C	C	As
	AS	B	S	C	C	C	B
	AS	B	S	C	C	C	Br
	AS	B	S	C	C	C	Cl
	AS	B	S	C	C	C	F
	AS	B	S	C	C	C	I
	AS	B	S	C	C	C	N
	AS	B	S	C	C	C	O
	AS	B	S	C	C	C	P
	AS	B	S	C	C	C	S
	AS	B	S	C	C	C	Se
	AS	B	S	C	C	C	Si
	AS	B	S	C	C	C	Te
	AS	B	S	C	C	Cl	
	AS	B	S	C	C	F	
	AS	B	S	C	C	I	
	AS	B	S	C	C	N	
	AS	B	S	C	C	O	

# Screen Number Order

Screen Number	Fragment Definition						Frequency Percent
310	AS	B	S	C	C	P	2.38 (continued)
	AS	B	S	C	C	S	
	AS	B	S	C	C	Se	
	AS	B	S	C	C	Si	
	AS	B	S	C	C	Te	
	AS	Br	C	C	C	O As	
	AS	Br	C	C	C	O B	
	AS	Br	C	C	C	O P	
	AS	Br	C	C	C	O Se	
	AS	Br	C	C	C	O Si	
	AS	Br	C	C	C	O Te	
	AS	Br	C	C	C	S As	
	AS	Br	C	C	C	S B	
	AS	Br	C	C	C	S P	
	AS	Br	C	C	C	S Se	
	AS	Br	C	C	C	S Si	
	AS	Br	C	C	C	S Te	
	AS	Br	C	C	O	As	
	AS	Br	C	C	O	B	
	AS	Br	C	C	O	P	
	AS	Br	C	C	O	Se	
	AS	Br	C	C	O	Si	
	AS	Br	C	C	O	Te	
	AS	Br	C	C	S	As	
	AS	Br	C	C	S	B	
	AS	Br	C	C	S	P	
	AS	Br	C	C	S	Se	
	AS	Br	C	C	S	Si	
	AS	Br	C	C	S	Te	
	AS	Cl	C	C	C	O As	
	AS	Cl	C	C	C	O B	
	AS	Cl	C	C	C	O P	
	AS	Cl	C	C	C	O Se	
	AS	Cl	C	C	C	O Si	
	AS	Cl	C	C	C	O Te	
	AS	Cl	C	C	C	S As	
	AS	Cl	C	C	C	S B	
	AS	Cl	C	C	C	S P	
	AS	Cl	C	C	C	S Se	
	AS	Cl	C	C	C	S Si	
	AS	Cl	C	C	C	S Te	
	AS	Cl	C	C	O	As	
	AS	Cl	C	C	O	B	
	AS	Cl	C	C	O	P	
	AS	Cl	C	C	O	Se	
	AS	Cl	C	C	O	Si	
	AS	Cl	C	C	O	Te	
	AS	Cl	C	C	S	As	
	AS	Cl	C	C	S	B	
	AS	Cl	C	C	S	P	
	AS	Cl	C	C	S	Se	
	AS	Cl	C	C	S	Si	
	AS	Cl	C	C	S	Te	
	AS	F	C	C	C	O As	
	AS	F	C	C	C	O B	

# Screen Number Order

Screen Number	Fragment Definition							Frequency Percent
310	AS	F	C	C	C	O	P	2.38 (continued)
	AS	F	C	C	C	O	Se	
	AS	F	C	C	C	O	Si	
	AS	F	C	C	C	O	Te	
	AS	F	C	C	C	S	As	
	AS	F	C	C	C	S	B	
	AS	F	C	C	C	S	P	
	AS	F	C	C	C	S	Se	
	AS	F	C	C	C	S	Si	
	AS	F	C	C	C	S	Te	
	AS	F	C	C	O	As		
	AS	F	C	C	O	B		
	AS	F	C	C	O	P		
	AS	F	C	C	O	Se		
	AS	F	C	C	O	Si		
	AS	F	C	C	O	Te		
	AS	F	C	C	S	As		
	AS	F	C	C	S	B		
	AS	F	C	C	S	P		
	AS	F	C	C	S	Se		
	AS	F	C	C	S	Si		
	AS	F	C	C	S	Te		
	AS	I	C	C	C	O	As	
	AS	I	C	C	C	O	B	
	AS	I	C	C	C	O	P	
	AS	I	C	C	C	O	Se	
	AS	I	C	C	C	O	Si	
	AS	I	C	C	C	O	Te	
	AS	I	C	C	C	S	As	
	AS	I	C	C	C	S	B	
	AS	I	C	C	C	S	P	
	AS	I	C	C	C	S	Se	
	AS	I	C	C	C	S	Si	
	AS	I	C	C	C	S	Te	
	AS	I	C	C	O	As		
	AS	I	C	C	O	B		
	AS	I	C	C	O	P		
	AS	I	C	C	O	Se		
	AS	I	C	C	O	Si		
	AS	I	C	C	O	Te		
	AS	I	C	C	S	As		
	AS	I	C	C	S	B		
	AS	I	C	C	S	P		
	AS	I	C	C	S	Se		
	AS	I	C	C	S	Si		
	AS	I	C	C	S	Te		
	AS	N	C	C	C	O	As	
	AS	N	C	C	C	O	B	
	AS	N	C	C	C	O	P	
	AS	N	C	C	C	O	Se	
	AS	N	C	C	C	O	Si	
	AS	N	C	C	C	O	Te	
	AS	N	C	C	C	S	As	
	AS	N	C	C	C	S	B	
	AS	N	C	C	C	S	P	

# Screen Number Order

Screen Number	Fragment Definition							Frequency Percent
310	AS	N	C	C	C	S	Se	2.38 (continued)
	AS	N	C	C	C	S	Si	
	AS	N	C	C	C	S	Te	
	AS	N	C	C	O	As		
	AS	N	C	C	O	B		
	AS	N	C	C	O	P		
	AS	N	C	C	O	Se		
	AS	N	C	C	O	Si		
	AS	N	C	C	O	Te		
	AS	N	C	C	S	As		
	AS	N	C	C	S	B		
	AS	N	C	C	S	P		
	AS	N	C	C	S	Se		
	AS	N	C	C	S	Si		
	AS	N	C	C	S	Te		
	AS	O	C	C	C	O	As	
	AS	O	C	C	C	O	B	
	AS	O	C	C	C	O	P	
	AS	O	C	C	C	O	Se	
	AS	O	C	C	C	O	Si	
	AS	O	C	C	C	O	Te	
	AS	O	C	C	C	S	As	
	AS	O	C	C	C	S	B	
	AS	O	C	C	C	S	P	
	AS	O	C	C	C	S	Se	
	AS	O	C	C	C	S	Si	
	AS	O	C	C	C	S	Te	
	AS	O	C	C	O	As		
	AS	O	C	C	O	B		
	AS	O	C	C	O	P		
	AS	O	C	C	O	Se		
	AS	O	C	C	O	Si		
	AS	O	C	C	O	Te		
	AS	O	C	C	S	As		
	AS	O	C	C	S	B		
	AS	O	C	C	S	P		
	AS	O	C	C	S	Se		
	AS	O	C	C	S	Si		
	AS	O	C	C	S	Te		
	AS	P	C	C	C	O	As	
	AS	P	C	C	C	O	B	
	AS	P	C	C	C	O	P	
	AS	P	C	C	C	O	Se	
	AS	P	C	C	C	O	Si	
	AS	P	C	C	C	O	Te	
	AS	P	C	C	C	S	As	
	AS	P	C	C	C	S	B	
	AS	P	C	C	C	S	P	
	AS	P	C	C	C	S	Se	
	AS	P	C	C	C	S	Si	
	AS	P	C	C	C	S	Te	
	AS	P	C	C	O	As		
	AS	P	C	C	O	B		
	AS	P	C	C	O	P		
	AS	P	C	C	O	Se		

# Screen Number Order

Screen Number	Fragment Definition						Frequency Percent
310	AS	P	C	C	O	Si	2.38 (continued)
	AS	P	C	C	O	Te	
	AS	P	C	C	S	As	
	AS	P	C	C	S	B	
	AS	P	C	C	S	P	
	AS	P	C	C	S	Se	
	AS	P	C	C	S	Si	
	AS	P	C	C	S	Te	
	AS	P	O	C	C	As	
	AS	P	O	C	C	B	
	AS	P	O	C	C	Br	
	AS	P	O	C	C	C	As
	AS	P	O	C	C	C	B
	AS	P	O	C	C	C	Br
	AS	P	O	C	C	C	Cl
	AS	P	O	C	C	C	F
	AS	P	O	C	C	C	I
	AS	P	O	C	C	C	N
	AS	P	O	C	C	C	O
	AS	P	O	C	C	C	P
	AS	P	O	C	C	C	S
	AS	P	O	C	C	C	Se
	AS	P	O	C	C	C	Si
	AS	P	O	C	C	C	Te
	AS	P	O	C	C	Cl	
	AS	P	O	C	C	F	
	AS	P	O	C	C	I	
	AS	P	O	C	C	N	
	AS	P	O	C	C	O	
	AS	P	O	C	C	P	
	AS	P	O	C	C	S	
	AS	P	O	C	C	Se	
	AS	P	O	C	C	Si	
	AS	P	O	C	C	Te	
	AS	P	S	C	C	As	
	AS	P	S	C	C	B	
	AS	P	S	C	C	Br	
	AS	P	S	C	C	C	As
	AS	P	S	C	C	C	B
	AS	P	S	C	C	C	Br
	AS	P	S	C	C	C	Cl
	AS	P	S	C	C	C	F
	AS	P	S	C	C	C	I
	AS	P	S	C	C	C	N
	AS	P	S	C	C	C	O
	AS	P	S	C	C	C	P
	AS	P	S	C	C	C	S
	AS	P	S	C	C	C	Se
	AS	P	S	C	C	C	Si
	AS	P	S	C	C	C	Te
	AS	P	S	C	C	Cl	
	AS	P	S	C	C	F	
	AS	P	S	C	C	I	
	AS	P	S	C	C	N	
	AS	P	S	C	C	O	

# Screen Number Order

Screen Number	Fragment Definition						Frequency Percent
310	AS	P	S	C	C	P	2.38 (continued)
	AS	P	S	C	C	S	
	AS	P	S	C	C	Se	
	AS	P	S	C	C	Si	
	AS	P	S	C	C	Te	
	AS	S	C	C	C	O As	
	AS	S	C	C	C	O B	
	AS	S	C	C	C	O P	
	AS	S	C	C	C	O Se	
	AS	S	C	C	C	O Si	
	AS	S	C	C	C	O Te	
	AS	S	C	C	C	S As	
	AS	S	C	C	C	S B	
	AS	S	C	C	C	S P	
	AS	S	C	C	C	S Se	
	AS	S	C	C	C	S Si	
	AS	S	C	C	C	S Te	
	AS	S	C	C	O	As	
	AS	S	C	C	O	B	
	AS	S	C	C	O	P	
	AS	S	C	C	O	Se	
	AS	S	C	C	O	Si	
	AS	S	C	C	O	Te	
	AS	S	C	C	S	As	
	AS	S	C	C	S	B	
	AS	S	C	C	S	P	
	AS	S	C	C	S	Se	
	AS	S	C	C	S	Si	
	AS	S	C	C	S	Te	
	AS	Se	C	C	C	O As	
	AS	Se	C	C	C	O B	
	AS	Se	C	C	C	O P	
	AS	Se	C	C	C	O Se	
	AS	Se	C	C	C	O Si	
	AS	Se	C	C	C	O Te	
	AS	Se	C	C	C	S As	
	AS	Se	C	C	C	S B	
	AS	Se	C	C	C	S P	
	AS	Se	C	C	C	S Se	
	AS	Se	C	C	C	S Si	
	AS	Se	C	C	C	S Te	
	AS	Se	C	C	O	As	
	AS	Se	C	C	O	B	
	AS	Se	C	C	O	P	
	AS	Se	C	C	O	Se	
	AS	Se	C	C	O	Si	
	AS	Se	C	C	O	Te	
	AS	Se	C	C	S	As	
	AS	Se	C	C	S	B	
	AS	Se	C	C	S	P	
	AS	Se	C	C	S	Se	
	AS	Se	C	C	S	Si	
	AS	Se	C	C	S	Te	
	AS	Se	O	C	C	As	
	AS	Se	O	C	C	B	

# Screen Number Order

Screen Number	Fragment Definition						Frequency Percent	
310	AS	Se	O	C	C	Br	2.38	(continued)
	AS	Se	O	C	C	C		As
	AS	Se	O	C	C	C		B
	AS	Se	O	C	C	C		Br
	AS	Se	O	C	C	C		Cl
	AS	Se	O	C	C	C		F
	AS	Se	O	C	C	C		I
	AS	Se	O	C	C	C		N
	AS	Se	O	C	C	C		O
	AS	Se	O	C	C	C		P
	AS	Se	O	C	C	C		S
	AS	Se	O	C	C	C		Se
	AS	Se	O	C	C	C		Si
	AS	Se	O	C	C	C		Te
	AS	Se	O	C	C	Cl		
	AS	Se	O	C	C	F		
	AS	Se	O	C	C	I		
	AS	Se	O	C	C	N		
	AS	Se	O	C	C	O		
	AS	Se	O	C	C	P		
	AS	Se	O	C	C	S		
	AS	Se	O	C	C	Se		
	AS	Se	O	C	C	Si		
	AS	Se	O	C	C	Te		
	AS	Se	S	C	C	As		
	AS	Se	S	C	C	B		
	AS	Se	S	C	C	Br		
	AS	Se	S	C	C	C		As
	AS	Se	S	C	C	C		B
	AS	Se	S	C	C	C		Br
	AS	Se	S	C	C	C		Cl
	AS	Se	S	C	C	C		F
	AS	Se	S	C	C	C		I
	AS	Se	S	C	C	C		N
	AS	Se	S	C	C	C		O
	AS	Se	S	C	C	C		P
	AS	Se	S	C	C	C		S
	AS	Se	S	C	C	C		Se
	AS	Se	S	C	C	C		Si
	AS	Se	S	C	C	C		Te
	AS	Se	S	C	C	Cl		
	AS	Se	S	C	C	F		
	AS	Se	S	C	C	I		
	AS	Se	S	C	C	N		
	AS	Se	S	C	C	O		
	AS	Se	S	C	C	P		
	AS	Se	S	C	C	S		
	AS	Se	S	C	C	Se		
	AS	Se	S	C	C	Si		
	AS	Se	S	C	C	Te		
	AS	Si	C	C	C	O		As
	AS	Si	C	C	C	O		B
	AS	Si	C	C	C	O		P
	AS	Si	C	C	C	O		Se
	AS	Si	C	C	C	O		Si



# Screen Number Order

Screen Number	Fragment Definition							Frequency Percent
310	AS	Si	C	C	C	O	Te	2.38 (continued)
	AS	Si	C	C	C	S	As	
	AS	Si	C	C	C	S	B	
	AS	Si	C	C	C	S	P	
	AS	Si	C	C	C	S	Se	
	AS	Si	C	C	C	S	Si	
	AS	Si	C	C	C	S	Te	
	AS	Si	C	C	O	As		
	AS	Si	C	C	O	B		
	AS	Si	C	C	O	P		
	AS	Si	C	C	O	Se		
	AS	Si	C	C	O	Si		
	AS	Si	C	C	O	Te		
	AS	Si	C	C	S	As		
	AS	Si	C	C	S	B		
	AS	Si	C	C	S	P		
	AS	Si	C	C	S	Se		
	AS	Si	C	C	S	Si		
	AS	Si	C	C	S	Te		
	AS	Si	O	C	C	As		
	AS	Si	O	C	C	B		
	AS	Si	O	C	C	Br		
	AS	Si	O	C	C	C	As	
	AS	Si	O	C	C	C	B	
	AS	Si	O	C	C	C	Br	
	AS	Si	O	C	C	C	Cl	
	AS	Si	O	C	C	C	F	
	AS	Si	O	C	C	C	I	
	AS	Si	O	C	C	C	N	
	AS	Si	O	C	C	C	O	
	AS	Si	O	C	C	C	P	
	AS	Si	O	C	C	C	S	
	AS	Si	O	C	C	C	Se	
	AS	Si	O	C	C	C	Si	
	AS	Si	O	C	C	C	Te	
	AS	Si	O	C	C	Cl		
	AS	Si	O	C	C	F		
	AS	Si	O	C	C	I		
	AS	Si	O	C	C	N		
	AS	Si	O	C	C	O		
	AS	Si	O	C	C	P		
	AS	Si	O	C	C	S		
	AS	Si	O	C	C	Se		
	AS	Si	O	C	C	Si		
	AS	Si	O	C	C	Te		
	AS	Si	S	C	C	As		
	AS	Si	S	C	C	B		
	AS	Si	S	C	C	Br		
	AS	Si	S	C	C	C	As	
	AS	Si	S	C	C	C	B	
	AS	Si	S	C	C	C	Br	
	AS	Si	S	C	C	C	Cl	
	AS	Si	S	C	C	C	F	
	AS	Si	S	C	C	C	I	
	AS	Si	S	C	C	C	N	

# Screen Number Order

Screen Number	Fragment Definition							Frequency Percent
310	AS	Si	S	C	C	C	O	2.38 (continued)
	AS	Si	S	C	C	C	P	
	AS	Si	S	C	C	C	S	
	AS	Si	S	C	C	C	Se	
	AS	Si	S	C	C	C	Si	
	AS	Si	S	C	C	C	Te	
	AS	Si	S	C	C	Cl		
	AS	Si	S	C	C	F		
	AS	Si	S	C	C	I		
	AS	Si	S	C	C	N		
	AS	Si	S	C	C	O		
	AS	Si	S	C	C	P		
	AS	Si	S	C	C	S		
	AS	Si	S	C	C	Se		
	AS	Si	S	C	C	Si		
	AS	Si	S	C	C	Te		
	AS	Te	C	C	C	O	As	
	AS	Te	C	C	C	O	B	
	AS	Te	C	C	C	O	P	
	AS	Te	C	C	C	O	Se	
	AS	Te	C	C	C	O	Si	
	AS	Te	C	C	C	O	Te	
	AS	Te	C	C	C	S	As	
	AS	Te	C	C	C	S	B	
	AS	Te	C	C	C	S	P	
	AS	Te	C	C	C	S	Se	
	AS	Te	C	C	C	S	Si	
	AS	Te	C	C	C	S	Te	
	AS	Te	C	C	O	As		
	AS	Te	C	C	O	B		
	AS	Te	C	C	O	P		
	AS	Te	C	C	O	Se		
	AS	Te	C	C	O	Si		
	AS	Te	C	C	O	Te		
	AS	Te	C	C	S	As		
	AS	Te	C	C	S	B		
	AS	Te	C	C	S	P		
	AS	Te	C	C	S	Se		
	AS	Te	C	C	S	Si		
	AS	Te	C	C	S	Te		
	AS	Te	O	C	C	As		
	AS	Te	O	C	C	B		
	AS	Te	O	C	C	Br		
	AS	Te	O	C	C	C	As	
	AS	Te	O	C	C	C	B	
	AS	Te	O	C	C	C	Br	
	AS	Te	O	C	C	C	Cl	
	AS	Te	O	C	C	C	F	
	AS	Te	O	C	C	C	I	
	AS	Te	O	C	C	C	N	
	AS	Te	O	C	C	C	O	
	AS	Te	O	C	C	C	P	
	AS	Te	O	C	C	C	S	
	AS	Te	O	C	C	C	Si	
	AS	Te	O	C	C	C	Se	

# Screen Number Order

Screen Number	Fragment Definition							Frequency Percent
310	AS	Te	O	C	C	C	Te	2.38 (continued)
	AS	Te	O	C	C	Cl		
	AS	Te	O	C	C	F		
	AS	Te	O	C	C	I		
	AS	Te	O	C	C	N		
	AS	Te	O	C	C	O		
	AS	Te	O	C	C	P		
	AS	Te	O	C	C	S		
	AS	Te	O	C	C	Se		
	AS	Te	O	C	C	Si		
	AS	Te	O	C	C	Te		
	AS	Te	S	C	C	As		
	AS	Te	S	C	C	B		
	AS	Te	S	C	C	Br		
	AS	Te	S	C	C	C	As	
	AS	Te	S	C	C	C	B	
	AS	Te	S	C	C	C	Br	
	AS	Te	S	C	C	C	Cl	
	AS	Te	S	C	C	C	F	
	AS	Te	S	C	C	C	I	
	AS	Te	S	C	C	C	N	
	AS	Te	S	C	C	C	O	
	AS	Te	S	C	C	C	P	
	AS	Te	S	C	C	C	S	
	AS	Te	S	C	C	C	Se	
	AS	Te	S	C	C	C	Si	
	AS	Te	S	C	C	C	Te	
	AS	Te	S	C	C	Cl		
	AS	Te	S	C	C	F		
	AS	Te	S	C	C	I		
	AS	Te	S	C	C	N		
	AS	Te	S	C	C	O		
	AS	Te	S	C	C	P		
	AS	Te	S	C	C	S		
	AS	Te	S	C	C	Se		
	AS	Te	S	C	C	Si		
	AS	Te	S	C	C	Te		
311	AS	As	C	C	C	As		1.14
	AS	As	C	C	C	B		
	AS	As	C	C	C	Br		
	AS	As	C	C	C	Cl		
	AS	As	C	C	C	F		
	AS	As	C	C	C	I		
	AS	As	C	C	C	N		
	AS	As	C	C	C	O		
	AS	As	C	C	C	P		
	AS	As	C	C	C	S		
	AS	As	C	C	C	Se		
	AS	As	C	C	C	Si		
	AS	As	C	C	C	Te		
	AS	B	C	C	C	As		
	AS	B	C	C	C	B		
	AS	B	C	C	C	Br		
	AS	B	C	C	C	Cl		

# Screen Number Order

Screen Number	Fragment Definition						Frequency Percent
311	AS	B	C	C	C	F	1.14 (continued)
	AS	B	C	C	C	I	
	AS	B	C	C	C	N	
	AS	B	C	C	C	O	
	AS	B	C	C	C	P	
	AS	B	C	C	C	S	
	AS	B	C	C	C	Se	
	AS	B	C	C	C	Si	
	AS	B	C	C	C	Te	
	AS	Br	C	C	C	As	
	AS	Br	C	C	C	B	
	AS	Br	C	C	C	P	
	AS	Br	C	C	C	Se	
	AS	Br	C	C	C	Si	
	AS	Br	C	C	C	Te	
	AS	Cl	C	C	C	As	
	AS	Cl	C	C	C	B	
	AS	Cl	C	C	C	P	
	AS	Cl	C	C	C	Se	
	AS	Cl	C	C	C	Si	
	AS	Cl	C	C	C	Te	
	AS	F	C	C	C	As	
	AS	F	C	C	C	B	
	AS	F	C	C	C	P	
	AS	F	C	C	C	Se	
	AS	F	C	C	C	Si	
	AS	F	C	C	C	Te	
	AS	I	C	C	C	As	
	AS	I	C	C	C	B	
	AS	I	C	C	C	P	
	AS	I	C	C	C	Se	
	AS	I	C	C	C	Si	
	AS	I	C	C	C	Te	
	AS	N	C	C	C	As	
	AS	N	C	C	C	B	
	AS	N	C	C	C	P	
	AS	N	C	C	C	Se	
	AS	N	C	C	C	Si	
	AS	N	C	C	C	Te	
	AS	O	C	C	C	As	
	AS	O	C	C	C	B	
	AS	O	C	C	C	P	
	AS	O	C	C	C	Se	
	AS	O	C	C	C	Si	
	AS	O	C	C	C	Te	
	AS	P	C	C	C	As	
	AS	P	C	C	C	B	
	AS	P	C	C	C	Br	
	AS	P	C	C	C	Cl	
	AS	P	C	C	C	F	
	AS	P	C	C	C	I	
	AS	P	C	C	C	N	
	AS	P	C	C	C	O	
	AS	P	C	C	C	P	
	AS	P	C	C	C	S	

# Screen Number Order

Screen Number	Fragment Definition						Frequency Percent
311	AS	P	C	C	C	Se	1.14 (continued)
	AS	P	C	C	C	Si	
	AS	P	C	C	C	Te	
	AS	S	C	C	C	As	
	AS	S	C	C	C	B	
	AS	S	C	C	C	P	
	AS	S	C	C	C	Se	
	AS	S	C	C	C	Si	
	AS	S	C	C	C	Te	
	AS	Se	C	C	C	As	
	AS	Se	C	C	C	B	
	AS	Se	C	C	C	Br	
	AS	Se	C	C	C	Cl	
	AS	Se	C	C	C	F	
	AS	Se	C	C	C	I	
	AS	Se	C	C	C	N	
	AS	Se	C	C	C	O	
	AS	Se	C	C	C	P	
	AS	Se	C	C	C	S	
	AS	Se	C	C	C	Se	
	AS	Se	C	C	C	Si	
	AS	Se	C	C	C	Te	
	AS	Si	C	C	C	As	
	AS	Si	C	C	C	B	
	AS	Si	C	C	C	Br	
	AS	Si	C	C	C	Cl	
	AS	Si	C	C	C	F	
	AS	Si	C	C	C	I	
	AS	Si	C	C	C	N	
	AS	Si	C	C	C	O	
	AS	Si	C	C	C	P	
	AS	Si	C	C	C	S	
	AS	Si	C	C	C	Se	
	AS	Si	C	C	C	Si	
	AS	Si	C	C	C	Te	
	AS	Te	C	C	C	As	
	AS	Te	C	C	C	B	
	AS	Te	C	C	C	Br	
	AS	Te	C	C	C	Cl	
	AS	Te	C	C	C	F	
	AS	Te	C	C	C	I	
	AS	Te	C	C	C	N	
	AS	Te	C	C	C	O	
	AS	Te	C	C	C	P	
	AS	Te	C	C	C	S	
	AS	Te	C	C	C	Se	
	AS	Te	C	C	C	Si	
	AS	Te	C	C	C	Te	
312	AS	Br-	C	*	C	- Br	2.00
	AS	Br-	C	*	C	- Cl	
	AS	Br-	C	*	C	- F	
	AS	Br-	C	*	C	- I	
	AS	Cl-	C	*	C	- Br	
	AS	Cl-	C	*	C	- Cl	

# Screen Number Order

Screen Number	Fragment Definition	Frequency Percent
312	AS Cl- C * C - F	2.00 (continued)
	AS Cl- C * C - I	
	AS F - C * C - Br	
	AS F - C * C - Cl	
	AS F - C * C - F	
	AS F - C * C - I	
	AS I - C * C - Br	
	AS I - C * C - Cl	
	AS I - C * C - F	
	AS I - C * C - I	
313	AS Br- C - C - Br	0.90
	AS Br- C - C - Cl	
	AS Br- C - C - F	
	AS Br- C - C - I	
	AS Cl- C - C - Br	
	AS Cl- C - C - Cl	
	AS Cl- C - C - F	
	AS Cl- C - C - I	
	AS F - C - C - Br	
	AS F - C - C - Cl	
	AS F - C - C - F	
	AS F - C - C - I	
	AS I - C - C - Br	
	AS I - C - C - Cl	
	AS I - C - C - F	
	AS I - C - C - I	
314	AS Br- C * C * N	1.48
	AS Cl- C * C * N	
	AS F - C * C * N	
	AS I - C * C * N	
	AS N * C * C - Br	
	AS N * C * C - Cl	
	AS N * C * C - F	
	AS N * C * C - I	
315	AS Br- C * C - N	2.34
	AS Cl- C * C - N	
	AS F - C * C - N	
	AS I - C * C - N	
	AS N - C * C - Br	
	AS N - C * C - Cl	
	AS N - C * C - F	
	AS N - C * C - I	
316	AS Br- C - C * N	0.64
	AS Cl- C - C * N	
	AS F - C - C * N	
	AS I - C - C * N	
	AS N * C - C - Br	
	AS N * C - C - Cl	
	AS N * C - C - F	
	AS N * C - C - I	

		Screen Number Order											
Screen Number		Fragment Definition						Frequency Percent					
317	AS	Br-	C	-	C	-	N	1.12					
	AS	Cl-	C	-	C	-	N						
	AS	F	-	C	-	C	-		N				
	AS	I	-	C	-	C	-		N				
	AS	N	-	C	-	C	-		Br				
	AS	N	-	C	-	C	-		Cl				
	AS	N	-	C	-	C	-		F				
	AS	N	-	C	-	C	-		I				
318	AS	Br	C		C	N	C	N	1.48				
	AS	Cl	C		C	N	C	N					
	AS	F	C		C	N	C	N					
	AS	I	C		C	N	C	N					
	AS	N	C		N	C	C	Br					
	AS	N	C		N	C	C	Cl					
	AS	N	C		N	C	C	F					
	AS	N	C		N	C	C	I					
319	AS	Br	C		C	N	C	O	1.84				
	AS	Br	C		C	N	C	S					
	AS	Cl	C		C	N	C	O					
	AS	Cl	C		C	N	C	S					
	AS	F	C		C	N	C	O					
	AS	F	C		C	N	C	S					
	AS	I	C		C	N	C	O					
	AS	I	C		C	N	C	S					
	AS	O	C		N	C	C	Br					
	AS	O	C		N	C	C	Cl					
	AS	O	C		N	C	C	F					
	AS	O	C		N	C	C	I					
	AS	S	C		N	C	C	Br					
	AS	S	C		N	C	C	Cl					
	AS	S	C		N	C	C	F					
	AS	S	C		N	C	C	I					
320	AS	Br-	C	*	C	-	N	-	C	-	O	0.72	
	AS	Br-	C	*	C	-	N	-	C	-	S		
	AS	Cl-	C	*	C	-	N	-	C	-	O		
	AS	Cl-	C	*	C	-	N	-	C	-	S		
	AS	F	-	C	*	C	-	N	-	C	-		O
	AS	F	-	C	*	C	-	N	-	C	-		S
	AS	I	-	C	*	C	-	N	-	C	-		O
	AS	I	-	C	*	C	-	N	-	C	-		S
	AS	O	-	C	-	N	-	C	*	C	-		Br
	AS	O	-	C	-	N	-	C	*	C	-		Cl
	AS	O	-	C	-	N	-	C	*	C	-		F
	AS	O	-	C	-	N	-	C	*	C	-		I
	AS	S	-	C	-	N	-	C	*	C	-		Br
	AS	S	-	C	-	N	-	C	*	C	-		Cl
	AS	S	-	C	-	N	-	C	*	C	-		F
	AS	S	-	C	-	N	-	C	*	C	-		I

Screen Number Order							
Screen Number	Fragment Definition						Frequency Percent
321	AS	Br	C	C	N	N	0.82
	AS	Cl	C	C	N	N	
	AS	F	C	C	N	N	
	AS	I	C	C	N	N	
	AS	N	N	C	C	Br	
	AS	N	N	C	C	Cl	
	AS	N	N	C	C	F	
	AS	N	N	C	C	I	
322	AS	Br	C	C	N	O	0.39
	AS	Br	C	C	N	S	
	AS	Cl	C	C	N	O	
	AS	Cl	C	C	N	S	
	AS	F	C	C	N	O	
	AS	F	C	C	N	S	
	AS	I	C	C	N	O	
	AS	I	C	C	N	S	
	AS	O	N	C	C	Br	
	AS	O	N	C	C	Cl	
	AS	O	N	C	C	F	
	AS	O	N	C	C	I	
	AS	S	N	C	C	Br	
	AS	S	N	C	C	Cl	
	AS	S	N	C	C	F	
	AS	S	N	C	C	I	
323	AS	Br-	C *	C *	O	0.61	
	AS	Br-	C *	C *	S		
	AS	Cl-	C *	C *	O		
	AS	Cl-	C *	C *	S		
	AS	F -	C *	C *	O		
	AS	F -	C *	C *	S		
	AS	I -	C *	C *	O		
	AS	I -	C *	C *	S		
	AS	O *	C *	C -	Br		
	AS	O *	C *	C -	Cl		
	AS	O *	C *	C -	F		
	AS	O *	C *	C -	I		
	AS	S *	C *	C -	Br		
	AS	S *	C *	C -	Cl		
	AS	S *	C *	C -	F		
	AS	S *	C *	C -	I		
324	AS	Br-	C *	C -	O	2.95	
	AS	Br-	C *	C -	S		
	AS	Cl-	C *	C -	O		
	AS	Cl-	C *	C -	S		
	AS	F -	C *	C -	O		
	AS	F -	C *	C -	S		
	AS	I -	C *	C -	O		
	AS	I -	C *	C -	S		
	AS	O -	C *	C -	Br		
	AS	O -	C *	C -	Cl		
	AS	O -	C *	C -	F		
	AS	O -	C *	C -	I		



# Screen Number Order

Screen Number	Fragment Definition	Frequency Percent
324	AS S - C * C - Br	2.95 (continued)
	AS S - C * C - Cl	
	AS S - C * C - F	
	AS S - C * C - I	
325	AS Br- C - C * O	0.45
	AS Br- C - C * S	
	AS Cl- C - C * O	
	AS Cl- C - C * S	
	AS F - C - C * O	
	AS F - C - C * S	
	AS I - C - C * O	
	AS I - C - C * S	
	AS O * C - C - Br	
	AS O * C - C - Cl	
	AS O * C - C - F	
	AS O * C - C - I	
	AS S * C - C - Br	
	AS S * C - C - Cl	
	AS S * C - C - F	
	AS S * C - C - I	
326	AS Br- C - C - O	2.53
	AS Br- C - C - S	
	AS Cl- C - C - O	
	AS Cl- C - C - S	
	AS F - C - C - O	
	AS F - C - C - S	
	AS I - C - C - O	
	AS I - C - C - S	
	AS O - C - C - Br	
	AS O - C - C - Cl	
	AS O - C - C - F	
	AS O - C - C - I	
	AS S - C - C - Br	
	AS S - C - C - Cl	
	AS S - C - C - F	
	AS S - C - C - I	
327	AS Br C C O C N	0.27
	AS Br C C S C N	
	AS Cl C C O C N	
	AS Cl C C S C N	
	AS F C C O C N	
	AS F C C S C N	
	AS I C C O C N	
	AS I C C S C N	
	AS N C O C C Br	
	AS N C O C C Cl	
	AS N C O C C F	
	AS N C O C C I	
	AS N C S C C Br	
	AS N C S C C Cl	
	AS N C S C C F	
	AS N C S C C I	

# Screen Number Order

Screen Number	Fragment Definition							Frequency Percent
328	AS	Br	C	C	O	C	O	0.64
	AS	Br	C	C	O	C	S	
	AS	Br	C	C	S	C	O	
	AS	Br	C	C	S	C	S	
	AS	Cl	C	C	O	C	O	
	AS	Cl	C	C	O	C	S	
	AS	Cl	C	C	S	C	O	
	AS	Cl	C	C	S	C	S	
	AS	F	C	C	O	C	O	
	AS	F	C	C	O	C	S	
	AS	F	C	C	S	C	O	
	AS	F	C	C	S	C	S	
	AS	I	C	C	O	C	O	
	AS	I	C	C	O	C	S	
	AS	I	C	C	S	C	O	
	AS	I	C	C	S	C	S	
	AS	O	C	O	C	C	Br	
	AS	O	C	O	C	C	Cl	
	AS	O	C	O	C	C	F	
	AS	O	C	O	C	C	I	
	AS	O	C	S	C	C	Br	
	AS	O	C	S	C	C	Cl	
	AS	O	C	S	C	C	F	
	AS	O	C	S	C	C	I	
	AS	S	C	O	C	C	Br	
	AS	S	C	O	C	C	Cl	
	AS	S	C	O	C	C	F	
	AS	S	C	O	C	C	I	
	AS	S	C	S	C	C	Br	
	AS	S	C	S	C	C	Cl	
	AS	S	C	S	C	C	F	
	AS	S	C	S	C	C	I	
329	AS	Br	C	C	O	N		0.30
	AS	Br	C	C	S	N		
	AS	Cl	C	C	O	N		
	AS	Cl	C	C	S	N		
	AS	F	C	C	O	N		
	AS	F	C	C	S	N		
	AS	I	C	C	O	N		
	AS	I	C	C	S	N		
	AS	N	O	C	C	Br		
	AS	N	O	C	C	Cl		
	AS	N	O	C	C	F		
	AS	N	O	C	C	I		
	AS	N	S	C	C	Br		
	AS	N	S	C	C	Cl		
	AS	N	S	C	C	F		
	AS	N	S	C	C	I		
330	AS	Br	C	C	O	O		0.43
	AS	Br	C	C	O	S		
	AS	Br	C	C	S	O		
	AS	Br	C	C	S	S		
	AS	Cl	C	C	O	O		

# Screen Number Order

Screen Number	Fragment Definition						Frequency Percent
330	AS	Cl	C	C	O	S	0.43 (continued)
	AS	Cl	C	C	S	O	
	AS	Cl	C	C	S	S	
	AS	F	C	C	O	O	
	AS	F	C	C	O	S	
	AS	F	C	C	S	O	
	AS	F	C	C	S	S	
	AS	I	C	C	O	O	
	AS	I	C	C	O	S	
	AS	I	C	C	S	O	
	AS	I	C	C	S	S	
	AS	O	O	C	C	Br	
	AS	O	O	C	C	Cl	
	AS	O	O	C	C	F	
	AS	O	O	C	C	I	
	AS	O	S	C	C	Br	
	AS	O	S	C	C	Cl	
	AS	O	S	C	C	F	
	AS	O	S	C	C	I	
	AS	S	O	C	C	Br	
	AS	S	O	C	C	Cl	
	AS	S	O	C	C	F	
	AS	S	O	C	C	I	
	AS	S	S	C	C	Br	
	AS	S	S	C	C	Cl	
	AS	S	S	C	C	F	
	AS	S	S	C	C	I	
331	AS	As	C	C	As		1.39
	AS	As	C	C	B		
	AS	As	C	C	Br		
	AS	As	C	C	Cl		
	AS	As	C	C	F		
	AS	As	C	C	I		
	AS	As	C	C	N		
	AS	As	C	C	O		
	AS	As	C	C	P		
	AS	As	C	C	S		
	AS	As	C	C	Se		
	AS	As	C	C	Si		
	AS	As	C	C	Te		
	AS	B	C	C	As		
	AS	B	C	C	B		
	AS	B	C	C	Br		
	AS	B	C	C	Cl		
	AS	B	C	C	F		
	AS	B	C	C	I		
	AS	B	C	C	N		
	AS	B	C	C	O		
	AS	B	C	C	P		
	AS	B	C	C	S		
	AS	B	C	C	Se		
	AS	B	C	C	Si		
	AS	B	C	C	Te		
	AS	Br	C	C	As		

# Screen Number Order

Screen Number	Fragment Definition					Frequency Percent
331	AS	Br	C	C	B	1.39 (continued)
	AS	Br	C	C	P	
	AS	Br	C	C	Se	
	AS	Br	C	C	Si	
	AS	Br	C	C	Te	
	AS	Cl	C	C	As	
	AS	Cl	C	C	B	
	AS	Cl	C	C	P	
	AS	Cl	C	C	Se	
	AS	Cl	C	C	Si	
	AS	Cl	C	C	Te	
	AS	F	C	C	As	
	AS	F	C	C	B	
	AS	F	C	C	P	
	AS	F	C	C	Se	
	AS	F	C	C	Si	
	AS	F	C	C	Te	
	AS	I	C	C	As	
	AS	I	C	C	B	
	AS	I	C	C	P	
	AS	I	C	C	Se	
	AS	I	C	C	Si	
	AS	I	C	C	Te	
	AS	N	C	C	As	
	AS	N	C	C	B	
	AS	N	C	C	P	
	AS	N	C	C	Se	
	AS	N	C	C	Si	
	AS	N	C	C	Te	
	AS	O	C	C	As	
	AS	O	C	C	B	
	AS	O	C	C	P	
	AS	O	C	C	Se	
	AS	O	C	C	Si	
	AS	O	C	C	Te	
	AS	P	C	C	As	
	AS	P	C	C	B	
	AS	P	C	C	Br	
	AS	P	C	C	Cl	
	AS	P	C	C	F	
	AS	P	C	C	I	
	AS	P	C	C	N	
	AS	P	C	C	O	
	AS	P	C	C	P	
	AS	P	C	C	S	
	AS	P	C	C	Se	
	AS	P	C	C	Si	
	AS	P	C	C	Te	
	AS	S	C	C	As	
	AS	S	C	C	B	
	AS	S	C	C	P	
	AS	S	C	C	Se	
	AS	S	C	C	Si	
	AS	S	C	C	Te	
	AS	Se	C	C	As	

# Screen Number Order

Screen Number	Fragment Definition					Frequency Percent
331	AS	Se	C	C	B	1.39 (continued)
	AS	Se	C	C	Br	
	AS	Se	C	C	Cl	
	AS	Se	C	C	F	
	AS	Se	C	C	I	
	AS	Se	C	C	N	
	AS	Se	C	C	O	
	AS	Se	C	C	P	
	AS	Se	C	C	S	
	AS	Se	C	C	Se	
	AS	Se	C	C	Si	
	AS	Se	C	C	Te	
	AS	Si	C	C	As	
	AS	Si	C	C	B	
	AS	Si	C	C	Br	
	AS	Si	C	C	Cl	
	AS	Si	C	C	F	
	AS	Si	C	C	I	
	AS	Si	C	C	N	
	AS	Si	C	C	O	
	AS	Si	C	C	P	
	AS	Si	C	C	S	
	AS	Si	C	C	Se	
	AS	Si	C	C	Si	
	AS	Si	C	C	Te	
	AS	Te	C	C	As	
	AS	Te	C	C	B	
	AS	Te	C	C	Br	
	AS	Te	C	C	Cl	
	AS	Te	C	C	F	
	AS	Te	C	C	I	
	AS	Te	C	C	N	
	AS	Te	C	C	O	
	AS	Te	C	C	P	
	AS	Te	C	C	S	
	AS	Te	C	C	Se	
	AS	Te	C	C	Si	
	AS	Te	C	C	Te	
332	AS	Br	C	N	C	0.12
	AS	Br	C	N	C	
	AS	Br	C	N	C	
	AS	Br	C	N	C	
	AS	Cl	C	N	C	
	AS	Cl	C	N	C	
	AS	Cl	C	N	C	
	AS	Cl	C	N	C	
	AS	Cl	C	N	C	
	AS	F	C	N	C	
	AS	F	C	N	C	
	AS	F	C	N	C	
	AS	F	C	N	C	
	AS	F	C	N	C	
	AS	I	C	N	C	
	AS	I	C	N	C	
	AS	I	C	N	C	
	AS	I	C	N	C	

Screen Number Order							Frequency Percent
Screen Number	Fragment Definition						
333	AS	Br	C	N	C	N	0.53
	AS	Cl	C	N	C	N	
	AS	F	C	N	C	N	
	AS	I	C	N	C	N	
	AS	N	C	N	C	Br	
	AS	N	C	N	C	Cl	
	AS	N	C	N	C	F	
	AS	N	C	N	C	I	
334	AS	Br	C	N	C	O	0.18
	AS	Br	C	N	C	S	
	AS	Cl	C	N	C	O	
	AS	Cl	C	N	C	S	
	AS	F	C	N	C	O	
	AS	F	C	N	C	S	
	AS	I	C	N	C	O	
	AS	I	C	N	C	S	
	AS	O	C	N	C	Br	
	AS	O	C	N	C	Cl	
	AS	O	C	N	C	F	
	AS	O	C	N	C	I	
	AS	S	C	N	C	Br	
	AS	S	C	N	C	Cl	
	AS	S	C	N	C	F	
	AS	S	C	N	C	I	
335	AS	Br	C	N	O		0.09
	AS	Br	C	N	S		
	AS	Cl	C	N	O		
	AS	Cl	C	N	S		
	AS	F	C	N	O		
	AS	F	C	N	S		
	AS	I	C	N	O		
	AS	I	C	N	S		
	AS	O	N	C	Br		
	AS	O	N	C	Cl		
	AS	O	N	C	F		
	AS	O	N	C	I		
	AS	S	N	C	Br		
	AS	S	N	C	Cl		
	AS	S	N	C	F		
	AS	S	N	C	I		
336	AS	Br	C	O	O		0.37
	AS	Br	C	O	S		
	AS	Br	C	S	O		
	AS	Br	C	S	S		
	AS	Cl	C	O	O		
	AS	Cl	C	O	S		
	AS	Cl	C	S	O		
	AS	Cl	C	S	S		
	AS	F	C	O	O		
	AS	F	C	O	S		
	AS	F	C	S	O		
	AS	F	C	S	S		

		Screen Number Order						
Screen Number		Fragment Definition					Frequency Percent	
336	AS	I	C	O	O		0.37	(continued)
	AS	I	C	O	S			
	AS	I	C	S	O			
	AS	I	C	S	S			
	AS	O	O	C	Br			
	AS	O	O	C	Cl			
	AS	O	O	C	F			
	AS	O	O	C	I			
	AS	O	S	C	Br			
	AS	O	S	C	Cl			
	AS	O	S	C	F			
	AS	O	S	C	I			
	AS	S	O	C	Br			
	AS	S	O	C	Cl			
	AS	S	O	C	F			
	AS	S	O	C	I			
	AS	S	S	C	Br			
	AS	S	S	C	Cl			
	AS	S	S	C	F			
	AS	S	S	C	I			
337	AS	N	C	C	C	C N	14.57	
338	AS	N * C * C * C * C - N					2.18	
	AS	N - C * C * C * C * N						
339	AS	N * C * C * C - C * N					0.58	
	AS	N * C - C * C * C * N						
340	AS	N * C * C * C - C - N					1.89	
	AS	N - C - C * C * C * N						
341	AS	N * C * C - C * C * N					0.18	
342	AS	N - C * C * C * C - N					2.33	
343	AS	N - C * C * C - C - N					1.25	
	AS	N - C - C * C * C - N						
344	AS	N - C - C - C - C - N					3.17	
345	AS	N	C	C	C	C O	25.91	
	AS	N	C	C	C	C S		
	AS	O	C	C	C	C N		
	AS	S	C	C	C	C N		
346	AS	N * C * C * C * C - O					5.92	
	AS	N * C * C * C * C - S						
	AS	O - C * C * C * C * N						
	AS	S - C * C * C * C * N						
347	AS	N - C * C * C * C * O					2.82	
	AS	N - C * C * C * C * S						
	AS	O * C * C * C * C - N						
	AS	S * C * C * C * C - N						

		Screen Number Order											
Screen Number		Fragment Definition										Frequency Percent	
348	AS	N	-	C	*	C	*	C	*	C	-	O	5.24
	AS	N	-	C	*	C	*	C	*	C	-	S	
	AS	O	-	C	*	C	*	C	*	C	-	N	
	AS	S	-	C	*	C	*	C	*	C	-	N	
349	AS	N	-	C	*	C	*	C	-	C	-	O	1.64
	AS	N	-	C	*	C	*	C	-	C	-	S	
	AS	O	-	C	-	C	*	C	*	C	-	N	
	AS	S	-	C	-	C	*	C	*	C	-	N	
350	AS	N	-	C	-	C	*	C	*	C	-	O	1.95
	AS	N	-	C	-	C	*	C	*	C	-	S	
	AS	O	-	C	*	C	*	C	-	C	-	N	
	AS	S	-	C	*	C	*	C	-	C	-	N	
351	AS	N	-	C	-	C	*	C	-	C	-	O	0.50
	AS	N	-	C	-	C	*	C	-	C	-	S	
	AS	O	-	C	-	C	*	C	-	C	-	N	
	AS	S	-	C	-	C	*	C	-	C	-	N	
352	AS	N	-	C	-	C	-	C	*	C	-	O	0.41
	AS	N	-	C	-	C	-	C	*	C	-	S	
	AS	O	-	C	*	C	-	C	-	C	-	N	
	AS	S	-	C	*	C	-	C	-	C	-	N	
353	AS	N	-	C	-	C	-	C	-	C	-	O	4.12
	AS	N	-	C	-	C	-	C	-	C	-	S	
	AS	O	-	C	-	C	-	C	-	C	-	N	
	AS	S	-	C	-	C	-	C	-	C	-	N	
354	AS	N	*	C	*	C	*	C	*	C	*	N	11.18
355	AS	N	*	C	*	C	*	C	*	C	-	N	4.85
	AS	N	-	C	*	C	*	C	*	C	*	N	
356	AS	N	*	C	*	C	-	C	*	C	*	N	0.63
	AS	N	*	C	-	C	*	C	*	C	*	N	
357	AS	N	*	C	*	C	-	C	-	C	-	N	3.16
	AS	N	-	C	-	C	*	C	*	C	*	N	
358	AS	N	*	C	-	C	*	C	-	C	-	N	0.16
	AS	N	-	C	*	C	-	C	*	C	*	N	
359	AS	N	*	C	-	C	-	C	*	C	*	N	0.19
360	AS	N	*	C	-	C	-	C	-	C	-	N	1.65
	AS	N	-	C	-	C	-	C	*	C	*	N	
361	AS	N	-	C	*	C	*	C	-	C	-	N	1.84
362	AS	N	-	C	*	C	-	C	-	C	-	N	1.32
	AS	N	-	C	-	C	*	C	-	C	-	N	
363	AS	N	-	C	-	C	-	C	-	C	-	N	3.46



		Screen Number Order						
Screen Number		Fragment Definition						Frequency Percent
364	AS	N	C	C	C	N	N	3.16
	AS	N	N	C	C	C	N	
365	AS	N	C	C	C	N	O	2.43
	AS	N	C	C	C	N	S	
	AS	O	N	C	C	C	N	
	AS	S	N	C	C	C	N	
366	AS	N * C * C * C - N - O						0.35
	AS	N * C * C * C - N - S						
	AS	O - N - C * C * C * N						
	AS	S - N - C * C * C * N						
367	AS	N - C * C * C - N - O						1.02
	AS	N - C * C * C - N - S						
	AS	O - N - C * C * C - N						
	AS	S - N - C * C * C - N						
368	AS	N * C * C * C * O					4.16	
	AS	N * C * C * C * S						
	AS	O * C * C * C * N						
	AS	S * C * C * C * N						
369	AS	N * C * C * C - O					9.05	
	AS	N * C * C * C - S						
	AS	O - C * C * C * N						
	AS	S - C * C * C * N						
370	AS	N * C * C - C * O					2.56	
	AS	N * C - C * C * O						
	AS	N * C - C - C * O						
	AS	N - C * C - C * O						
	AS	N - C - C * C * O						
	AS	N - C - C - C * O						
	AS	N * C * C - C * S						
	AS	N * C - C * C * S						
	AS	N * C - C - C * S						
	AS	N - C * C - C * S						
	AS	N - C - C * C * S						
	AS	N - C - C - C * S						
	AS	O * C * C - C * N						
	AS	O * C * C - C - N						
	AS	O * C - C * C * N						
	AS	O * C - C * C - N						
	AS	O * C - C - C * N						
	AS	O * C - C - C - N						
	AS	S * C * C - C * N						
	AS	S * C * C - C - N						
	AS	S * C - C * C * N						
	AS	S * C - C * C - N						
	AS	S * C - C - C * N						
	AS	S * C - C - C - N						

		Screen Number Order										
Screen Number		Fragment Definition						Frequency Percent				
371	AS	N	*	C	*	C	-	C	-	O	4.73	
	AS	N	*	C	*	C	-	C	-	S		
	AS	O	-	C	-	C	*	C	*	N		
	AS	S	-	C	-	C	*	C	*	N		
372	AS	N	*	C	-	C	*	C	-	O	0.73	
	AS	N	*	C	-	C	*	C	-	S		
	AS	O	-	C	*	C	-	C	*	N		
	AS	S	-	C	*	C	-	C	*	N		
373	AS	N	*	C	-	C	-	C	-	O	1.07	
	AS	N	*	C	-	C	-	C	-	S		
	AS	O	-	C	-	C	-	C	*	N		
	AS	S	-	C	-	C	-	C	*	N		
374	AS	N	-	C	*	C	*	C	*	O	1.65	
	AS	N	-	C	*	C	*	C	*	S		
	AS	O	*	C	*	C	*	C	-	N		
	AS	S	*	C	*	C	*	C	-	N		
375	AS	N	-	C	*	C	*	C	-	O	4.45	
	AS	N	-	C	*	C	*	C	-	S		
	AS	O	-	C	*	C	*	C	-	N		
	AS	S	-	C	*	C	*	C	-	N		
376	AS	N	-	C	*	C	-	C	-	O	1.92	
	AS	N	-	C	*	C	-	C	-	S		
	AS	O	-	C	-	C	*	C	-	N		
	AS	S	-	C	-	C	*	C	-	N		
377	AS	N	-	C	-	C	*	C	-	O	2.93	
	AS	N	-	C	-	C	*	C	-	S		
	AS	O	-	C	*	C	-	C	-	N		
	AS	S	-	C	*	C	-	C	-	N		
378	AS	N	-	C	-	C	-	C	-	O	7.21	
	AS	N	-	C	-	C	-	C	-	S		
	AS	O	-	C	-	C	-	C	-	N		
	AS	S	-	C	-	C	-	C	-	N		
379	AS	N		C		C		C		O	N	0.80
	AS	N		C		C		C		S	N	
	AS	N		O		C		C		C	N	
	AS	N		S		C		C		C	N	
380	AS	N		C		C		C		O	O	1.74
	AS	N		C		C		C		O	S	
	AS	N		C		C		C		S	O	
	AS	N		C		C		C		S	S	
	AS	O		O		C		C		C	N	
	AS	O		S		C		C		C	N	
	AS	S		O		C		C		C	N	
	AS	S		S		C		C		C	N	

		Screen Number Order											
Screen Number		Fragment Definition										Frequency Percent	
381	AS	N	-	C	*	C	*	C	-	O	-	O	0.76
	AS	N	-	C	*	C	*	C	-	O	-	S	
	AS	N	-	C	*	C	*	C	-	S	-	O	
	AS	N	-	C	*	C	*	C	-	S	-	S	
	AS	O	-	O	-	C	*	C	*	C	-	N	
	AS	O	-	S	-	C	*	C	*	C	-	N	
	AS	S	-	O	-	C	*	C	*	C	-	N	
	AS	S	-	S	-	C	*	C	*	C	-	N	
382	AS	N	*	C	*	C	*	N				12.36	
383	AS	N	*	C	*	C	-	N				4.10	
	AS	N	-	C	*	C	*	N					
384	AS	N	*	C	-	C	*	N				0.52	
385	AS	N	*	C	-	C	-	N				4.56	
	AS	N	-	C	-	C	*	N					
386	AS	N	-	C	*	C	-	N				1.42	
387	AS	N	-	C	-	C	-	N				8.72	
388	AS	N		C		C		N		C		5.86	
	AS	N		C		N		C		C			
389	AS	N		C		C		N		C		12.87	
	AS	N		C		C		N		C			
	AS	O		C		N		C		C			
	AS	S		C		N		C		C			
390	AS	N	*	C	*	C	*	N	-	C	-	O	1.34
	AS	N	*	C	*	C	*	N	-	C	-	S	
	AS	O	-	C	-	N	*	C	*	C	*	N	
	AS	S	-	C	-	N	*	C	*	C	*	N	
391	AS	N	-	C	*	C	-	N	-	C	-	O	0.42
	AS	N	-	C	*	C	-	N	-	C	-	S	
	AS	O	-	C	-	N	-	C	*	C	-	N	
	AS	S	-	C	-	N	-	C	*	C	-	N	
392	AS	N	-	C	-	C	-	N	-	C	-	O	5.48
	AS	N	-	C	-	C	-	N	-	C	-	S	
	AS	O	-	C	-	N	-	C	-	C	-	N	
	AS	S	-	C	-	N	-	C	-	C	-	N	
393	AS	N		C		C		N		N		3.65	
	AS	N		N		C		C		N			
394	AS	N		C		C		N		O		3.00	
	AS	N		C		C		N		S			
	AS	O		N		C		C		N			
	AS	S		N		C		C		N			

Screen Number Order				
Screen Number		Fragment Definition	Frequency Percent	
395	AS	N * C * C - N - O	0.48	
	AS	N * C * C - N - S		
	AS	O - N - C * C * N		
	AS	S - N - C * C * N		
396	AS	N - C * C - N - O	0.72	
	AS	N - C * C - N - S		
	AS	O - N - C * C - N		
	AS	S - N - C * C - N		
397	AS	N - C - C - N - O	0.82	
	AS	N - C - C - N - S		
	AS	O - N - C - C - N		
	AS	S - N - C - C - N		
398	AS	N * C * C * O	8.97	
	AS	N * C * C * S		
	AS	O * C * C * N		
	AS	S * C * C * N		
399	AS	N * C * C - O	5.41	
	AS	N * C * C - S		
	AS	O - C * C * N		
	AS	S - C * C * N		
400	AS	N * C - C * O	0.73	
	AS	N * C - C * S		
	AS	O * C - C * N		
	AS	S * C - C * N		
401	AS	N * C - C - O	6.21	
	AS	N * C - C - S		
	AS	O - C - C * N		
	AS	S - C - C * N		
402	AS	N - C * C * O	1.91	
	AS	N - C * C * S		
	AS	O * C * C - N		
	AS	S * C * C - N		
403	AS	N - C * C - O	6.11	
	AS	N - C * C - S		
	AS	O - C * C - N		
	AS	S - C * C - N		
404	AS	N - C - C * O	2.34	
	AS	N - C - C * S		
	AS	O * C - C - N		
	AS	S * C - C - N		
405	AS	N - C - C - O	16.92	
	AS	N - C - C - S		
	AS	O - C - C - N		
	AS	S - C - C - N		

		Screen Number Order						
Screen Number		Fragment Definition						Frequency Percent
406	AS	N	C	C	O	C	N	4.07
	AS	N	C	C	S	C	N	
	AS	N	C	O	C	C	N	
	AS	N	C	S	C	C	N	
407	AS	N - C - C - O - C - N						0.13
	AS	N - C - C - S - C - N						
	AS	N - C - O - C - C - N						
	AS	N - C - S - C - C - N						
408	AS	N	C	C	O	C	O	4.14
	AS	N	C	C	O	C	S	
	AS	N	C	C	S	C	O	
	AS	N	C	C	S	C	S	
	AS	O	C	O	C	C	N	
	AS	O	C	S	C	C	N	
	AS	S	C	O	C	C	N	
	AS	S	C	S	C	C	N	
409	AS	N - C * C - O - C - O						0.36
	AS	N - C * C - O - C - S						
	AS	N - C * C - S - C - O						
	AS	N - C * C - S - C - S						
	AS	O - C - O - C * C - N						
	AS	O - C - S - C * C - N						
	AS	S - C - O - C * C - N						
	AS	S - C - S - C * C - N						
410	AS	N - C - C - O - C - O						1.42
	AS	N - C - C - O - C - S						
	AS	N - C - C - S - C - O						
	AS	N - C - C - S - C - S						
	AS	O - C - O - C - C - N						
	AS	O - C - S - C - C - N						
	AS	S - C - O - C - C - N						
	AS	S - C - S - C - C - N						
411	AS	N	C	C	O	N		0.75
	AS	N	C	C	S	N		
	AS	N	O	C	C	N		
	AS	N	S	C	C	N		
412	AS	N	C	C	O	O		1.53
	AS	N	C	C	O	S		
	AS	N	C	C	S	O		
	AS	N	C	C	S	S		
	AS	O	O	C	C	N		
	AS	O	S	C	C	N		
	AS	S	O	C	C	N		
	AS	S	S	C	C	N		

		Screen Number Order											
Screen Number		Fragment Definition						Frequency Percent					
413	AS	N	*	C	*	C	-	O	-	O	0.27		
	AS	N	*	C	*	C	-	O	-	S			
	AS	N	*	C	*	C	-	S	-	O			
	AS	N	*	C	*	C	-	S	-	S			
	AS	O	-	O	-	C	*	C	*	N			
	AS	O	-	S	-	C	*	C	*	N			
	AS	S	-	O	-	C	*	C	*	N			
	AS	S	-	S	-	C	*	C	*	N			
414	AS	N	-	C	*	C	-	O	-	O	0.52		
	AS	N	-	C	*	C	-	O	-	S			
	AS	N	-	C	*	C	-	S	-	O			
	AS	N	-	C	*	C	-	S	-	S			
	AS	O	-	O	-	C	*	C	-	N			
	AS	O	-	S	-	C	*	C	-	N			
	AS	S	-	O	-	C	*	C	-	N			
	AS	S	-	S	-	C	*	C	-	N			
415	AS	N		C		N		C		C	O	7.06	
	AS	N		C		N		C		C	S		
	AS	O		C		C		N		C	N		
	AS	S		C		C		N		C	N		
416	AS	N	*	C	*	N	*	C	*	C	-	O	1.32
	AS	N	*	C	*	N	*	C	*	C	-	S	
	AS	O	-	C	*	C	*	N	*	C	*	N	
	AS	S	-	C	*	C	*	N	*	C	*	N	
417	AS	N	*	C	*	N	*	C	-	C	-	O	0.56
	AS	N	*	C	*	N	*	C	-	C	-	S	
	AS	O	-	C	-	C	*	N	*	C	*	N	
	AS	S	-	C	-	C	*	N	*	C	*	N	
418	AS	N	-	C	-	N	-	C	*	C	-	O	0.25
	AS	N	-	C	-	N	-	C	*	C	-	S	
	AS	O	-	C	*	C	-	N	-	C	-	N	
	AS	S	-	C	*	C	-	N	-	C	-	N	
419	AS	N	-	C	-	N	-	C	-	C	-	O	0.42
	AS	N	-	C	-	N	-	C	-	C	-	S	
	AS	O	-	C	-	C	-	N	-	C	-	N	
	AS	S	-	C	-	C	-	N	-	C	-	N	
420	AS	N		C		N		C		N		6.57	
421	AS	N	*	C	*	N	*	C	-	N		3.26	
	AS	N	-	C	*	N	*	C	*	N			
422	AS	N	*	C	-	N	-	C	*	N		0.08	
423	AS	N	-	C	*	N	*	C	-	N		0.98	
424	AS	N	-	C	-	N	-	C	-	N		0.19	

		Screen Number Order						
Screen Number		Fragment Definition						Frequency Percent
425	AS	N	C	N	C	O	9.70	
	AS	N	C	N	C	S		
	AS	O	C	N	C	N		
	AS	S	C	N	C	N		
426	AS	N * C * N * C - O	5.47					
	AS	N * C * N * C - S						
	AS	O - C * N * C * N						
	AS	S - C * N * C * N						
427	AS	N * C * N - C - O	0.50					
	AS	N * C * N - C - S						
	AS	O - C - N * C * N						
	AS	S - C - N * C * N						
428	AS	N * C - N - C - O	1.59					
	AS	N * C - N - C - S						
	AS	O - C - N - C * N						
	AS	S - C - N - C * N						
429	AS	N - C * N * C - O	1.44					
	AS	N - C * N * C - S						
	AS	O - C * N * C - N						
	AS	S - C * N * C - N						
430	AS	N - C - N - C - O	0.75					
	AS	N - C - N - C - S						
	AS	O - C - N - C - N						
	AS	S - C - N - C - N						
431	AS	N	C	N	N	3.67		
	AS	N	N	C	N			
432	AS	N * C * N * N	3.24					
	AS	N * N * C * N						
433	AS	N * C - N - N	0.55					
	AS	N - N - C * N						
434	AS	N - C * N * N	1.27					
	AS	N * N * C - N						
435	AS	N - C - N - N	0.73					
	AS	N - N - C - N						
436	AS	N	C	N	N	C	N	0.65
437	AS	N	C	N	O	1.66		
	AS	N	C	N	S			
	AS	O	N	C	N			
	AS	S	N	C	N			
438	AS	N * C * N * O	0.48					
	AS	N * C * N * S						
	AS	O * N * C * N						
	AS	S * N * C * N						

		Screen Number Order							
Screen Number		Fragment Definition						Frequency Percent	
439	AS	N	*	C	-	N	-	O	0.35
	AS	N	*	C	-	N	-	S	
	AS	O	-	N	-	C	*	N	
	AS	S	-	N	-	C	*	N	
440	AS	N	-	C	-	N	-	O	0.51
	AS	N	-	C	-	N	-	S	
	AS	O	-	N	-	C	-	N	
	AS	S	-	N	-	C	-	N	
441	AS	N	C	O	C	C	O	4.35	
	AS	N	C	O	C	C	S		
	AS	N	C	S	C	C	O		
	AS	N	C	S	C	C	S		
	AS	O	C	C	O	C	N		
	AS	O	C	C	S	C	N		
	AS	S	C	C	O	C	N		
	AS	S	C	C	S	C	N		
442	AS	N	C	O	C	N	1.12		
	AS	N	C	S	C	N			
443	AS	N	C	O	C	O	0.95		
	AS	N	C	O	C	S			
	AS	N	C	S	C	O			
	AS	N	C	S	C	S			
	AS	O	C	O	C	N			
	AS	O	C	S	C	N			
	AS	S	C	O	C	N			
	AS	S	C	S	C	N			
444	AS	N	*	C	*	O	*	N	0.42
	AS	N	*	C	*	S	*	N	
	AS	N	*	O	*	C	*	N	
	AS	N	*	S	*	C	*	N	
445	AS	N	-	C	-	O	-	N	0.06
	AS	N	-	C	-	S	-	N	
	AS	N	-	O	-	C	-	N	
	AS	N	-	S	-	C	-	N	
446	AS	N	C	O	O			0.48	
	AS	N	C	O	S				
	AS	N	C	S	O				
	AS	N	C	S	S				
	AS	O	O	C	N				
	AS	O	S	C	N				
	AS	S	O	C	N				
	AS	S	S	C	N				
447	AS	N	N	C	C	C	O	3.35	
	AS	N	N	C	C	C	S		
	AS	O	C	C	C	N	N		
	AS	S	C	C	C	N	N		



		Screen Number Order											
Screen Number		Fragment Definition										Frequency Percent	
448	AS	N	-	N	-	C	*	C	*	C	-	O	0.33
	AS	N	-	N	-	C	*	C	*	C	-	S	
	AS	O	-	C	*	C	*	C	-	N	-	N	
	AS	S	-	C	*	C	*	C	-	N	-	N	
449	AS	N		N		C		C		N		N	0.42
450	AS	N		N		C		C		N		O	0.51
	AS	N		N		C		C		N		S	
	AS	O		N		C		C		N		N	
	AS	S		N		C		C		N		N	
451	AS	N		N		C		C		O			4.22
	AS	N		N		C		C		S			
	AS	O		C		C		N		N			
	AS	S		C		C		N		N			
452	AS	N	*	N	*	C	*	C	*	C	-	O	0.46
	AS	N	*	N	*	C	*	C	*	C	-	S	
	AS	O	-	C	*	C	*	N	*	N			
	AS	S	-	C	*	C	*	N	*	N			
453	AS	N	*	N	*	C	-	C	-	O			0.74
	AS	N	*	N	*	C	-	C	-	S			
	AS	O	-	C	-	C	*	N	*	N			
	AS	S	-	C	-	C	*	N	*	N			
454	AS	N	-	N	-	C	*	C	-	O			0.91
	AS	N	-	N	-	C	*	C	-	S			
	AS	O	-	C	*	C	-	N	-	N			
	AS	S	-	C	*	C	-	N	-	N			
455	AS	N	-	N	-	C	-	C	-	O			0.80
	AS	N	-	N	-	C	-	C	-	S			
	AS	O	-	C	-	C	-	N	-	N			
	AS	S	-	C	-	C	-	N	-	N			
456	AS	N		N		C		C		O		O	0.36
	AS	N		N		C		C		O		S	
	AS	N		N		C		C		S		O	
	AS	N		N		C		C		S		S	
	AS	O		O		C		C		N		N	
	AS	O		S		C		C		N		N	
	AS	S		O		C		C		N		N	
	AS	S		S		C		C		N		N	
457	AS	N		N		C		N		N			1.08
458	AS	N		N		C		N		O			0.17
	AS	N		N		C		N		S			
	AS	O		N		C		N		N			
	AS	S		N		C		N		N			

		Screen Number Order							
Screen Number		Fragment Definition						Frequency Percent	
459	AS	N	N	C	O			6.66	
	AS	N	N	C	S				
	AS	O	C	N	N				
	AS	S	C	N	N				
460	AS	N	*	N	*	C	*	1.19	
	AS	N	*	N	*	C	*		
	AS	O	*	C	*	N	*		
	AS	S	*	C	*	N	*		
461	AS	N	*	N	*	C	-	2.61	
	AS	N	*	N	*	C	-		
	AS	O	-	C	*	N	*		
	AS	S	-	C	*	N	*		
462	AS	N	*	N	-	C	-	0.41	
	AS	N	*	N	-	C	-		
	AS	O	-	C	-	N	*		
	AS	S	-	C	-	N	*		
463	AS	N	-	N	-	C	-	2.57	
	AS	N	-	N	-	C	-		
	AS	O	-	C	-	N	-		
	AS	S	-	C	-	N	-		
464	AS	N	N	N	N			0.60	
465	AS	N	N	O	O			0.17	
	AS	N	N	O	S				
	AS	N	N	S	O				
	AS	N	N	S	S				
	AS	O	O	N	N				
	AS	O	S	N	N				
	AS	S	O	N	N				
	AS	S	S	N	N				
466	AS	N	O	C	C	C	O	0.71	
	AS	N	O	C	C	C	S		
	AS	N	S	C	C	C	O		
	AS	N	S	C	C	C	S		
	AS	O	C	C	C	O	N		
	AS	O	C	C	C	S	N		
	AS	S	C	C	C	O	N		
	AS	S	C	C	C	S	N		
467	AS	N	O	C	C	O		0.63	
	AS	N	O	C	C	S			
	AS	N	S	C	C	O			
	AS	N	S	C	C	S			
	AS	O	C	C	O	N			
	AS	O	C	C	S	N			
	AS	S	C	C	O	N			
	AS	S	C	C	S	N			

Screen Number Order						
Screen Number				Fragment Definition		Frequency Percent
468	AS	N	O	C	O	0.58
	AS	N	O	C	S	
	AS	N	S	C	O	
	AS	N	S	C	S	
	AS	O	C	O	N	
	AS	O	C	S	N	
	AS	S	C	O	N	
	AS	S	C	S	N	
469	AS	O * C * C * C * C - O	5.73			
	AS	O - C * C * C * C * O				
	AS	O * C * C * C * C - S				
	AS	O - C * C * C * C * S				
	AS	S * C * C * C * C - O				
	AS	S - C * C * C * C * O				
	AS	S * C * C * C * C - S				
	AS	S - C * C * C * C * S				
470	AS	O - C * C * C * C - O	7.27			
	AS	O - C * C * C * C - S				
	AS	S - C * C * C * C - O				
	AS	S - C * C * C * C - S				
471	AS	O - C * C * C - C - O	4.77			
	AS	O - C - C * C * C - O				
	AS	O - C * C * C - C - S				
	AS	O - C - C * C * C - S				
	AS	S - C * C * C - C - O				
	AS	S - C - C * C * C - O				
	AS	S - C * C * C - C - S				
	AS	S - C - C * C * C - S				
472	AS	O - C * C - C * C - O	0.22			
	AS	O - C * C - C * C - S				
	AS	S - C * C - C * C - O				
	AS	S - C * C - C * C - S				
473	AS	O - C * C - C - C - O	0.86			
	AS	O - C - C - C * C - O				
	AS	O - C * C - C - C - S				
	AS	O - C - C - C * C - S				
	AS	S - C * C - C - C - O				
	AS	S - C - C - C * C - O				
	AS	S - C * C - C - C - S				
	AS	S - C - C - C * C - S				
474	AS	O - C - C * C - C - O	1.17			
	AS	O - C - C * C - C - S				
	AS	S - C - C * C - C - O				
	AS	S - C - C * C - C - S				
475	AS	O - C - C - C - C - O	4.56			
	AS	O - C - C - C - C - S				
	AS	S - C - C - C - C - O				
	AS	S - C - C - C - C - S				

		Screen Number Order						
Screen Number		Fragment Definition						Frequency Percent
476	AS	O	C	C	C	N	O	2.08
	AS	O	C	C	C	N	S	
	AS	O	N	C	C	C	O	
	AS	O	N	C	C	C	S	
	AS	S	C	C	C	N	O	
	AS	S	C	C	C	N	S	
	AS	S	N	C	C	C	O	
	AS	S	N	C	C	C	S	
477	AS	O - C * C * C - N - O						0.52
	AS	O - C * C * C - N - S						
	AS	O - N - C * C * C - O						
	AS	O - N - C * C * C - S						
	AS	S - C * C * C - N - O						
	AS	S - C * C * C - N - S						
	AS	S - N - C * C * C - O						
	AS	S - N - C * C * C - S						
478	AS	O * C * C * C * O						2.29
	AS	O * C * C * C * S						
	AS	S * C * C * C * O						
	AS	S * C * C * C * S						
479	AS	O * C * C * C - O						7.38
	AS	O - C * C * C * O						
	AS	O * C * C * C - S						
	AS	O - C * C * C * S						
	AS	S * C * C * C - O						
	AS	S - C * C * C * O						
	AS	S * C * C * C - S						
	AS	S - C * C * C * S						
480	AS	O * C * C - C - O						3.12
	AS	O - C - C * C * O						
	AS	O * C * C - C - S						
	AS	O - C - C * C * S						
	AS	S * C * C - C - O						
	AS	S - C - C * C * O						
	AS	S * C * C - C - S						
	AS	S - C - C * C * S						
481	AS	O * C - C - C * O						0.19
	AS	O * C - C - C * S						
	AS	S * C - C - C * O						
	AS	S * C - C - C * S						
482	AS	O - C * C * C - O						6.67
	AS	O - C * C * C - S						
	AS	S - C * C * C - O						
	AS	S - C * C * C - S						

		Screen Number Order											
Screen Number		Fragment Definition						Frequency Percent					
483	AS	O	-	C	*	C	-	C	-	O	6.12		
	AS	O	-	C	-	C	*	C	-	O			
	AS	O	-	C	*	C	-	C	-	S			
	AS	O	-	C	-	C	*	C	-	S			
	AS	S	-	C	*	C	-	C	-	O			
	AS	S	-	C	-	C	*	C	-	O			
	AS	S	-	C	*	C	-	C	-	S			
	AS	S	-	C	-	C	*	C	-	S			
484	AS	O	-	C	-	C	-	C	-	O	6.65		
	AS	O	-	C	-	C	-	C	-	S			
	AS	S	-	C	-	C	-	C	-	O			
	AS	S	-	C	-	C	-	C	-	S			
485	AS	O		C		C		C		O	O	1.62	
	AS	O		C		C		C		O	S		
	AS	O		C		C		C		S	O		
	AS	O		C		C		C		S	S		
	AS	O	O		C		C		C		O		
	AS	O	O		C		C		C		S		
	AS	O	S		C		C		C		O		
	AS	O	S		C		C		C		S		
	AS	S	C		C		C		O		O		
	AS	S	C		C		C		O		S		
	AS	S	C		C		C		S		O		
	AS	S	C		C		C		S		S		
	AS	S	O		C		C		C		O		
	AS	S	O		C		C		C		S		
	AS	S	S		C		C		C		O		
	AS	S	S		C		C		C		S		
486	AS	O		C		C		N		C	O	14.96	
	AS	O		C		C		N		C	S		
	AS	O		C		N		C		C	O		
	AS	O		C		N		C		C	S		
	AS	S		C		C		N		C	O		
	AS	S		C		C		N		C	S		
	AS	S		C		N		C		C	O		
	AS	S		C		N		C		C	S		
487	AS	O	-	C	*	C	-	N	-	C	-	O	2.07
	AS	O	-	C	*	C	-	N	-	C	-	S	
	AS	O	-	C	-	N	-	C	*	C	-	O	
	AS	O	-	C	-	N	-	C	*	C	-	S	
	AS	S	-	C	*	C	-	N	-	C	-	O	
	AS	S	-	C	*	C	-	N	-	C	-	S	
	AS	S	-	C	-	N	-	C	*	C	-	O	
	AS	S	-	C	-	N	-	C	*	C	-	S	
488	AS	O	-	C	-	C	-	N	-	C	-	O	7.07
	AS	O	-	C	-	C	-	N	-	C	-	S	
	AS	O	-	C	-	N	-	C	-	C	-	O	
	AS	O	-	C	-	N	-	C	-	C	-	S	
	AS	S	-	C	-	C	-	N	-	C	-	O	
	AS	S	-	C	-	C	-	N	-	C	-	S	
	AS	S	-	C	-	N	-	C	-	C	-	O	
	AS	S	-	C	-	N	-	C	-	C	-	S	

		Screen Number Order					
Screen Number		Fragment Definition					Frequency Percent
489	AS	O	C	C	N	O	2.88
	AS	O	C	C	N	S	
	AS	O	N	C	C	O	
	AS	O	N	C	C	S	
	AS	S	C	C	N	O	
	AS	S	C	C	N	S	
	AS	S	N	C	C	O	
	AS	S	N	C	C	S	
490	AS	O - C * C - N - O					0.94
	AS	O - C * C - N - S					
	AS	O - N - C * C - O					
	AS	O - N - C * C - S					
	AS	S - C * C - N - O					
	AS	S - C * C - N - S					
	AS	S - N - C * C - O					
	AS	S - N - C * C - S					
491	AS	O - C - C - N - O					1.05
	AS	O - C - C - N - S					
	AS	O - N - C - C - O					
	AS	O - N - C - C - S					
	AS	S - C - C - N - O					
	AS	S - C - C - N - S					
	AS	S - N - C - C - O					
	AS	S - N - C - C - S					
492	AS	O * C * C * O					4.00
	AS	O * C * C * S					
	AS	S * C * C * O					
	AS	S * C * C * S					
493	AS	O * C * C - O					6.17
	AS	O - C * C * O					
	AS	O * C * C - S					
	AS	O - C * C * S					
	AS	S * C * C - O					
	AS	S - C * C * O					
	AS	S * C * C - S					
	AS	S - C * C * S					
494	AS	O * C - C * O					0.42
	AS	O * C - C * S					
	AS	S * C - C * O					
	AS	S * C - C * S					
495	AS	O * C - C - O					5.40
	AS	O - C - C * O					
	AS	O * C - C - S					
	AS	O - C - C * S					
	AS	S * C - C - O					
	AS	S - C - C * O					
	AS	S * C - C - S					
	AS	S - C - C * S					

		Screen Number Order						
Screen Number		Fragment Definition						Frequency Percent
496	AS	O - C * C - O						7.98
	AS	O - C * C - S						
	AS	S - C * C - O						
	AS	S - C * C - S						
497	AS	O - C - C - O						9.90
	AS	O - C - C - S						
	AS	S - C - C - O						
	AS	S - C - C - S						
498	AS	O	C	C	O	C	O	7.30
	AS	O	C	C	O	C	S	
	AS	O	C	C	S	C	O	
	AS	O	C	C	S	C	S	
	AS	O	C	O	C	C	O	
	AS	O	C	O	C	C	S	
	AS	O	C	S	C	C	O	
	AS	O	C	S	C	C	S	
	AS	S	C	C	O	C	O	
	AS	S	C	C	O	C	S	
	AS	S	C	C	S	C	O	
	AS	S	C	C	S	C	S	
	AS	S	C	O	C	C	O	
	AS	S	C	O	C	C	S	
	AS	S	C	S	C	C	O	
	AS	S	C	S	C	C	S	
499	AS	O	C	C	O	O	1.31	
	AS	O	C	C	O	S		
	AS	O	C	C	S	O		
	AS	O	C	C	S	S		
	AS	O	O	C	C	O		
	AS	O	O	C	C	S		
	AS	O	S	C	C	O		
	AS	O	S	C	C	S		
	AS	S	C	C	O	O		
	AS	S	C	C	O	S		
	AS	S	C	C	S	O		
	AS	S	C	C	S	S		
	AS	S	O	C	C	O		
	AS	S	O	C	C	S		
	AS	S	S	C	C	O		
	AS	S	S	C	C	S		
500	AS	O	C	N	C	O	8.18	
	AS	O	C	N	C	S		
	AS	S	C	N	C	O		
	AS	S	C	N	C	S		
501	AS	O - C * N * C - O						4.24
	AS	O - C * N * C - S						
	AS	S - C * N * C - O						
	AS	S - C * N * C - S						

Screen Number Order												
Screen Number		Fragment Definition								Frequency Percent		
502	AS	O	-	C	*	N	-	C	-	O	0.50	
	AS	O	-	C	-	N	*	C	-	O		
	AS	O	-	C	*	N	-	C	-	S		
	AS	O	-	C	-	N	*	C	-	S		
	AS	S	-	C	*	N	-	C	-	O		
	AS	S	-	C	-	N	*	C	-	O		
	AS	S	-	C	*	N	-	C	-	S		
	AS	S	-	C	-	N	*	C	-	S		
503	AS	O	-	C	-	N	-	C	-	O	0.77	
	AS	O	-	C	-	N	-	C	-	S		
	AS	S	-	C	-	N	-	C	-	O		
	AS	S	-	C	-	N	-	C	-	S		
504	AS	O		C		N		N		C	O	1.09
	AS	O		C		N		N		C	S	
	AS	S		C		N		N		C	O	
	AS	S		C		N		N		C	S	
505	AS	O		C		N		O			1.66	
	AS	O		C		N		S				
	AS	O		N		C		O				
	AS	O		N		C		S				
	AS	S		C		N		O				
	AS	S		C		N		S				
	AS	S		N		C		O				
	AS	S		N		C		S				
506	AS	O	*	C	*	N	*	O			0.08	
	AS	O	*	C	*	N	*	S				
	AS	O	*	N	*	C	*	O				
	AS	O	*	N	*	C	*	S				
	AS	S	*	C	*	N	*	O				
	AS	S	*	C	*	N	*	S				
	AS	S	*	N	*	C	*	O				
	AS	S	*	N	*	C	*	S				
507	AS	O	*	C	-	N	-	O			0.24	
	AS	O	*	C	-	N	-	S				
	AS	O	-	N	-	C	*	O				
	AS	O	-	N	-	C	*	S				
	AS	S	*	C	-	N	-	O				
	AS	S	*	C	-	N	-	S				
	AS	S	-	N	-	C	*	O				
	AS	S	-	N	-	C	*	S				
508	AS	O	-	C	*	N	*	O			0.24	
	AS	O	-	C	*	N	*	S				
	AS	O	*	N	*	C	-	O				
	AS	O	*	N	*	C	-	S				
	AS	S	-	C	*	N	*	O				
	AS	S	-	C	*	N	*	S				
	AS	S	*	N	*	C	-	O				
	AS	S	*	N	*	C	-	S				



Screen Number Order								
Screen Number		Fragment Definition						Frequency Percent
509	AS	O - C - N - O						0.83
	AS	O - C - N - S						
	AS	O - N - C - O						
	AS	O - N - C - S						
	AS	S - C - N - O						
	AS	S - C - N - S						
	AS	S - N - C - O						
	AS	S - N - C - S						
510	AS	O	C	O	C	O	1.46	
	AS	O	C	O	C	S		
	AS	O	C	S	C	O		
	AS	O	C	S	C	S		
	AS	S	C	O	C	O		
	AS	S	C	O	C	S		
	AS	S	C	S	C	O		
	AS	S	C	S	C	S		
511	AS	O	C	O	O	0.48		
	AS	O	C	O	S			
	AS	O	C	S	O			
	AS	O	C	S	S			
	AS	O	O	C	O			
	AS	O	O	C	S			
	AS	O	S	C	O			
	AS	O	S	C	S			
	AS	S	C	O	O			
	AS	S	C	O	S			
	AS	S	C	S	O			
	AS	S	C	S	S			
	AS	S	O	C	O			
	AS	S	O	C	S			
	AS	S	S	C	O			
	AS	S	S	C	S			
512	AS	O	N	C	C	N	O	0.33
	AS	O	N	C	C	N	S	
	AS	S	N	C	C	N	O	
	AS	S	N	C	C	N	S	
513	CS	1 - 2 - 2 - 2 - 2 - 1						0.16
514	CS	1 - 2 - 2 - 2 - 2 - 2						5.75
	CS	2 - 2 - 2 - 2 - 2 - 1						
515	CS	1 - 2 - 2 - 2 - 2 - 3						3.74
	CS	3 - 2 - 2 - 2 - 2 - 1						
516	CS	1 - 2 - 2 - 2 - 3						5.04
	CS	3 - 2 - 2 - 2 - 1						
517	CS	1	2	2	2	4	0.88	
	CS	4	2	2	2	1		

		Screen Number Order											
Screen Number		Fragment Definition					Frequency Percent						
518	CS	1	-	2	-	2	-	3	-	1	5.12		
	CS	1	-	3	-	2	-	2	-	1			
519	CS	1	-	2	-	2	-	3	*	2	3.51		
	CS	2	*	3	-	2	-	2	-	1			
520	CS	1	-	2	-	2	-	3	-	2	3.25		
	CS	2	-	3	-	2	-	2	-	1			
521	CS	1	-	2	-	2	-	3	*	3	2.60		
	CS	3	*	3	-	2	-	2	-	1			
522	CS	1	-	2	-	2	-	3	-	3	4.06		
	CS	3	-	3	-	2	-	2	-	1			
523	CS	1		2		2		3		4	0.61		
	CS	4		3		2		2		1			
524	CS	1		2		2		4		1	0.95		
	CS	1		4		2		2		1			
525	CS	1		2		2		4		2	1.19		
	CS	2		4		2		2		1			
526	CS	1	-	2	-	3	-	2	-	1	2.00		
527	CS	1	-	2	-	3	-	2	-	2	3.69		
	CS	2	-	2	-	3	-	2	-	1			
528	CS	1	-	2	-	3	*	2	*	2	*	2	3.10
	CS	2	*	2	*	2	*	3	-	2	-	1	
529	CS	1	-	2	-	3	*	2	*	2	*	3	7.71
	CS	3	*	2	*	2	*	3	-	2	-	1	
530	CS	1	-	2	-	3	-	2	-	2	-	3	1.46
	CS	3	-	2	-	2	-	3	-	2	-	1	
531	CS	1	-	2	-	3	*	2	*	3		9.36	
	CS	3	*	2	*	3	-	2	-	1			
532	CS	1	-	2	-	3	-	2	-	3		4.54	
	CS	3	-	2	-	3	-	2	-	1			
533	CS	1	-	2	-	3	*	3				12.00	
	CS	3	*	3	-	2	-	1					
534	CS	1	-	2	-	3	-	3				10.15	
	CS	3	-	3	-	2	-	1					
535	CS	1	-	2	-	3	-	3	-	1		4.42	
	CS	1	-	3	-	3	-	2	-	1			
536	CS	1	-	2	-	3	-	3	*	2		3.69	
	CS	2	*	3	-	3	-	2	-	1			

		Screen Number Order								
Screen Number		Fragment Definition								Frequency Percent
537	CS	1 - 2 - 3 - 3 - 2								4.54
	CS	2 - 3 - 3 - 2 - 1								
538	CS	1 - 2 - 3 - 3 * 3								2.36
	CS	3 * 3 - 3 - 2 - 1								
539	CS	1 - 2 - 3 - 3 - 3								3.11
	CS	3 - 3 - 3 - 2 - 1								
540	CS	1	2	3	4				1.45	
	CS	4	3	2	1					
541	CS	1	2	4				3.93		
	CS	4	2	1						
542	CS	1 - 3 - 2 - 2 - 2 - 2								8.38
	CS	2 - 2 - 2 - 2 - 3 - 1								
543	CS	1 - 3 * 2 * 2 * 3 - 1								1.79
544	CS	1 - 3 - 2 - 2 - 3 - 1								5.14
545	CS	1 - 3 * 2 * 2 * 3 - 2								8.51
	CS	2 - 3 * 2 * 2 * 3 - 1								
546	CS	1 - 3 - 2 - 2 - 3 - 2								5.61
	CS	2 - 3 - 2 - 2 - 3 - 1								
547	CS	1 - 3 * 2 * 2 * 3 - 3								8.12
	CS	3 - 3 * 2 * 2 * 3 - 1								
548	CS	1 - 3 * 2 * 2 * 3 - 4								3.16
	CS	1 - 3 * 2 * 3 * 3 - 4								
	CS	1 - 3 * 3 * 2 * 3 - 4								
	CS	1 - 3 * 3 * 3 * 3 - 4								
	CS	4 - 3 * 2 * 2 * 3 - 1								
	CS	4 - 3 * 2 * 3 * 3 - 1								
	CS	4 - 3 * 3 * 2 * 3 - 1								
	CS	4 - 3 * 3 * 3 * 3 - 1								
549	CS	1 - 3 * 2 * 3 - 1								7.34
550	CS	1 - 3 - 2 - 3 - 1								4.92
551	CS	1 - 3 * 2 * 3 - 2								9.61
	CS	2 - 3 * 2 * 3 - 1								
552	CS	1 - 3 - 2 - 3 * 2								16.48
	CS	2 * 3 - 2 - 3 - 1								
553	CS	1 - 3 - 2 - 3 - 2								9.26
	CS	2 - 3 - 2 - 3 - 1								
554	CS	1 - 3 - 2 - 3 - 2 - 2								5.66
	CS	2 - 2 - 3 - 2 - 3 - 1								

		Screen Number Order								
Screen Number		Fragment Definition					Frequency Percent			
555	CS	1	-	3	*	2	* 3 - 3	8.64		
	CS	3	-	3	*	2	* 3 - 1			
556	CS	1	-	3	-	2	- 3 * 3	10.21		
	CS	3	*	3	-	2	- 3 - 1			
557	CS	1	-	3	-	2	- 3 - 3	9.58		
	CS	3	-	3	-	2	- 3 - 1			
558	CS	1	-	3	*	2	* 3 * 3 - 1	5.64		
	CS	1	-	3	*	3	* 2 * 3 - 1			
559	CS	1	-	3	*	2	* 3 * 3 - 2	4.75		
	CS	2	-	3	*	3	* 2 * 3 - 1			
560	CS	1	-	3	*	2	* 3 * 3 - 3	3.92		
	CS	3	-	3	*	3	* 2 * 3 - 1			
561	CS	1		3		2		3	4	4.25
	CS	4		3		2		3	1	
562	CS	1	-	3	*	2	* 3 - 4	1.86		
	CS	1	-	3	*	3	* 3 - 4			
	CS	4	-	3	*	2	* 3 - 1			
	CS	4	-	3	*	3	* 3 - 1			
563	CS	1		3		2		4	6.81	
	CS	4		2		3		1		
564	CS	1		3		2		4	1	4.90
	CS	1		4		2		3	1	
565	CS	1	-	3	*	3	- 1			9.71
566	CS	1	-	3	-	3	- 1			9.12
567	CS	1	-	3	*	3	- 2			19.66
	CS	2	-	3	*	3	- 1			
568	CS	1	-	3	-	3	- 2 - 2			8.72
	CS	2	-	2	-	3	- 3 - 1			
569	CS	1	-	3	-	3	* 2 * 2 * 2			11.24
	CS	2	*	2	*	2	* 3 - 3 - 1			
570	CS	1	-	3	-	3	* 2 * 2 * 3			14.08
	CS	3	*	2	*	2	* 3 - 3 - 1			
571	CS	1	-	3	-	3	* 2 * 3			14.13
	CS	3	*	2	*	3	- 3 - 1			
572	CS	1	-	3	-	3	- 2 - 3			10.45
	CS	3	-	2	-	3	- 3 - 1			

		Screen Number Order												
Screen Number		Fragment Definition										Frequency Percent		
573	CS	1	-	3	*	3	*	2	*	3	-	2	6.02	
	CS	2	-	3	*	2	*	3	*	3	-	1		
574	CS	1	-	3	*	3	*	2	*	3	-	3	5.24	
	CS	3	-	3	*	2	*	3	*	3	-	1		
575	CS	1	-	3	*	3	-	3					15.42	
	CS	3	-	3	*	3	-	1						
576	CS	1	-	3	-	3	*	3					18.41	
	CS	3	*	3	-	3	-	1						
577	CS	1	-	3	-	3	-	3					9.33	
	CS	3	-	3	-	3	-	1						
578	CS	1	-	3	*	3	*	3	-	1				9.40
579	CS	1	-	3	-	3	-	3	-	1				4.71
580	CS	1	-	3	*	3	*	3	-	2				7.26
	CS	2	-	3	*	3	*	3	-	1				
581	CS	1	-	3	-	3	-	3	-	2				4.79
	CS	2	-	3	-	3	-	3	-	1				
582	CS	1	-	3	*	3	*	3	-	3				6.31
	CS	3	-	3	*	3	*	3	-	1				
583	CS	1	-	3	*	3	*	3	*	3	-	1	5.57	
584	CS	1	-	3	*	3	*	3	*	3	-	2	6.50	
	CS	2	-	3	*	3	*	3	*	3	-	1		
585	CS	1	-	3	*	3	*	3	*	3	-	3	4.88	
	CS	3	-	3	*	3	*	3	*	3	-	1		
586	CS	1	-	3	*	3	-	4					1.75	
	CS	4	-	3	*	3	-	1						
587	CS	1		3		4							8.58	
	CS	4		3		1								
588	CS	1		4		1							27.09	
589	CS	1	-	4	*	2							7.98	
	CS	2	*	4	-	1								
590	CS	1		4		2		2		2				4.04
	CS	2		2		2		4		1				
591	CS	1	-	4	*	3							7.10	
	CS	3	*	4	-	1								
592	CS	1		4		3		2		3		2	7.50	
	CS	2		3		2		3		4		1		

		Screen Number Order							
Screen Number		Fragment Definition							Frequency Percent
593	CS	2 - 2 - 2 - 2 - 2							8.75
594	CS	2 * 2 * 2 * 2 * 2 * 2							1.48
595	CS	2 - 2 - 2 - 2 - 2 - 2							6.35
596	CS	2 * 2 * 2 * 2 * 2 * 2 * 3							29.58
	CS	3 * 2 * 2 * 2 * 2 * 2 * 2							
597	CS	2 - 2 - 2 - 2 - 2 - 2 - 3							7.57
	CS	3 - 2 - 2 - 2 - 2 - 2 - 2							
598	CS	2 * 2 * 2 * 2 * 3 - 2							20.16
	CS	2 - 3 * 2 * 2 * 2 * 2							
599	CS	2 - 2 - 2 - 2 - 3 * 2							5.76
	CS	2 * 3 - 2 - 2 - 2 - 2							
600	CS	2 * 2 * 2 * 2 * 3 * 3							21.07
	CS	3 * 3 * 2 * 2 * 2 * 2							
601	CS	2 * 2 * 2 * 2 * 3 - 3							18.36
	CS	3 - 3 * 2 * 2 * 2 * 2							
602	CS	2      2      2      2      4							3.60
	CS	4      2      2      2      2							
603	CS	2 - 2 - 2 - 3 * 2							11.91
	CS	2 * 3 - 2 - 2 - 2							
604	CS	2 - 2 - 2 - 3 - 2							10.91
	CS	2 - 3 - 2 - 2 - 2							
605	CS	2 * 2 * 2 * 3 * 2 * 3							15.52
	CS	3 * 2 * 3 * 2 * 2 * 2							
606	CS	2 - 2 - 2 - 3 * 3							7.09
	CS	3 * 3 - 2 - 2 - 2							
607	CS	2 - 2 - 2 - 3 - 3							9.62
	CS	3 - 3 - 2 - 2 - 2							
608	CS	2 * 2 * 2 * 3 * 3 * 3							18.39
	CS	3 * 3 * 3 * 2 * 2 * 2							
609	CS	2      2      2      3      4							9.00
	CS	4      3      2      2      2							
610	CS	2      2      2      4      2      2							2.71
	CS	2      2      4      2      2      2							
611	CS	2 - 2 - 3 - 2 - 2							6.69
612	CS	2 * 2 * 3 * 2 * 2 * 3							30.31
	CS	3 * 2 * 2 * 3 * 2 * 2							

		Screen Number Order											
Screen Number		Fragment Definition										Frequency Percent	
613	CS	2	-	2	-	3	-	2	-	2	-	3	4.05
	CS	3	-	2	-	2	-	3	-	2	-	2	
614	CS	2	-	2	-	3	-	2	-	3			11.92
	CS	3	-	2	-	3	-	2	-	2			
615	CS	2	-	2	-	3	-	2	-	3	*	2	4.78
	CS	2	*	3	-	2	-	3	-	2	-	2	
616	CS	2	*	2	*	3	*	2	*	3	*	3	26.19
	CS	3	*	3	*	2	*	3	*	2	*	2	
617	CS	2		2		3		2		3		4	5.82
	CS	4		3		2		3		2		2	
618	CS	2	-	2	-	3	-	3	*	2			9.84
	CS	2	*	3	-	3	-	2	-	2			
619	CS	2	-	2	-	3	-	3	-	2			7.18
	CS	2	-	3	-	3	-	2	-	2			
620	CS	2	-	2	-	3	-	3	*	3			5.14
	CS	3	*	3	-	3	-	2	-	2			
621	CS	2	-	2	-	3	-	3	-	3			3.49
	CS	3	-	3	-	3	-	2	-	2			
622	CS	2	*	2	*	3	*	3	*	3	*	3	18.21
	CS	3	*	3	*	3	*	3	*	2	*	2	
623	CS	2		2		4		2		3			4.49
	CS	3		2		4		2		2			
624	CS	2	*	3	-	2	-	2	-	3			16.28
	CS	3	-	2	-	2	-	3	*	2			
625	CS	2	*	3	-	2	-	2	-	3	*	2	7.26
	CS	2	*	3	-	2	-	2	-	3	*	3	
	CS	3	*	3	-	2	-	2	-	3	*	2	
	CS	3	*	3	-	2	-	2	-	3	*	3	
626	CS	2	-	3	*	2	*	2	*	3	-	2	7.61
627	CS	2	-	3	-	2	-	2	-	3	-	2	1.66
628	CS	2	-	3	*	2	*	2	*	3	-	3	12.20
	CS	3	-	3	*	2	*	2	*	3	-	2	
629	CS	2	-	3	*	2	*	2	*	3	-	4	3.11
	CS	2	-	3	*	2	*	3	*	3	-	4	
	CS	2	-	3	*	3	*	2	*	3	-	4	
	CS	2	-	3	*	3	*	3	*	3	-	4	
	CS	4	-	3	*	2	*	2	*	3	-	2	
	CS	4	-	3	*	2	*	3	*	3	-	2	
	CS	4	-	3	*	3	*	2	*	3	-	2	
	CS	4	-	3	*	3	*	3	*	3	-	2	

		Screen Number Order										
Screen Number		Fragment Definition										Frequency Percent
630	CS	2 * 3 - 2 - 3 * 2										8.16
631	CS	2 * 3 - 2 - 3 -										12.19
	CS	2 - 3 - 2 - 3 *										
632	CS	2 - 3 * 2 * 3 - 2										7.31
633	CS	2 - 3 - 2 - 3 - 2										4.05
634	CS	2 * 3 * 2 * 3 * 2 * 3										10.75
	CS	3 * 2 * 3 * 2 * 3 * 2										
635	CS	2 * 3 - 2 - 3 * 3										8.27
	CS	3 * 3 - 2 - 3 * 2										
636	CS	2 * 3 - 2 - 3 - 3										12.48
	CS	3 - 3 - 2 - 3 * 2										
637	CS	2 - 3 * 2 * 3 - 3										9.61
	CS	3 - 3 * 2 * 3 - 2										
638	CS	2 - 3 - 2 - 3 * 3										5.52
	CS	3 * 3 - 2 - 3 - 2										
639	CS	2 - 3 - 2 - 3 - 3										7.60
	CS	3 - 3 - 2 - 3 - 2										
640	CS	2 * 3 - 2 - 3 * 3 - 2										2.57
	CS	2 - 3 * 3 - 2 - 3 * 2										
	CS	2 - 3 * 3 - 2 - 3 * 3										
	CS	3 * 3 - 2 - 3 * 3 - 2										
641	CS	2 * 3 - 2 - 3 - 3 * 2										6.65
	CS	2 * 3 - 2 - 3 - 3 * 3										
	CS	2 * 3 - 3 - 2 - 3 * 2										
	CS	2 * 3 - 3 - 2 - 3 * 3										
	CS	3 * 3 - 2 - 3 - 3 * 2										
	CS	3 * 3 - 2 - 3 - 3 * 3										
	CS	3 * 3 - 3 - 2 - 3 * 2										
	CS	3 * 3 - 3 - 2 - 3 * 3										
642	CS	2 - 3 * 2 * 3 * 3 - 2										6.04
	CS	2 - 3 * 3 * 2 * 3 - 2										
643	CS	2 * 3 * 2 * 3 * 3 * 3										19.19
	CS	3 * 3 * 3 * 2 * 3 * 2										
644	CS	2 * 3 - 2 - 3 * 3 - 3										1.81
	CS	3 * 3 - 2 - 3 * 3 - 3										
	CS	3 - 3 * 3 - 2 - 3 * 2										
	CS	3 - 3 * 3 - 2 - 3 * 3										
645	CS	2 - 3 * 2 * 3 * 3 - 3										3.14
	CS	3 - 3 * 3 * 2 * 3 - 2										



		Screen Number Order										
Screen Number		Fragment Definition										Frequency Percent
646	CS	2	-	3	*	2	*	3	-	4	2.00	
	CS	2	-	3	*	3	*	3	-	4		
	CS	4	-	3	*	2	*	3	-	2		
	CS	4	-	3	*	3	*	3	-	2		
647	CS	2		3		2		4			11.56	
	CS	4		2		3		2				
648	CS	2	*	3	-	3	*	2			16.88	
649	CS	2	-	3	*	3	-	2			10.47	
650	CS	2	-	3	-	3	-	2			10.14	
651	CS	2	*	3	-	3	-	2	-	3	10.75	
	CS	3	-	2	-	3	-	3	*	2		
652	CS	2	-	3	-	3	-	2	-	3	8.39	
	CS	3	-	2	-	3	-	3	-	2		
653	CS	2	*	3	*	3	*	2	*	3	15.08	
	CS	3	*	3	*	2	*	3	*	3		
654	CS	2	-	3	*	3	*	2	*	3	5.08	
	CS	3	-	3	*	2	*	3	*	3		
655	CS	2	*	3	-	3	*	3			15.68	
	CS	3	*	3	-	3	*	2				
656	CS	2	*	3	-	3	-	3			11.02	
	CS	3	-	3	-	3	*	2				
657	CS	2	-	3	*	3	-	3			10.72	
	CS	3	-	3	*	3	-	2				
658	CS	2	-	3	-	3	*	3			11.95	
	CS	3	*	3	-	3	-	2				
659	CS	2	-	3	-	3	-	3			8.93	
	CS	3	-	3	-	3	-	2				
660	CS	2	*	3	-	3	*	3	-	2	4.50	
	CS	2	-	3	*	3	-	3	*	2		
661	CS	2	*	3	-	3	-	3	*	2	4.23	
662	CS	2	-	3	*	3	*	3	-	2	4.50	
663	CS	2	-	3	-	3	-	3	-	2	2.35	
664	CS	2	*	3	-	3	*	3	-	3	3.93	
	CS	3	-	3	*	3	-	3	*	2		
665	CS	2	*	3	-	3	-	3	*	3	2.75	
	CS	3	*	3	-	3	-	3	*	2		

		Screen Number Order											
Screen Number		Fragment Definition						Frequency Percent					
666	CS	2	-	3	*	3	*	3	-	3	4.43		
	CS	3	-	3	*	3	*	3	-	2			
667	CS	2	-	3	*	3	-	3	*	3	1.37		
	CS	3	*	3	-	3	*	3	-	2			
668	CS	2	*	3	-	3	-	3	*	3	-	2	0.60
	CS	2	-	3	*	3	-	3	-	3	*	2	
	CS	2	-	3	*	3	-	3	-	3	*	3	
	CS	3	*	3	-	3	-	3	*	3	-	2	
669	CS	2	*	3	-	3	-	3	-	3	*	2	0.80
	CS	2	*	3	-	3	-	3	-	3	*	3	
	CS	3	*	3	-	3	-	3	-	3	*	2	
	CS	3	*	3	-	3	-	3	-	3	*	3	
670	CS	2	-	3	*	3	*	3	*	3	-	2	2.95
671	CS	2	*	3	*	3	*	3	*	3	*	3	15.97
	CS	3	*	3	*	3	*	3	*	3	*	2	
672	CS	2	*	3	-	3	-	3	*	3	-	3	0.96
	CS	3	-	3	*	3	-	3	-	3	*	2	
	CS	3	*	3	-	3	-	3	*	3	-	3	
	CS	3	-	3	*	3	-	3	-	3	*	3	
673	CS	2	-	3	*	3	*	3	*	3	-	3	3.75
	CS	3	-	3	*	3	*	3	*	3	-	2	
674	CS	2	-	3	*	3	-	4					1.37
	CS	4	-	3	*	3	-	2					
675	CS	2	*	3	*	4							7.98
	CS	4	*	3	*	2							
676	CS	2	*	3	-	4							14.83
	CS	4	-	3	*	2							
677	CS	2	-	3	*	4							2.36
	CS	4	*	3	-	2							
678	CS	2	-	3	-	4							4.44
	CS	4	-	3	-	2							
679	CS	2	*	4	-	2							3.49
	CS	2	-	4	*	2							
680	CS	2		4		2		3					8.39
	CS	3		2		4		2					
681	CS	2	*	4	*	3							7.86
	CS	3	*	4	*	2							
682	CS	2	*	4	-	3							3.23
	CS	3	-	4	*	2							

		Screen Number Order					
Screen Number		Fragment Definition					Frequency Percent
683	CS	2 - 4 * 3					2.54
	CS	3 * 4 - 2					
684	CS	2 - 4 - 3					6.98
	CS	3 - 4 - 2					
685	CS	3 - 2 - 2 - 2 - 2 - 3					4.23
686	CS	3 - 2 - 2 - 2 - 3					6.76
687	CS	3	2	2	2	4	2.05
	CS	4	2	2	2	3	
688	CS	3 - 2 - 2 - 3 - 2 - 3					6.96
	CS	3 - 2 - 3 - 2 - 2 - 3					
689	CS	3 - 2 - 2 - 3 * 3					9.91
	CS	3 * 3 - 2 - 2 - 3					
690	CS	3 - 2 - 2 - 3 - 3					9.42
	CS	3 - 3 - 2 - 2 - 3					
691	CS	3	2	2	3	4	10.08
	CS	4	3	2	2	3	
692	CS	3	2	2	4		8.19
	CS	4	2	2	3		
693	CS	3 - 2 - 3 - 2 - 3					7.87
694	CS	3	2	3	2	3 4	3.99
	CS	4	3	2	3	2 3	
695	CS	3 - 2 - 3 - 3 - 3					5.68
	CS	3 - 3 - 3 - 2 - 3					
696	CS	3 - 3 * 2 * 2 * 3 - 3					4.81
697	CS	3 - 3 * 2 * 2 * 3 - 4					2.13
	CS	3 - 3 * 2 * 3 * 3 - 4					
	CS	3 - 3 * 3 * 2 * 3 - 4					
	CS	3 - 3 * 3 * 3 * 3 - 4					
	CS	4 - 3 * 2 * 2 * 3 - 3					
	CS	4 - 3 * 2 * 3 * 3 - 3					
	CS	4 - 3 * 3 * 2 * 3 - 3					
	CS	4 - 3 * 3 * 3 * 3 - 3					
698	CS	3 * 3 - 2 - 3 * 3					2.62
699	CS	3 * 3 - 2 - 3 - 3					5.51
	CS	3 - 3 - 2 - 3 * 3					
700	CS	3 - 3 * 2 * 3 - 3					5.43

		Screen Number Order											
Screen Number		Fragment Definition										Frequency Percent	
701	CS	3	-	3	-	2	-	3	-	3		5.59	
702	CS	3	-	3	*	2	*	3	*	3	-	3	2.80
	CS	3	-	3	*	3	*	2	*	3	-	3	
703	CS	3		3		2		3		4		7.93	
	CS	4		3		2		3		3			
704	CS	3	-	3	*	2	*	3	-	4		1.89	
	CS	3	-	3	*	3	*	3	-	4			
	CS	4	-	3	*	2	*	3	-	3			
	CS	4	-	3	*	3	*	3	-	3			
705	CS	3		3		2		4				9.47	
	CS	4		2		3		3					
706	CS	3	*	3	-	3	*	3				3.65	
707	CS	3	*	3	-	3	-	3				6.09	
	CS	3	-	3	-	3	*	3					
708	CS	3	-	3	*	3	-	3				7.00	
709	CS	3	-	3	-	3	-	3				2.79	
710	CS	3	*	3	-	3	*	3	-	3		1.08	
	CS	3	-	3	*	3	-	3	*	3			
711	CS	3	*	3	-	3	-	3	*	3		0.75	
712	CS	3	-	3	*	3	*	3	-	3		2.35	
713	CS	3	*	3	*	3	*	3	*	3	*	3	7.52
714	CS	3	-	3	*	3	*	3	*	3	-	3	1.64
715	CS	3		3		3		4				10.43	
	CS	4		3		3		3					
716	CS	3	-	3	*	3	-	4				1.02	
	CS	4	-	3	*	3	-	3					
	CS	4	-	3	*	3	-	4					
717	CS	3		3		4						15.49	
	CS	4		3		3							
718	CS	3		4		3						13.57	
719	CS	3	*	4	-	3						2.12	
	CS	3	-	4	*	3							

		Screen Number Order											
Screen Number		Fragment Definition							Frequency Percent				
720	CS	4	2	2	2	2	4	3.12					
	CS	4	2	2	2	3	4						
	CS	4	2	2	3	2	4						
	CS	4	2	2	3	3	4						
	CS	4	2	3	2	2	4						
	CS	4	2	3	2	3	4						
	CS	4	2	3	3	2	4						
	CS	4	2	3	3	3	4						
	CS	4	3	2	2	2	4						
	CS	4	3	2	2	3	4						
	CS	4	3	2	3	2	4						
	CS	4	3	2	3	3	4						
	CS	4	3	3	2	2	4						
	CS	4	3	3	2	3	4						
	CS	4	3	3	3	2	4						
	CS	4	3	3	3	3	4						
721	CS	4	2	2	2	4	5.18						
	CS	4	2	2	3	4							
	CS	4	2	3	2	4							
	CS	4	2	3	3	4							
	CS	4	3	2	2	4							
	CS	4	3	2	3	4							
	CS	4	3	3	2	4							
722	CS	4	2	2	4	3.29							
	CS	4	2	3	4								
	CS	4	3	2	4								
	CS	4	3	3	4								
723	CS	4	2	4			2.20						
724	CS	4	-	3	*	2	*	2	*	3	-	4	0.32
	CS	4	-	3	*	2	*	3	*	3	-	4	
	CS	4	-	3	*	3	*	2	*	3	-	4	
	CS	4	-	3	*	3	*	3	*	3	-	4	
725	CS	4	-	3	*	2	*	3	-	4	0.78		
	CS	4	-	3	*	3	*	3	-	4			
726	CS	4		3	4							1.90	
727	CS	4		4								5.62	
728	BS	A	*1A	*1A	*2A							33.57	
	BS	A	*2A	*1A	*1A								
729	BS	A	*1A	*1A	*4A							25.91	
	BS	A	*4A	*1A	*1A								
730	BS	A	*1A	*4A	*1A							23.66	
731	BS	A	*2A	*1A	*2A							14.60	

		Screen Number Order				
Screen Number		Fragment Definition				Frequency Percent
732	BS	A	*2A	*1A	*4A	12.99
	BS	A	*4A	*1A	*2A	
733	BS	A	*4A	*1A	*4A	3.43
734	BS	A	*1A	*1A	*1A *1A	46.26
735	BS	A	*1A	*1A	*1A *2A	18.26
	BS	A	*2A	*1A	*1A *1A	
736	BS	A	*1A	*1A	*1A *4A	15.85
	BS	A	*4A	*1A	*1A *1A	
737	BS	A	*1A	*1A	*4A *1A	23.12
	BS	A	*1A	*4A	*1A *1A	
738	BS	A	*1A	*4A	*1A *4A	3.11
	BS	A	*4A	*1A	*4A *1A	
739	BS	A	*1A	*4A	*4A *1A	5.55
740	BS	A	*2A	*1A	*1A *2A	15.67
741	BS	A	*2A	*1A	*1A *4A	10.64
	BS	A	*4A	*1A	*1A *2A	
742	BS	A	*4A	*1A	*1A *4A	5.18
743	BS	A	*4A	*4A	*4A *4A	70.68
744	BS	A	*1A	*1A	*1A *1A *1A	32.33
745	BS	A	*1A	*1A	*1A *1A *2A	11.68
	BS	A	*2A	*1A	*1A *1A *1A	
746	BS	A	*1A	*1A	*2A *1A *1A	12.39
747	BS	A	*1A	*1A	*4A *1A *1A	8.65
748	BS	A	*1A	*4A	*4A *4A *1A	1.67
749	BS	A	*2A	*1A	*1A *1A *2A	4.86
750	BS	A	*2A	*1A	*1A *1A *4A	5.71
	BS	A	*4A	*1A	*1A *1A *2A	
	BS	A	*4A	*1A	*1A *1A *4A	
751	BS	A	*2A	*1A	*2A *1A *2A	1.80
752	BS	A	*2A	*1A	*2A *1A *4A	1.61
	BS	A	*2A	*1A	*4A *1A *2A	
	BS	A	*2A	*1A	*4A *1A *4A	
	BS	A	*4A	*1A	*2A *1A *2A	
	BS	A	*4A	*1A	*2A *1A *4A	
	BS	A	*4A	*1A	*4A *1A *2A	
	BS	A	*4A	*1A	*4A *1A *4A	

		Screen Number Order						
Screen Number		Fragment Definition						Frequency Percent
753	BS	A	*1A	*4A	*4A	*4A	-1A	11.30
	BS	A	*1A	*4A	*4A	*4A	-4A	
	BS	A	-1A	*4A	*4A	*4A	*1A	
	BS	A	-4A	*4A	*4A	*4A	*1A	
754	BS	A	*2A	*1A	*1A	*1A	-1A	16.45
	BS	A	*4A	*1A	*1A	*1A	-1A	
	BS	A	-1A	*1A	*1A	*1A	*2A	
	BS	A	-1A	*1A	*1A	*1A	*4A	
755	BS	A	*2A	*1A	*1A	*1A	-2A	7.52
	BS	A	*2A	*1A	*1A	*1A	-4A	
	BS	A	*4A	*1A	*1A	*1A	-2A	
	BS	A	*4A	*1A	*1A	*1A	-4A	
	BS	A	-2A	*1A	*1A	*1A	*2A	
	BS	A	-2A	*1A	*1A	*1A	*4A	
	BS	A	-4A	*1A	*1A	*1A	*2A	
	BS	A	-4A	*1A	*1A	*1A	*4A	
756	BS	A	*2A	*1A	*1A	*2A	-1A	8.46
	BS	A	-1A	*2A	*1A	*1A	*2A	
757	BS	A	*2A	*1A	*1A	*4A	-1A	7.07
	BS	A	*4A	*1A	*1A	*2A	-1A	
	BS	A	*4A	*1A	*1A	*4A	-1A	
	BS	A	-1A	*2A	*1A	*1A	*4A	
	BS	A	-1A	*4A	*1A	*1A	*2A	
	BS	A	-1A	*4A	*1A	*1A	*4A	
758	BS	A	*2A	*1A	*1A	*4A	-4A	0.97
	BS	A	*4A	*1A	*1A	*4A	-4A	
	BS	A	-4A	*4A	*1A	*1A	*2A	
	BS	A	-4A	*4A	*1A	*1A	*4A	
759	BS	A	*2A	*1A	*2A	*1A	-1A	13.23
	BS	A	*2A	*1A	*4A	*1A	-1A	
	BS	A	*4A	*1A	*2A	*1A	-1A	
	BS	A	*4A	*1A	*4A	*1A	-1A	
	BS	A	-1A	*1A	*2A	*1A	*2A	
	BS	A	-1A	*1A	*2A	*1A	*4A	
	BS	A	-1A	*1A	*4A	*1A	*2A	
	BS	A	-1A	*1A	*4A	*1A	*4A	
760	BS	A	*2A	*1A	*2A	*1A	-2A	4.14
	BS	A	*2A	*1A	*2A	*1A	-4A	
	BS	A	*2A	*1A	*4A	*1A	-2A	
	BS	A	*2A	*1A	*4A	*1A	-4A	
	BS	A	*4A	*1A	*2A	*1A	-2A	
	BS	A	*4A	*1A	*2A	*1A	-4A	
	BS	A	*4A	*1A	*4A	*1A	-2A	
	BS	A	*4A	*1A	*4A	*1A	-4A	
	BS	A	-2A	*1A	*2A	*1A	*2A	
	BS	A	-2A	*1A	*2A	*1A	*4A	
	BS	A	-2A	*1A	*4A	*1A	*2A	
	BS	A	-2A	*1A	*4A	*1A	*4A	

		Screen Number Order							
Screen Number		Fragment Definition						Frequency Percent	
760	BS	A	-4A	*1A	*2A	*1A	*2A	4.14	(continued)
	BS	A	-4A	*1A	*2A	*1A	*4A		
	BS	A	-4A	*1A	*4A	*1A	*2A		
	BS	A	-4A	*1A	*4A	*1A	*4A		
761	BS	A	*2A	*1A	*4A	*4A	-1A	3.88	
	BS	A	*4A	*1A	*4A	*4A	-1A		
	BS	A	-1A	*4A	*4A	*1A	*2A		
	BS	A	-1A	*4A	*4A	*1A	*4A		
762	BS	A	*2A	*1A	*4A	*4A	-4A	0.88	
	BS	A	*4A	*1A	*4A	*4A	-4A		
	BS	A	-4A	*4A	*4A	*1A	*2A		
	BS	A	-4A	*4A	*4A	*1A	*4A		
763	BS	A	*1A	*1A	*1A	-1A		43.32	
	BS	A	-1A	*1A	*1A	*1A			
764	BS	A	*1A	*1A	*1A	-2A		16.95	
	BS	A	*1A	*1A	*1A	-4A			
	BS	A	-2A	*1A	*1A	*1A			
	BS	A	-4A	*1A	*1A	*1A			
765	BS	A	*1A	*1A	*2A	-1A		24.92	
	BS	A	*1A	*1A	*4A	-1A			
	BS	A	*1A	*1A	*4A	-4A			
	BS	A	-1A	*2A	*1A	*1A			
	BS	A	-1A	*4A	*1A	*1A			
	BS	A	-4A	*4A	*1A	*1A			
766	BS	A	*1A	*4A	*1A	-1A		15.89	
	BS	A	*1A	*4A	*1A	-2A			
	BS	A	*1A	*4A	*1A	-4A			
	BS	A	-1A	*1A	*4A	*1A			
	BS	A	-2A	*1A	*4A	*1A			
	BS	A	-4A	*1A	*4A	*1A			
767	BS	A	*1A	*4A	*4A	-1A		14.13	
	BS	A	*1A	*4A	*4A	-4A			
	BS	A	-1A	*4A	*4A	*1A			
	BS	A	-4A	*4A	*4A	*1A			
768	BS	A	*2A	*1A	*1A	-1A		26.83	
	BS	A	*4A	*1A	*1A	-1A			
	BS	A	-1A	*1A	*1A	*2A			
	BS	A	-1A	*1A	*1A	*4A			
769	BS	A	*2A	*1A	*1A	-2A		10.73	
	BS	A	*2A	*1A	*1A	-4A			
	BS	A	*4A	*1A	*1A	-2A			
	BS	A	*4A	*1A	*1A	-4A			
	BS	A	-2A	*1A	*1A	*2A			
	BS	A	-2A	*1A	*1A	*4A			
	BS	A	-4A	*1A	*1A	*2A			
	BS	A	-4A	*1A	*1A	*4A			



		Screen Number Order				
Screen Number		Fragment Definition				Frequency Percent
770	BS	A	*2A	*1A	*2A -1A	17.24
	BS	A	*2A	*1A	*4A -1A	
	BS	A	*4A	*1A	*2A -1A	
	BS	A	*4A	*1A	*4A -1A	
	BS	A	-1A	*2A	*1A *2A	
	BS	A	-1A	*2A	*1A *4A	
	BS	A	-1A	*4A	*1A *2A	
	BS	A	-1A	*4A	*1A *4A	
771	BS	A	*2A	*1A	*4A -4A	3.22
	BS	A	*4A	*1A	*4A -4A	
	BS	A	-4A	*4A	*1A *2A	
	BS	A	-4A	*4A	*1A *4A	
772	BS	A	*4A	*4A	*1A -1A	12.57
	BS	A	-1A	*1A	*4A *4A	
773	BS	A	*4A	*4A	*1A -2A	5.73
	BS	A	*4A	*4A	*1A -4A	
	BS	A	-2A	*1A	*4A *4A	
	BS	A	-4A	*1A	*4A *4A	
774	BS	A	*1A	*1A	*1A -1A -1A	31.09
	BS	A	-1A	-1A	*1A *1A *1A	
775	BS	A	*1A	*1A	*1A -1A -2A	15.47
	BS	A	*1A	*1A	*1A -1A -4A	
	BS	A	-2A	-1A	*1A *1A *1A	
	BS	A	-4A	-1A	*1A *1A *1A	
776	BS	A	*1A	*4A	*4A -1A -2A	3.05
	BS	A	*1A	*4A	*4A -1A -4A	
	BS	A	-2A	-1A	*4A *4A *1A	
	BS	A	-4A	-1A	*4A *4A *1A	
777	BS	A	*2A	*1A	*1A -1A -2A	4.54
	BS	A	*2A	*1A	*1A -1A -4A	
	BS	A	-2A	-1A	*1A *1A *2A	
	BS	A	-4A	-1A	*1A *1A *2A	
778	BS	A	*4A	*1A	*1A -1A -2A	2.25
	BS	A	*4A	*1A	*1A -1A -4A	
	BS	A	-2A	-1A	*1A *1A *4A	
	BS	A	-4A	-1A	*1A *1A *4A	
779	BS	A	*4A	*1A	*2A -1A -2A	1.43
	BS	A	*4A	*1A	*2A -1A -4A	
	BS	A	-2A	-1A	*2A *1A *4A	
	BS	A	-4A	-1A	*2A *1A *4A	
780	BS	A	*4A	*1A	*4A -1A -2A	0.18
	BS	A	*4A	*1A	*4A -1A -4A	
	BS	A	-2A	-1A	*4A *1A *4A	
	BS	A	-4A	-1A	*4A *1A *4A	

		Screen Number Order				
Screen Number		Fragment Definition				Frequency Percent
781	BS	A	*2A	*1A	-1A	20.76
	BS	A	-1A	*1A	*2A	
782	BS	A	*2A	*1A	-2A	7.00
	BS	A	-2A	*1A	*2A	
783	BS	A	*2A	*1A	-4A	1.11
	BS	A	-4A	*1A	*2A	
784	BS	A	*1A	*1A	-1A -1A	38.04
	BS	A	-1A	-1A	*1A *1A	
785	BS	A	*1A	*1A	-1A -2A	19.91
	BS	A	*1A	*1A	-1A -4A	
	BS	A	-2A	-1A	*1A *1A	
	BS	A	-4A	-1A	*1A *1A	
786	BS	A	*1A	*1A	-2A -1A	4.41
	BS	A	*1A	*1A	-4A -1A	
	BS	A	-1A	-2A	*1A *1A	
	BS	A	-1A	-4A	*1A *1A	
787	BS	A	*1A	*4A	-1A -1A	2.71
	BS	A	-1A	-1A	*4A *1A	
788	BS	A	*1A	*4A	-1A -2A	0.92
	BS	A	*1A	*4A	-1A -4A	
	BS	A	-2A	-1A	*4A *1A	
	BS	A	-4A	-1A	*4A *1A	
789	BS	A	*2A	*1A	-1A -1A	15.32
	BS	A	*4A	*1A	-1A -1A	
	BS	A	-1A	-1A	*1A *2A	
	BS	A	-1A	-1A	*1A *4A	
790	BS	A	*2A	*1A	-1A -2A	6.14
	BS	A	*2A	*1A	-1A -4A	
	BS	A	*4A	*1A	-1A -2A	
	BS	A	*4A	*1A	-1A -4A	
	BS	A	-2A	-1A	*1A *2A	
	BS	A	-2A	-1A	*1A *4A	
	BS	A	-4A	-1A	*1A *2A	
	BS	A	-4A	-1A	*1A *4A	
791	BS	A	*2A	*1A	-2A -1A	2.06
	BS	A	*2A	*1A	-4A -1A	
	BS	A	*4A	*1A	-2A -1A	
	BS	A	*4A	*1A	-4A -1A	
	BS	A	-1A	-2A	*1A *2A	
	BS	A	-1A	-2A	*1A *4A	
	BS	A	-1A	-4A	*1A *2A	
	BS	A	-1A	-4A	*1A *4A	
792	BS	A	*4A	*4A	-1A -1A	50.44
	BS	A	-1A	-1A	*4A *4A	

		Screen Number Order				
Screen Number		Fragment Definition				Frequency Percent
793	BS	A	*4A	*4A	-1A -2A	21.99
	BS	A	-2A	-1A	*4A *4A	
794	BS	A	*4A	*4A	-1A -4A	14.39
	BS	A	-4A	-1A	*4A *4A	
795	BS	A	*	A	- A * A	24.19
796	BS	A	*1A	-1A	*1A	4.83
797	BS	A	*1A	-1A	*2A	2.29
	BS	A	*2A	-1A	*1A	
798	BS	A	*1A	-1A	*4A	17.07
	BS	A	*4A	-1A	*1A	
799	BS	A	*1A	-2A	*1A	0.27
800	BS	A	*2A	-1A	*2A	0.82
801	BS	A	*2A	-1A	*4A	6.81
	BS	A	*4A	-1A	*2A	
802	BS	A	*4A	-1A	*4A	4.33
803	BS	A	*	A	- A * A * A - A	16.99
	BS	A	- A	* A	* A - A * A	
804	BS	A	*	A	- A * A - A	15.25
	BS	A	- A	* A	- A * A	
805	BS	A	*	A	- A * A - A * A	1.90
806	BS	A	*1A	-1A	-3A	3.87
	BS	A	*2A	-1A	-3A	
	BS	A	*4A	-1A	-3A	
	BS	A	-3A	-1A	*1A	
	BS	A	-3A	-1A	*2A	
	BS	A	-3A	-1A	*4A	
807	BS	A	*1A	-4A	-4A	1.54
	BS	A	*4A	-4A	-4A	
	BS	A	-4A	-4A	*1A	
	BS	A	-4A	-4A	*4A	
808	BS	A	*2A	-1A	-1A	14.59
	BS	A	-1A	-1A	*2A	
809	BS	A	*2A	-1A	-2A	8.95
	BS	A	*2A	-1A	-4A	
	BS	A	-2A	-1A	*2A	
	BS	A	-4A	-1A	*2A	
810	BS	A	*4A	-4A	-1A	2.32
	BS	A	-1A	-4A	*4A	

Screen Number Order				
Screen Number			Fragment Definition	Frequency Percent
811	BS	A	* A - A - A * A	20.58
812	BS	A	*1A -1A -1A *1A	3.71
813	BS	A	*1A -1A -1A *2A	1.34
	BS	A	*2A -1A -1A *1A	
814	BS	A	*1A -1A -1A *4A	8.26
	BS	A	*4A -1A -1A *1A	
815	BS	A	*1A -1A -2A *1A	1.79
	BS	A	*1A -1A -4A *1A	
	BS	A	*1A -1A -4A *4A	
	BS	A	*1A -2A -1A *1A	
	BS	A	*1A -4A -1A *1A	
	BS	A	*1A -4A -4A *1A	
	BS	A	*1A -4A -4A *4A	
	BS	A	*2A -1A -4A *4A	
	BS	A	*4A -1A -4A *4A	
	BS	A	*4A -4A -1A *1A	
	BS	A	*4A -4A -1A *2A	
	BS	A	*4A -4A -1A *4A	
	BS	A	*4A -4A -4A *1A	
	BS	A	*4A -4A -4A *4A	
816	BS	A	*1A -2A -1A *2A	2.34
	BS	A	*1A -2A -1A *4A	
	BS	A	*1A -4A -1A *2A	
	BS	A	*1A -4A -1A *4A	
	BS	A	*2A -1A -2A *1A	
	BS	A	*2A -1A -4A *1A	
	BS	A	*4A -1A -2A *1A	
	BS	A	*4A -1A -4A *1A	
817	BS	A	*2A -1A -1A *2A	0.35
818	BS	A	*2A -1A -1A *4A	1.80
	BS	A	*4A -1A -1A *2A	
819	BS	A	*4A -1A -1A *4A	7.50
820	BS	A	* A - A - A * A - A	11.11
	BS	A	- A * A - A - A * A	
821	BS	A	*1A -1A -1A -1A	29.59
	BS	A	*2A -1A -1A -1A	
	BS	A	-1A -1A -1A *1A	
	BS	A	-1A -1A -1A *2A	
822	BS	A	*1A -1A -1A -2A	6.54
	BS	A	*2A -1A -1A -2A	
	BS	A	-2A -1A -1A *1A	
	BS	A	-2A -1A -1A *2A	

Screen Number Order													
Screen Number				Fragment Definition		Frequency Percent							
823	BS	A	*1A	-1A	-1A	-4A	3.08						
	BS	A	*2A	-1A	-1A	-4A							
	BS	A	-4A	-1A	-1A	*1A							
	BS	A	-4A	-1A	-1A	*2A							
824	BS	A	*1A	-1A	-1A	-3A	1.16						
	BS	A	*1A	-2A	-1A	-3A							
	BS	A	*1A	-4A	-1A	-3A							
	BS	A	*2A	-1A	-1A	-3A							
	BS	A	*4A	-1A	-1A	-3A							
	BS	A	*4A	-4A	-1A	-3A							
	BS	A	-3A	-1A	-1A	*1A							
	BS	A	-3A	-1A	-1A	*2A							
	BS	A	-3A	-1A	-1A	*4A							
	BS	A	-3A	-1A	-2A	*1A							
	BS	A	-3A	-1A	-4A	*1A							
	BS	A	-3A	-1A	-4A	*4A							
	825	BS	A	*1A	-1A	-2A		-1A	9.84				
BS		A	*1A	-1A	-4A	-1A							
BS		A	*2A	-1A	-2A	-1A							
BS		A	*2A	-1A	-4A	-1A							
BS		A	-1A	-2A	-1A	*1A							
BS		A	-1A	-2A	-1A	*2A							
BS		A	-1A	-4A	-1A	*1A							
BS		A	-1A	-4A	-1A	*2A							
826	BS	A	*1A	-1A	-4A	-4A	3.47						
	BS	A	*2A	-1A	-4A	-4A							
	BS	A	-4A	-4A	-1A	*1A							
	BS	A	-4A	-4A	-1A	*2A							
827	BS	A	*4A	-1A	-1A	-1A	32.93						
	BS	A	-1A	-1A	-1A	*4A							
828	BS	A	*4A	-1A	-1A	-2A	6.41						
	BS	A	-2A	-1A	-1A	*4A							
829	BS	A	*4A	-1A	-1A	-4A	3.12						
	BS	A	-4A	-1A	-1A	*4A							
830	BS	A	*4A	-1A	-2A	-1A	7.09						
	BS	A	-1A	-2A	-1A	*4A							
831	BS	A	*4A	-1A	-4A	-1A	9.50						
	BS	A	-1A	-4A	-1A	*4A							
832	BS	A	*4A	-1A	-4A	-4A	8.33						
	BS	A	-4A	-4A	-1A	*4A							
833	BS	A	*	A	-	A	-	A	-	A	*	A	16.30

		Screen Number Order						
Screen Number		Fragment Definition					Frequency Percent	
834	BS	A	*1A	-1A	-1A	-1A	*1A	9.08
	BS	A	*1A	-1A	-1A	-1A	*2A	
	BS	A	*1A	-1A	-1A	-1A	*4A	
	BS	A	*2A	-1A	-1A	-1A	*1A	
	BS	A	*2A	-1A	-1A	-1A	*2A	
	BS	A	*2A	-1A	-1A	-1A	*4A	
	BS	A	*4A	-1A	-1A	-1A	*1A	
	BS	A	*4A	-1A	-1A	-1A	*2A	
	BS	A	*4A	-1A	-1A	-1A	*4A	
835	BS	A	*1A	-1A	-1A	-1A	*1A	2.29
	BS	A	*1A	-1A	-1A	-2A	*1A	
	BS	A	*1A	-1A	-1A	-4A	*1A	
	BS	A	*1A	-1A	-2A	-1A	*1A	
	BS	A	*1A	-1A	-4A	-1A	*1A	
	BS	A	*1A	-1A	-4A	-4A	*1A	
	BS	A	*1A	-2A	-1A	-1A	*1A	
	BS	A	*1A	-2A	-1A	-2A	*1A	
	BS	A	*1A	-2A	-1A	-4A	*1A	
	BS	A	*1A	-4A	-1A	-1A	*1A	
	BS	A	*1A	-4A	-1A	-2A	*1A	
	BS	A	*1A	-4A	-1A	-4A	*1A	
	BS	A	*1A	-4A	-4A	-1A	*1A	
	BS	A	*1A	-4A	-4A	-4A	*1A	
	BS	A	*1A	-4A	-4A	-4A	*1A	
836	BS	A	*1A	-1A	-1A	-1A	*2A	1.05
	BS	A	*1A	-1A	-2A	-1A	*2A	
	BS	A	*1A	-1A	-4A	-1A	*2A	
	BS	A	*1A	-2A	-1A	-1A	*2A	
	BS	A	*1A	-4A	-1A	-1A	*2A	
	BS	A	*1A	-4A	-4A	-1A	*2A	
	BS	A	*2A	-1A	-1A	-1A	*1A	
	BS	A	*2A	-1A	-1A	-2A	*1A	
	BS	A	*2A	-1A	-1A	-4A	*1A	
	BS	A	*2A	-1A	-2A	-1A	*1A	
	BS	A	*2A	-1A	-4A	-1A	*1A	
	BS	A	*2A	-1A	-4A	-4A	*1A	
837	BS	A	*1A	-1A	-1A	-1A	*4A	7.61
	BS	A	*1A	-1A	-2A	-1A	*4A	
	BS	A	*1A	-1A	-4A	-1A	*4A	
	BS	A	*1A	-1A	-4A	-4A	*4A	
	BS	A	*1A	-2A	-1A	-1A	*4A	
	BS	A	*1A	-2A	-1A	-4A	*4A	
	BS	A	*1A	-4A	-1A	-1A	*4A	
	BS	A	*1A	-4A	-1A	-4A	*4A	
	BS	A	*1A	-4A	-4A	-1A	*4A	
	BS	A	*1A	-4A	-4A	-4A	*4A	
	BS	A	*4A	-1A	-1A	-1A	*1A	
	BS	A	*4A	-1A	-1A	-2A	*1A	
	BS	A	*4A	-1A	-1A	-4A	*1A	
	BS	A	*4A	-1A	-2A	-1A	*1A	
	BS	A	*4A	-1A	-2A	-1A	*1A	

		Screen Number Order						
Screen Number		Fragment Definition					Frequency Percent	
837	BS	A	*4A	-1A	-4A	-1A *1A	7.61	(continued)
	BS	A	*4A	-1A	-4A	-4A *1A		
	BS	A	*4A	-4A	-1A	-2A *1A		
	BS	A	*4A	-4A	-1A	-4A *1A		
	BS	A	*4A	-4A	-4A	-1A *1A		
	BS	A	*4A	-4A	-4A	-4A *1A		
838	BS	A	*1A	-1A	-1A	-2A *1A	0.72	
	BS	A	*1A	-1A	-1A	-4A *1A		
	BS	A	*1A	-1A	-1A	-4A *4A		
	BS	A	*1A	-2A	-1A	-1A *1A		
	BS	A	*1A	-2A	-1A	-1A *2A		
	BS	A	*1A	-2A	-1A	-1A *4A		
	BS	A	*1A	-4A	-1A	-1A *1A		
	BS	A	*1A	-4A	-1A	-1A *2A		
	BS	A	*1A	-4A	-1A	-1A *4A		
	BS	A	*2A	-1A	-1A	-2A *1A		
	BS	A	*2A	-1A	-1A	-4A *1A		
	BS	A	*2A	-1A	-1A	-4A *4A		
	BS	A	*4A	-1A	-1A	-2A *1A		
	BS	A	*4A	-1A	-1A	-4A *1A		
	BS	A	*4A	-1A	-1A	-4A *4A		
	BS	A	*4A	-4A	-1A	-1A *1A		
	BS	A	*4A	-4A	-1A	-1A *2A		
	BS	A	*4A	-4A	-1A	-1A *4A		
839	BS	A	*1A	-1A	-2A	-1A *1A	3.00	
	BS	A	*1A	-1A	-2A	-1A *2A		
	BS	A	*1A	-1A	-2A	-1A *4A		
	BS	A	*2A	-1A	-2A	-1A *1A		
	BS	A	*2A	-1A	-2A	-1A *2A		
	BS	A	*2A	-1A	-2A	-1A *4A		
	BS	A	*4A	-1A	-2A	-1A *1A		
	BS	A	*4A	-1A	-2A	-1A *2A		
	BS	A	*4A	-1A	-2A	-1A *4A		
840	BS	A	*1A	-1A	-4A	-1A *1A	3.51	
	BS	A	*1A	-1A	-4A	-1A *2A		
	BS	A	*1A	-1A	-4A	-1A *4A		
	BS	A	*2A	-1A	-4A	-1A *1A		
	BS	A	*2A	-1A	-4A	-1A *2A		
	BS	A	*2A	-1A	-4A	-1A *4A		
	BS	A	*4A	-1A	-4A	-1A *1A		
	BS	A	*4A	-1A	-4A	-1A *2A		
	BS	A	*4A	-1A	-4A	-1A *4A		
841	BS	A	*1A	-1A	-4A	-4A *1A	0.60	
	BS	A	*1A	-1A	-4A	-4A *4A		
	BS	A	*1A	-4A	-4A	-1A *1A		
	BS	A	*1A	-4A	-4A	-1A *2A		
	BS	A	*1A	-4A	-4A	-1A *4A		
	BS	A	*1A	-4A	-4A	-4A *1A		
	BS	A	*1A	-4A	-4A	-4A *4A		
	BS	A	*2A	-1A	-4A	-4A *1A		
	BS	A	*2A	-1A	-4A	-4A *4A		

		Screen Number Order						
Screen Number		Fragment Definition					Frequency Percent	
841	BS	A	*4A	-1A	-4A	-4A *1A	0.60	(continued)
	BS	A	*4A	-1A	-4A	-4A *4A		
	BS	A	*4A	-4A	-4A	-1A *1A		
	BS	A	*4A	-4A	-4A	-1A *2A		
	BS	A	*4A	-4A	-4A	-1A *4A		
	BS	A	*4A	-4A	-4A	-4A *1A		
	BS	A	*4A	-4A	-4A	-4A *4A		
842	BS	A	*1A	-2A	-1A	-2A *1A	0.16	
	BS	A	*1A	-2A	-1A	-4A *1A		
	BS	A	*1A	-2A	-1A	-4A *4A		
	BS	A	*1A	-4A	-1A	-2A *1A		
	BS	A	*1A	-4A	-1A	-4A *1A		
	BS	A	*1A	-4A	-1A	-4A *4A		
	BS	A	*4A	-4A	-1A	-2A *1A		
	BS	A	*4A	-4A	-1A	-4A *1A		
	BS	A	*4A	-4A	-1A	-4A *4A		
843	BS	A	*2A	-1A	-1A	-1A *2A	0.38	
	BS	A	*2A	-1A	-2A	-1A *2A		
	BS	A	*2A	-1A	-4A	-1A *2A		
844	BS	A	*2A	-1A	-1A	-1A *4A	2.50	
	BS	A	*2A	-1A	-1A	-4A *4A		
	BS	A	*2A	-1A	-2A	-1A *4A		
	BS	A	*2A	-1A	-4A	-1A *4A		
	BS	A	*2A	-1A	-4A	-4A *4A		
	BS	A	*4A	-1A	-1A	-1A *2A		
	BS	A	*4A	-1A	-2A	-1A *2A		
	BS	A	*4A	-1A	-4A	-1A *2A		
	BS	A	*4A	-4A	-1A	-1A *2A		
	BS	A	*4A	-4A	-4A	-1A *2A		
845	BS	A	*4A	-1A	-1A	-1A *4A	7.44	
	BS	A	*4A	-1A	-1A	-4A *4A		
	BS	A	*4A	-1A	-2A	-1A *4A		
	BS	A	*4A	-1A	-4A	-1A *4A		
	BS	A	*4A	-1A	-4A	-4A *4A		
	BS	A	*4A	-4A	-1A	-1A *4A		
	BS	A	*4A	-4A	-1A	-4A *4A		
	BS	A	*4A	-4A	-4A	-1A *4A		
	BS	A	*4A	-4A	-4A	-4A *4A		
846	BS	A	*	A	-	A - A - A	49.89	
	BS	A	-	A	-	A - A * A		
847	BS	A	*1A	-1A	-1A	-1A -1A	19.15	
	BS	A	*2A	-1A	-1A	-1A -1A		
	BS	A	-1A	-1A	-1A	-1A *1A		
	BS	A	-1A	-1A	-1A	-1A *2A		



# Screen Number Order

Screen Number	Fragment Definition	Frequency Percent
848	BS A *1A -1A -1A -1A -2A	7.95
	BS A *1A -1A -1A -1A -4A	
	BS A *2A -1A -1A -1A -2A	
	BS A *2A -1A -1A -1A -4A	
	BS A -2A -1A -1A -1A *1A	
	BS A -2A -1A -1A -1A *2A	
	BS A -4A -1A -1A -1A *1A	
	BS A -4A -1A -1A -1A *2A	
849	BS A *1A -1A -1A -1A -3A	1.26
	BS A *1A -1A -2A -1A -3A	
	BS A *1A -1A -3A -1A -3A	
	BS A *1A -1A -4A -1A -3A	
	BS A *1A -2A -1A -1A -3A	
	BS A *1A -4A -1A -1A -3A	
	BS A *1A -4A -4A -1A -3A	
	BS A *2A -1A -1A -1A -3A	
	BS A *2A -1A -2A -1A -3A	
	BS A *2A -1A -3A -1A -3A	
	BS A *2A -1A -4A -1A -3A	
	BS A *4A -1A -1A -1A -3A	
	BS A *4A -1A -2A -1A -3A	
	BS A *4A -1A -3A -1A -3A	
	BS A *4A -1A -4A -1A -3A	
	BS A *4A -4A -1A -1A -3A	
	BS A *4A -4A -4A -1A -3A	
	BS A -3A -1A -1A -1A *1A	
	BS A -3A -1A -1A -1A *2A	
	BS A -3A -1A -1A -1A *4A	
	BS A -3A -1A -1A -2A *1A	
	BS A -3A -1A -1A -4A *1A	
	BS A -3A -1A -1A -4A *4A	
	BS A -3A -1A -2A -1A *1A	
	BS A -3A -1A -2A -1A *2A	
	BS A -3A -1A -2A -1A *4A	
	BS A -3A -1A -3A -1A *1A	
	BS A -3A -1A -3A -1A *2A	
	BS A -3A -1A -3A -1A *4A	
	BS A -3A -1A -4A -1A *1A	
	BS A -3A -1A -4A -1A *2A	
	BS A -3A -1A -4A -1A *4A	
	BS A -3A -1A -4A -4A *1A	
	BS A -3A -1A -4A -4A *4A	
850	BS A *1A -1A -1A -2A -1A	6.05
	BS A *1A -1A -1A -4A -1A	
	BS A *2A -1A -1A -2A -1A	
	BS A *2A -1A -1A -4A -1A	
	BS A *4A -1A -1A -2A -1A	
	BS A *4A -1A -1A -4A -1A	
	BS A -1A -2A -1A -1A *1A	
	BS A -1A -2A -1A -1A *2A	
	BS A -1A -2A -1A -1A *4A	
	BS A -1A -4A -1A -1A *1A	
	BS A -1A -4A -1A -1A *2A	
	BS A -1A -4A -1A -1A *4A	

# Screen Number Order

Screen Number		Fragment Definition	Frequency Percent
851	BS	A *1A -1A -1A -4A -4A	4.86
	BS	A *1A -1A -4A -4A -1A	
	BS	A *1A -1A -4A -4A -4A	
	BS	A *1A -2A -1A -4A -4A	
	BS	A *1A -4A -1A -4A -4A	
	BS	A *1A -4A -4A -1A -1A	
	BS	A *1A -4A -4A -1A -2A	
	BS	A *1A -4A -4A -1A -4A	
	BS	A *1A -4A -4A -4A -1A	
	BS	A *1A -4A -4A -4A -4A	
	BS	A *2A -1A -1A -4A -4A	
	BS	A *2A -1A -4A -4A -1A	
	BS	A *2A -1A -4A -4A -4A	
	BS	A *4A -1A -1A -4A -4A	
	BS	A *4A -1A -4A -4A -1A	
	BS	A *4A -1A -4A -4A	
	BS	A *4A -4A -1A -4A -4A	
	BS	A *4A -4A -4A -1A -1A	
	BS	A *4A -4A -4A -1A -2A	
	BS	A *4A -4A -4A -1A -4A	
	BS	A *4A -4A -4A -4A -1A	
	BS	A *4A -4A -4A -4A -4A	
	BS	A -1A -1A -4A -4A *1A	
	BS	A -1A -1A -4A -4A *4A	
	BS	A -1A -4A -4A -1A *1A	
	BS	A -1A -4A -4A -1A *2A	
	BS	A -1A -4A -4A -1A *4A	
	BS	A -1A -4A -4A -4A *1A	
	BS	A -1A -4A -4A -4A *4A	
	BS	A -2A -1A -4A -4A *1A	
	BS	A -2A -1A -4A -4A *4A	
	BS	A -4A -1A -4A -4A *1A	
	BS	A -4A -1A -4A -4A *4A	
	BS	A -4A -4A -1A -1A *1A	
	BS	A -4A -4A -1A -1A *2A	
	BS	A -4A -4A -1A -1A *4A	
	BS	A -4A -4A -1A -2A *1A	
	BS	A -4A -4A -1A -4A *1A	
	BS	A -4A -4A -1A -4A *4A	
	BS	A -4A -4A -4A -1A *1A	
	BS	A -4A -4A -4A -1A *2A	
	BS	A -4A -4A -4A -1A *4A	
	BS	A -4A -4A -4A -4A *1A	
	BS	A -4A -4A -4A -4A *4A	
852	BS	A *1A -1A -2A -1A -1A	9.56
	BS	A *2A -1A -2A -1A -1A	
	BS	A *2A -1A -4A -1A -1A	
	BS	A *4A -1A -2A -1A -1A	
	BS	A *4A -1A -4A -1A -1A	
	BS	A -1A -1A -2A -1A *1A	
	BS	A -1A -1A -2A -1A *2A	
	BS	A -1A -1A -2A -1A *4A	
	BS	A -1A -1A -4A -1A *2A	
	BS	A -1A -1A -4A -1A *4A	
	BS	A -1A -1A -4A -1A *4A	

Screen Number Order								
Screen Number				Fragment Definition			Frequency Percent	
853	BS	A	*1A	-1A	-2A	-1A	-2A	3.89
	BS	A	*1A	-1A	-2A	-1A	-4A	
	BS	A	*2A	-1A	-2A	-1A	-2A	
	BS	A	*2A	-1A	-2A	-1A	-4A	
	BS	A	*4A	-1A	-2A	-1A	-2A	
	BS	A	*4A	-1A	-2A	-1A	-4A	
	BS	A	-2A	-1A	-2A	-1A	*1A	
	BS	A	-2A	-1A	-2A	-1A	*2A	
	BS	A	-2A	-1A	-2A	-1A	*4A	
	BS	A	-4A	-1A	-2A	-1A	*1A	
	BS	A	-4A	-1A	-2A	-1A	*2A	
	BS	A	-4A	-1A	-2A	-1A	*4A	
854	BS	A	*1A	-1A	-4A	-1A	-1A	5.30
	BS	A	*1A	-2A	-1A	-1A	-1A	
	BS	A	*1A	-4A	-1A	-1A	-1A	
	BS	A	*4A	-4A	-1A	-1A	-1A	
	BS	A	-1A	-1A	-1A	-2A	*1A	
	BS	A	-1A	-1A	-1A	-4A	*1A	
	BS	A	-1A	-1A	-1A	-4A	*4A	
	BS	A	-1A	-1A	-4A	-1A	*1A	
855	BS	A	*1A	-1A	-4A	-1A	-2A	1.69
	BS	A	*1A	-1A	-4A	-1A	-4A	
	BS	A	*2A	-1A	-4A	-1A	-2A	
	BS	A	*2A	-1A	-4A	-1A	-4A	
	BS	A	*4A	-1A	-4A	-1A	-2A	
	BS	A	*4A	-1A	-4A	-1A	-4A	
	BS	A	-2A	-1A	-4A	-1A	*1A	
	BS	A	-2A	-1A	-4A	-1A	*2A	
	BS	A	-2A	-1A	-4A	-1A	*4A	
	BS	A	-4A	-1A	-4A	-1A	*1A	
	BS	A	-4A	-1A	-4A	-1A	*2A	
	BS	A	-4A	-1A	-4A	-1A	*4A	
856	BS	A	*1A	-2A	-1A	-1A	-2A	0.24
	BS	A	*1A	-2A	-1A	-1A	-4A	
	BS	A	*1A	-4A	-1A	-1A	-2A	
	BS	A	*1A	-4A	-1A	-1A	-4A	
	BS	A	*4A	-4A	-1A	-1A	-2A	
	BS	A	*4A	-4A	-1A	-1A	-4A	
	BS	A	-2A	-1A	-1A	-2A	*1A	
	BS	A	-2A	-1A	-1A	-4A	*1A	
	BS	A	-2A	-1A	-1A	-4A	*4A	
	BS	A	-4A	-1A	-1A	-2A	*1A	
	BS	A	-4A	-1A	-1A	-4A	*1A	
	BS	A	-4A	-1A	-1A	-4A	*4A	
857	BS	A	*1A	-2A	-1A	-2A	-1A	0.76
	BS	A	*1A	-2A	-1A	-4A	-1A	
	BS	A	*1A	-4A	-1A	-2A	-1A	
	BS	A	*1A	-4A	-1A	-4A	-1A	
	BS	A	*4A	-4A	-1A	-2A	-1A	
	BS	A	*4A	-4A	-1A	-4A	-1A	
	BS	A	-1A	-2A	-1A	-2A	*1A	

		Screen Number Order						
Screen Number		Fragment Definition					Frequency Percent	
857	BS	A	-1A	-2A	-1A	-4A *1A	0.76	(continued)
	BS	A	-1A	-2A	-1A	-4A *4A		
	BS	A	-1A	-4A	-1A	-2A *1A		
	BS	A	-1A	-4A	-1A	-4A *1A		
	BS	A	-1A	-4A	-1A	-4A *4A		
858	BS	A	*4A	-1A	-1A	-1A -1A	19.79	
	BS	A	-1A	-1A	-1A	-1A *4A		
859	BS	A	*4A	-1A	-1A	-1A -2A	10.42	
	BS	A	*4A	-1A	-1A	-1A -4A		
	BS	A	-2A	-1A	-1A	-1A *4A		
	BS	A	-4A	-1A	-1A	-1A *4A		
860	BS	A	-	A *	A *	A * A - A	60.97	
861	BS	A	-1A	*1A	*1A	*1A -1A	18.92	
862	BS	A	-1A	*1A	*1A	*1A -2A	7.82	
	BS	A	-2A	*1A	*1A	*1A -1A		
863	BS	A	-1A	*1A	*1A	*1A -4A	0.85	
	BS	A	-4A	*1A	*1A	*1A -1A		
864	BS	A	-1A	*1A	*1A	*2A -1A	14.38	
	BS	A	-1A	*1A	*4A	*1A -1A		
	BS	A	-1A	*1A	*4A	*4A -1A		
	BS	A	-1A	*2A	*1A	*1A -1A		
	BS	A	-1A	*2A	*1A	*2A -1A		
	BS	A	-1A	*2A	*1A	*4A -1A		
	BS	A	-1A	*4A	*1A	*2A -1A		
	BS	A	-1A	*4A	*1A	*4A -1A		
	BS	A	-1A	*4A	*4A	*1A -1A		
865	BS	A	-1A	*1A	*1A	*4A -1A	5.70	
	BS	A	-1A	*1A	*2A	*1A -1A		
	BS	A	-1A	*4A	*1A	*1A -1A		
866	BS	A	-1A	*1A	*1A	*4A -4A	3.89	
	BS	A	-1A	*1A	*2A	*1A -4A		
	BS	A	-1A	*1A	*4A	*1A -4A		
	BS	A	-1A	*1A	*4A	*4A -4A		
	BS	A	-1A	*2A	*1A	*1A -4A		
	BS	A	-1A	*2A	*1A	*4A -4A		
	BS	A	-1A	*4A	*1A	*1A -4A		
	BS	A	-1A	*4A	*1A	*4A -4A		
	BS	A	-1A	*4A	*4A	*1A -4A		
	BS	A	-4A	*1A	*1A	*2A -1A		
	BS	A	-4A	*1A	*1A	*4A -1A		
	BS	A	-4A	*1A	*2A	*1A -1A		
	BS	A	-4A	*1A	*4A	*1A -1A		
	BS	A	-4A	*1A	*4A	*4A -1A		
	BS	A	-4A	*4A	*1A	*1A -1A		
	BS	A	-4A	*4A	*1A	*2A -1A		
	BS	A	-4A	*4A	*1A	*4A -1A		
	BS	A	-4A	*4A	*4A	*1A -1A		

Screen Number Order											
Screen Number				Fragment Definition			Frequency Percent				
867	BS	A	-1A	*1A	*2A	*1A	-2A	7.30			
	BS	A	-1A	*1A	*4A	*1A	-2A				
	BS	A	-1A	*2A	*1A	*1A	-2A				
	BS	A	-1A	*4A	*1A	*1A	-2A				
	BS	A	-1A	*4A	*4A	*1A	-2A				
	BS	A	-2A	*1A	*1A	*2A	-1A				
	BS	A	-2A	*1A	*1A	*4A	-1A				
	BS	A	-2A	*1A	*2A	*1A	-1A				
	BS	A	-2A	*1A	*4A	*1A	-1A				
	BS	A	-2A	*1A	*4A	*4A	-1A				
868	BS	A	-1A	*4A	*4A	*4A	-1A	35.57			
869	BS	A	-1A	*4A	*4A	*4A	-4A	0.88			
	BS	A	-4A	*4A	*4A	*4A	-1A				
870	BS	A	-2A	*1A	*1A	*1A	-2A	3.88			
	BS	A	-2A	*1A	*2A	*1A	-2A				
	BS	A	-2A	*1A	*4A	*1A	-2A				
871	BS	A	-2A	*1A	*1A	*1A	-4A	1.29			
	BS	A	-2A	*1A	*1A	*4A	-4A				
	BS	A	-2A	*1A	*2A	*1A	-4A				
	BS	A	-2A	*1A	*4A	*1A	-4A				
	BS	A	-2A	*1A	*4A	*4A	-4A				
	BS	A	-4A	*1A	*1A	*1A	-2A				
	BS	A	-4A	*1A	*1A	*1A	-4A				
	BS	A	-4A	*1A	*1A	*4A	-4A				
	BS	A	-4A	*1A	*2A	*1A	-2A				
	BS	A	-4A	*1A	*2A	*1A	-4A				
	BS	A	-4A	*1A	*4A	*1A	-2A				
	BS	A	-4A	*1A	*4A	*1A	-4A				
	BS	A	-4A	*1A	*4A	*4A	-4A				
	BS	A	-4A	*4A	*1A	*1A	-2A				
	BS	A	-4A	*4A	*1A	*1A	-4A				
	BS	A	-4A	*4A	*1A	*4A	-4A				
	BS	A	-4A	*4A	*4A	*1A	-2A				
	BS	A	-4A	*4A	*4A	*1A	-4A				
	BS	A	-4A	*4A	*4A	*4A	-4A				
872	BS	A	-	A	*	A	*	A	-	A	53.81
873	BS	A	-1A	*1A	*1A	-1A	20.93				
874	BS	A	-1A	*1A	*1A	-2A	12.22				
	BS	A	-1A	*2A	*1A	-2A					
	BS	A	-1A	*4A	*1A	-2A					
	BS	A	-2A	*1A	*1A	-1A					
	BS	A	-2A	*1A	*2A	-1A					
	BS	A	-2A	*1A	*4A	-1A					

		Screen Number Order					
Screen Number		Fragment Definition					Frequency Percent
875	BS	A	-1A	*1A	*1A	-4A	2.85
	BS	A	-1A	*1A	*4A	-4A	
	BS	A	-1A	*2A	*1A	-4A	
	BS	A	-1A	*4A	*1A	-4A	
	BS	A	-4A	*1A	*1A	-1A	
	BS	A	-4A	*1A	*2A	-1A	
	BS	A	-4A	*1A	*4A	-1A	
	BS	A	-4A	*4A	*1A	-1A	
876	BS	A	-1A	*1A	*2A	-1A	10.85
	BS	A	-1A	*1A	*4A	-1A	
	BS	A	-1A	*2A	*1A	-1A	
	BS	A	-1A	*4A	*1A	-1A	
877	BS	A	-1A	*4A	*4A	-1A	25.09
878	BS	A	-1A	*4A	*4A	-4A	2.01
	BS	A	-4A	*4A	*4A	-1A	
879	BS	A	-2A	*1A	*1A	-2A	3.77
880	BS	A	-2A	*1A	*1A	-4A	2.69
	BS	A	-2A	*1A	*4A	-4A	
	BS	A	-4A	*1A	*1A	-2A	
	BS	A	-4A	*1A	*1A	-4A	
	BS	A	-4A	*1A	*4A	-4A	
	BS	A	-4A	*4A	*1A	-2A	
	BS	A	-4A	*4A	*1A	-4A	
	BS	A	-4A	*4A	*4A	-4A	
881	BS	A	-1A	*4A	*4A	-1A -1A	15.57
	BS	A	-1A	-1A	*4A	*4A -1A	
882	BS	A	-1A	*4A	*4A	-1A -2A	7.58
	BS	A	-2A	-1A	*4A	*4A -1A	
883	BS	A	-1A	*4A	*4A	-1A -4A	5.64
	BS	A	-4A	-1A	*4A	*4A -1A	
884	BS	A	-	A	*	A - A	52.87
885	BS	A	-1A	*1A	-1A		23.45
886	BS	A	-1A	*1A	-2A		14.04
	BS	A	-2A	*1A	-1A		
887	BS	A	-1A	*1A	-4A		2.47
	BS	A	-4A	*1A	-1A		
888	BS	A	-1A	*2A	-1A		8.13
889	BS	A	-1A	*4A	-1A		24.67
890	BS	A	-1A	*4A	-4A		0.92
	BS	A	-4A	*4A	-1A		

Screen Number Order			Fragment Definition	Frequency Percent
891	BS	A -2A *1A -2A		1.95
892	BS	A -2A *1A -4A		0.54
	BS	A -4A *1A -2A		
	BS	A -4A *1A -4A		
	BS	A -4A *4A -4A		
893	BS	A - A * A - A * A - A		2.80
894	BS	A -1A *4A -1A -1A		16.03
	BS	A -1A -1A *4A -1A		
895	BS	A -1A *4A -1A -2A		7.01
	BS	A -2A -1A *4A -1A		
896	BS	A -1A *4A -1A -4A		5.42
	BS	A -4A -1A *4A -1A		
897	BS	A -1A -1A *4A -1A -1A		5.51
898	BS	A -1A -1A *4A -1A -2A		4.41
	BS	A -1A -1A *4A -1A -4A		
	BS	A -2A -1A *4A -1A -1A		
	BS	A -4A -1A *4A -1A -1A		
899	BS	A -2A -1A *4A -1A -2A		1.55
	BS	A -2A -1A *4A -1A -4A		
	BS	A -4A -1A *4A -1A -2A		
	BS	A -4A -1A *4A -1A -4A		
900	BS	A -1A -1A -2A		36.03
	BS	A -2A -1A -1A		
901	BS	A -1A -1A -4A		23.62
	BS	A -4A -1A -1A		
902	BS	A -1A -1A -3A		4.52
	BS	A -3A -1A -1A		
903	BS	A -1A -2A -1A		13.44
904	BS	A -1A -2A -2A		1.23
	BS	A -2A -2A -1A		
905	BS	A -1A -4A -1A		20.88
906	BS	A -1A -4A -4A		23.99
	BS	A -4A -4A -1A		
907	BS	A -1A -3A -1A		1.31
908	BS	A -2A -1A -2A		5.38
909	BS	A -2A -1A -4A		4.21
	BS	A -4A -1A -2A		

		Screen Number Order				
Screen Number		Fragment Definition				Frequency Percent
910	BS	A	-2A	-1A	-3A	1.19
	BS	A	-3A	-1A	-2A	
911	BS	A	-4A	-1A	-4A	0.72
912	BS	A	-4A	-4A	-4A	2.45
913	BS	A	-3A	-1A	-4A	0.00
	BS	A	-4A	-1A	-3A	
914	BS	A	-3A	-1A	-3A	0.09
915	BS	A	-1A	-1A	-1A -1A	45.77
916	BS	A	-1A	-1A	-1A -2A	26.16
	BS	A	-2A	-1A	-1A -1A	
917	BS	A	-1A	-1A	-1A -4A	18.40
	BS	A	-4A	-1A	-1A -1A	
918	BS	A	-1A	-1A	-1A -3A	2.42
	BS	A	-3A	-1A	-1A -1A	
919	BS	A	-1A	-1A	-2A -1A	23.74
	BS	A	-1A	-1A	-3A -1A	
	BS	A	-1A	-1A	-4A -1A	
	BS	A	-1A	-2A	-1A -1A	
	BS	A	-1A	-3A	-1A -1A	
	BS	A	-1A	-4A	-1A -1A	
920	BS	A	-1A	-1A	-4A -4A	12.63
	BS	A	-4A	-4A	-1A -1A	
921	BS	A	-1A	-2A	-1A -2A	7.65
	BS	A	-1A	-2A	-1A -3A	
	BS	A	-1A	-2A	-1A -4A	
	BS	A	-1A	-3A	-1A -2A	
	BS	A	-1A	-3A	-1A -3A	
	BS	A	-1A	-3A	-1A -4A	
	BS	A	-1A	-4A	-1A -2A	
	BS	A	-1A	-4A	-1A -3A	
	BS	A	-1A	-4A	-1A -4A	
	BS	A	-2A	-1A	-2A -1A	
	BS	A	-2A	-1A	-3A -1A	
	BS	A	-2A	-1A	-4A -1A	
	BS	A	-3A	-1A	-2A -1A	
	BS	A	-3A	-1A	-3A -1A	
	BS	A	-3A	-1A	-4A -1A	
	BS	A	-4A	-1A	-2A -1A	
	BS	A	-4A	-1A	-3A -1A	
	BS	A	-4A	-1A	-4A -1A	
922	BS	A	-1A	-4A	-4A -1A	2.48
	BS	A	-1A	-4A	-4A -4A	
	BS	A	-4A	-4A	-4A -1A	



		Screen Number Order										
Screen Number		Fragment Definition							Frequency Percent			
923	BS	A	-2A	-1A	-1A	-2A			9.54			
	BS	A	-2A	-1A	-1A	-4A						
	BS	A	-4A	-1A	-1A	-2A						
	BS	A	-4A	-1A	-1A	-4A						
924	BS	A	-2A	-1A	-1A	-3A			1.72			
	BS	A	-3A	-1A	-1A	-2A						
	BS	A	-3A	-1A	-1A	-3A						
	BS	A	-3A	-1A	-1A	-4A						
	BS	A	-4A	-1A	-1A	-3A						
925	BS	A	-2A	-1A	-4A	-4A			3.29			
	BS	A	-3A	-1A	-4A	-4A						
	BS	A	-4A	-1A	-4A	-4A						
	BS	A	-4A	-4A	-1A	-2A						
	BS	A	-4A	-4A	-1A	-3A						
	BS	A	-4A	-4A	-1A	-4A						
	BS	A	-4A	-4A	-4A	-4A						
926	BS	A	-	A	-	A	-	A	-	A		44.76
927	BS	A	-1A	-1A	-1A	-1A	-1A			30.55		
928	BS	A	-1A	-1A	-1A	-1A	-2A			24.95		
	BS	A	-1A	-1A	-1A	-1A	-3A					
	BS	A	-1A	-1A	-1A	-1A	-4A					
	BS	A	-2A	-1A	-1A	-1A	-1A					
	BS	A	-3A	-1A	-1A	-1A	-1A					
	BS	A	-4A	-1A	-1A	-1A	-1A					
929	BS	A	-1A	-1A	-1A	-2A	-1A			18.34		
	BS	A	-1A	-1A	-1A	-3A	-1A					
	BS	A	-1A	-1A	-1A	-4A	-1A					
	BS	A	-1A	-2A	-1A	-1A	-1A					
	BS	A	-1A	-3A	-1A	-1A	-1A					
	BS	A	-1A	-4A	-1A	-1A	-1A					
930	BS	A	-1A	-1A	-1A	-4A	-4A			9.93		
	BS	A	-4A	-4A	-1A	-1A	-1A					
931	BS	A	-1A	-1A	-2A	-1A	-1A			10.49		
	BS	A	-1A	-1A	-3A	-1A	-1A					
	BS	A	-1A	-1A	-4A	-1A	-1A					
932	BS	A	-1A	-2A	-1A	-2A	-1A			3.30		
	BS	A	-1A	-2A	-1A	-3A	-1A					
	BS	A	-1A	-2A	-1A	-4A	-1A					
	BS	A	-1A	-3A	-1A	-2A	-1A					
	BS	A	-1A	-3A	-1A	-3A	-1A					
	BS	A	-1A	-3A	-1A	-4A	-1A					
	BS	A	-1A	-4A	-1A	-2A	-1A					
	BS	A	-1A	-4A	-1A	-3A	-1A					
	BS	A	-1A	-4A	-1A	-4A	-1A					

Screen Number Order										
Screen Number	Fragment Definition						Frequency Percent			
933	BS	A	-2A	-1A	-1A	-1A	-2A	6.75		
	BS	A	-2A	-1A	-1A	-1A	-3A			
	BS	A	-2A	-1A	-1A	-1A	-4A			
	BS	A	-3A	-1A	-1A	-1A	-2A			
	BS	A	-3A	-1A	-1A	-1A	-3A			
	BS	A	-3A	-1A	-1A	-1A	-4A			
	BS	A	-4A	-1A	-1A	-1A	-2A			
	BS	A	-4A	-1A	-1A	-1A	-3A			
	BS	A	-4A	-1A	-1A	-1A	-4A			
934	BS	A	-2A	-1A	-2A	-1A	-2A	1.22		
	BS	A	-2A	-1A	-2A	-1A	-3A			
	BS	A	-2A	-1A	-2A	-1A	-4A			
	BS	A	-2A	-1A	-3A	-1A	-2A			
	BS	A	-2A	-1A	-3A	-1A	-3A			
	BS	A	-2A	-1A	-3A	-1A	-4A			
	BS	A	-2A	-1A	-4A	-1A	-2A			
	BS	A	-2A	-1A	-4A	-1A	-3A			
	BS	A	-2A	-1A	-4A	-1A	-4A			
	BS	A	-3A	-1A	-2A	-1A	-2A			
	BS	A	-3A	-1A	-2A	-1A	-3A			
	BS	A	-3A	-1A	-2A	-1A	-4A			
	BS	A	-3A	-1A	-3A	-1A	-2A			
	BS	A	-3A	-1A	-3A	-1A	-3A			
	BS	A	-3A	-1A	-3A	-1A	-4A			
	BS	A	-3A	-1A	-4A	-1A	-2A			
	BS	A	-3A	-1A	-4A	-1A	-3A			
	BS	A	-3A	-1A	-4A	-1A	-4A			
	BS	A	-4A	-1A	-2A	-1A	-2A			
	BS	A	-4A	-1A	-2A	-1A	-3A			
	BS	A	-4A	-1A	-2A	-1A	-4A			
	BS	A	-4A	-1A	-3A	-1A	-2A			
	BS	A	-4A	-1A	-3A	-1A	-3A			
	BS	A	-4A	-1A	-3A	-1A	-4A			
	BS	A	-4A	-1A	-4A	-1A	-2A			
	BS	A	-4A	-1A	-4A	-1A	-3A			
	BS	A	-4A	-1A	-4A	-1A	-4A			
935	AA	A	*2A				34.69			
936	AA	A	*4A				72.06			
937	AA	A	*3A				0.14			
938	AA	A	-2A				59.17			
939	AA	A	-4A				39.02			
940	AA	A	*	A	*	A	*	A	41.18	
941	AA	A	*	A	-	A	-	A	12.51	
942	AA	2	A	*	A	-	A	-	A	3.34
943	AA	3	A	*	A	-	A	-	A	1.07

Screen Number		Screen Number Order					Frequency Percent	
Screen Number			Fragment Definition					
944	AA		A	- A	- A	- A		73.89
945	AA		A	* A	* A	* A	* A	7.17
946	AA	2	A	* A	* A	* A	* A	1.92
947	AA		A	* A	* A	* A	- A	7.64
948	AA	2	A	* A	* A	* A	- A	3.57
949	AA	3	A	* A	* A	* A	- A	1.36
950	DC		5					5.63
951	HA		AlH2-1C					0.07
	HA		AlH -1C	-1C				
	HA		AsH2-1C					
	HA		AsH -1C	-1C				
	HA		B H2-1C					
	HA		B H -1C	-1C				
	HA		GeH3-1C					
	HA		GeH2-1C	-1C				
	HA		GeH -1C	-1C	-1C			
	HA		P H2-1C					
	HA		P H -1C	-1C				
	HA		SbH2-1C					
	HA		SbH -1C	-1C				
	HA		SeH -1C					
	HA		SiH3-1C					
	HA		SiH2-1C	-1C				
	HA		SiH -1C	-1C	-1C			
	HA		SnH3-1C					
	HA		SnH2-1C	-1C				
	HA		SnH -1C	-1C	-1C			
	HA		TeH -1C					
952	AA		As	X				0.53
	AA		B	X				
	AA		Se	X				
	AA		Si	X				
	AA		Te	X				
	AA		X	As				
	AA		X	B				
	AA		X	Se				
	AA		X	Si				
	AA		X	Te				
953	AA		B	- C				0.39
	AA		C	- B				
954	AA		B	N				0.22
	AA		N	B				

Screen Number		Screen Number Order				Fragment Definition		Frequency Percent	
955	AA		B	*	O			0.30	
	AA		B	-	O				
	AA		O	*	B				
	AA		O	-	B				
956	AA		Br		C			4.36	
	AA		C		Br				
957	AA	2	C		Br			0.80	
958	AA		C		Br	Br		0.09	
959	AA		C	-	Br	*	C	3.55	
960	AA	2	C	-	Br	*	C	0.64	
961	AA		C		Br	Cl		0.16	
	AA		C		Br	F			
	AA		C		Br	I			
	AA		C		Cl	F			
	AA		C		Cl	I			
	AA		C		F	I			
962	AA		C	-	Br	*	N	0.11	
963	HA		C	H3-1C				57.28	
964	HA	2	C	H3-1C				37.58	
965	HA	3	C	H3-1C				22.43	
966	HA	4	C	H3-1C				14.08	
967	HA	6	C	H3-1C				6.24	
968	AA		C	-2C				14.86	
969	AA	4	C	-2C				3.19	
970	HA		C	H2-2C				5.09	
971	AA	2	C	-3C				1.56	
972	AA	4	C	-3C				0.28	
973	HA		C	H -3C				0.52	
974	AA		C	*	C	*	C	83.26	
975	AA		C	*	C	-	C	70.68	
976	AA	2	C	*	C	-	C	51.36	
977	AA	3	C	*	C	-	C	30.91	

Screen Number Order							Frequency Percent
Screen Number	Fragment Definition						
978	AA	4	C	* C	– C		18.42
979	AA	5	C	* C	– C		9.80
980	AA		C	*1C	*1C		38.78
981	AA	2	C	*1C	*1C		32.27
982	AA	3	C	*1C	*1C		24.82
983	AA	4	C	*1C	*1C		18.90
984	AA	5	C	*1C	*1C		15.08
985	AA	6	C	*1C	*1C		12.75
986	AA	7	C	*1C	*1C		8.38
987	AA	10	C	*1C	*1C		4.88
988	AA	14	C	*1C	*1C		2.59
989	HA		C H2	*1C	*1C		27.77
990	HA	2	C H2	*1C	*1C		22.12
991	HA	3	C H2	*1C	*1C		14.50
992	AA		C	*1C	*2C		23.19
993	AA	2	C	*1C	*2C		16.26
994	AA	3	C	*1C	*2C		6.48
995	AA	4	C	*1C	*2C		4.73
996	HA		C H	*1C	*2C		12.78
997	HA	2	C H	*1C	*2C		6.93
998	AA		C	*4C	*4C		70.37
999	AA	4	C	*4C	*4C		68.05
1000	AA	7	C	*4C	*4C		46.29
1001	AA	9	C	*4C	*4C		44.62
1002	AA	12	C	*4C	*4C		41.35
1003	AA	15	C	*4C	*4C		18.54
1004	AA	18	C	*4C	*4C		16.22
1005	AA		C	– C	– C		59.87

		Screen Number Order				Frequency Percent
Screen Number			Fragment Definition			
1006	HA		C H2-1C	-1C		35.14
1007	HA	2	C H2-1C	-1C		22.54
1008	HA	3	C H2-1C	-1C		15.40
1009	HA	5	C H2-1C	-1C		9.31
1010	HA	8	C H2-1C	-1C		6.05
1011	AA		C	-1C	-2C	14.27
1012	AA	2	C	-1C	-2C	8.12
1013	AA	3	C	-1C	-2C	2.10
1014	AA	6	C	-1C	-2C	0.42
1015	HA		C H	-1C	-2C	12.02
1016	HA	2	C H	-1C	-2C	5.64
1017	HA	3	C H	-1C	-2C	1.54
1018	HA	4	C H	-1C	-2C	0.99
1019	AA		C	-1C	-3C	1.58
1020	AA		C	-2As	-2C	0.14
	AA		C	-2B	-2C	
	AA		C	-2C	-2C	
	AA		C	-2C	-2N	
	AA		C	-2C	-2O	
	AA		C	-2C	-2P	
	AA		C	-2C	-2S	
	AA		C	-2C	-2Se	
	AA		C	-2C	-2Si	
	AA		C	-2C	-2Te	
1021	AA		C	* C	* C * C	29.30
1022	AA	2	C	* C	* C * C	19.00
1023	AA	3	C	* C	* C * C	9.59
1024	AA	5	C	* C	* C * C	4.24
1025	AA		C	*1C	*1C *1C	7.74
1026	AA	2	C	*1C	*1C *1C	5.66
1027	AA	3	C	*1C	*1C *1C	3.23
1028	HA		C H	*1C	*1C *1C	6.09

		Screen Number Order					
Screen Number				Fragment Definition			Frequency Percent
1029	AA		C	*1C	*1C	*2C	3.99
1030	AA	2	C	*1C	*1C	*2C	0.98
1031	AA		C	*1C	*1C	-1C	16.17
1032	AA	2	C	*1C	*1C	-1C	6.87
1033	AA	3	C	*1C	*1C	-1C	2.67
1034	HA		C H	*1C	*1C	-1C	10.75
1035	AA		C	*1C	*1C	-2C	1.98
1036	AA		C	*1C	*2C	-1C	10.48
1037	AA	2	C	*1C	*2C	-1C	2.50
1038	AA		C	*1C	*4C	*4C	16.87
1039	AA	2	C	*1C	*4C	*4C	8.65
1040	AA	3	C	*1C	*4C	*4C	3.02
1041	AA		C	*4C	*4C	*4C	6.96
1042	AA	2	C	*4C	*4C	*4C	4.96
1043	AA	3	C	*4C	*4C	*4C	1.64
1044	AA		C	*4C	*4C	-1C	53.13
1045	AA	2	C	*4C	*4C	-1C	29.03
1046	AA	3	C	*4C	*4C	-1C	12.69
1047	AA	5	C	*4C	*4C	-1C	2.69
1048	AA		C	- C	- C	- C	21.56
1049	AA		C	-1C	-1C	-1C	18.17
1050	AA	2	C	-1C	-1C	-1C	6.13
1051	HA		C H	-1C	-1C	-1C	10.06
1052	HA	2	C H	-1C	-1C	-1C	3.43
1053	HA	3	C H	-1C	-1C	-1C	1.59
1054	AA		C	-1C	-1C	-2C	4.39
1055	AA	2	C	-1C	-1C	-2C	0.79
1056	AA		C	C	C	C	10.15

Screen Number Order								
Screen Number	Fragment Definition							Frequency Percent
1057	AA	2	C	C	C	C	C	3.79
1058	AA	3	C	C	C	C	C	0.96
1059	AA	4	C	C	C	C	C	0.56
1060	AA	5	C	C	C	C	C	0.25
1061	AA		C	* C	* C	* C	* C	1.01
1062	AA		C	* C	* C	* C	- C	3.22
1063	AA		C	* C	* C	- C	- C	3.52
1064	AA		C	- C	- C	- C	- C	3.78
1065	AA		C	C	C	C	X	0.41
1066	AA		C	* C	* C	- C	- N	1.87
	AA		C	* C	* C	- C	- O	
	AA		C	* C	* C	- C	- S	
	AA		C	* C	* C	- C	- X	
1067	AA		C	- C	- C	- C	- X	0.12
1068	AA		C	C	C	C	N	2.73
1069	AA	2	C	C	C	C	N	0.43
1070	AA		C	* C	- C	- C	* N	0.70
1071	AA		C	- C	- C	- C	- N	1.23
1072	AA		C	C	C	C	O	7.26
	AA		C	C	C	C	S	
1073	AA	2	C	C	C	C	O	1.18
	AA	2	C	C	C	C	S	
1074	AA	3	C	C	C	C	O	0.25
	AA	3	C	C	C	C	S	
1075	AA		C	* C	- C	- C	* O	1.18
	AA		C	* C	- C	- C	* S	
1076	AA		C	- C	- C	- C	- O	3.59
	AA		C	- C	- C	- C	- S	
1077	AA		C	* C	* C	- X		18.59
1078	HA		C H	*1C	*1C	-1X		0.47
1079	AA		C	- C	- C	- X		1.51
1080	AA	2	C	- C	- C	- X		0.55



Screen Number Order							
Screen Number	Fragment Definition						Frequency Percent
1081	AA	3	C	- C	- C	- X	0.35
1082	AA		C	-1C	-1C	-1X	1.18
1083	HA		C H	-1C	-1C	-1X	0.44
1084	AA		C	-1C	-2C	-1X	0.35
1085	AA		C	C	C	X X	0.86
1086	AA		C	* C	* C	- X - X	0.23
1087	AA		C	-1C	-1C	-2N	7.76
	AA		C	-1C	-1C	-1N -1N	
	AA		C	-1C	-1C	-1N -1O	
	AA		C	-1C	-1C	-1N -1S	
	AA		C	-1C	-1C	-1N -1X	
	AA		C	-1C	-1C	-2O	
	AA		C	-1C	-1C	-1O -1O	
	AA		C	-1C	-1C	-1O -1S	
	AA		C	-1C	-1C	-1O -1X	
	AA		C	-1C	-1C	-2S	
	AA		C	-1C	-1C	-1S -1S	
	AA		C	-1C	-1C	-1S -1X	
	AA		C	-1C	-1C	-1X -1X	
	1088	AA		C	C	C	
AA			C	C	C	O X	
AA			C	C	C	S X	
1089	AA		C	* C	* C	- N - N	0.08
	AA		C	* C	* C	- N - O	
	AA		C	* C	* C	- N - S	
	AA		C	* C	* C	- N - X	
	AA		C	* C	* C	- O - X	
	AA		C	* C	* C	- S - X	
1090	AA		C	* C	- C	* N - N	0.12
	AA		C	* C	- C	* N - O	
	AA		C	* C	- C	* N - S	
	AA		C	* C	- C	* N - X	
	AA		C	* C	* N	- N - N	
	AA		C	* C	* N	- N - O	
	AA		C	* C	* N	- N - S	
	AA		C	* C	* N	- N - X	
	AA		C	* C	* N	- O - O	
	AA		C	* C	* N	- O - S	
	AA		C	* C	* N	- O - X	
	AA		C	* C	* N	- S - S	
	AA		C	* C	* N	- S - X	
	AA		C	* C	* N	- X - X	

		Screen Number Order					Frequency Percent
Screen Number			Fragment Definition				
1091	AA		C	* C	- C	- N * O	0.12
	AA		C	* C	- C	- N * S	
	AA		C	* C	- C	* O - O	
	AA		C	* C	- C	* O - S	
	AA		C	* C	- C	- O * S	
	AA		C	* C	- C	* O - X	
	AA		C	* C	- C	* S - S	
	AA		C	* C	- C	* S - X	
	AA		C	* C	- N	- N * O	
	AA		C	* C	- N	- N * S	
	AA		C	* C	- N	* O - O	
	AA		C	* C	- N	* O - S	
	AA		C	* C	- N	- O * S	
	AA		C	* C	- N	* O - X	
	AA		C	* C	- N	* S - S	
	AA		C	* C	- N	* S - X	
	AA		C	* C	- O	- O - O	
	AA		C	* C	- O	- O - S	
	AA		C	* C	* O	- O - X	
	AA		C	* C	- O	- S - S	
	AA		C	* C	* O	- S - X	
	AA		C	* C	- O	* S - X	
	AA		C	* C	* O	- X - X	
	AA		C	* C	- S	- S - S	
	AA		C	* C	* S	- S - X	
	AA		C	* C	* S	- X - X	
1092	AA		C	* C	* C	* N	18.01
1093	AA	2	C	* C	* C	* N	7.34
1094	AA	3	C	* C	* C	* N	2.48
1095	AA	4	C	* C	* C	* N	1.63
1096	AA	5	C	* C	* C	* N	0.82
1097	AA		C	* C	* C	- N	28.97
1098	AA	2	C	* C	* C	- N	10.75
1099	AA		C	* C	- C	* N	19.54
1100	AA	2	C	* C	- C	* N	6.42
1101	AA		C	*1C	*1C	*1N	2.52
1102	HA		C H	*1C	*1C	*1N	3.90
	HA		C H	*1C	*1C	*1O	
	HA		C H	*1C	*1C	*1S	
1103	AA		C	*1C	*1C	*2N	0.63
1104	AA		C	*1C	*1C	-1N	5.62

		Screen Number Order					Frequency Percent
Screen Number				Fragment Definition			
1105	HA		C H	*1C	*1C	-1N	5.12
1106	AA		C	*1C	*1C	-2N	0.85
1107	AA		C	*1C	*2C	*1N	1.97
1108	AA		C	*1C	*2C	-1N	1.18
1109	AA		C	*1C	*4C	*4N	1.45
1110	AA		C	*1C	-1C	*1N	7.36
1111	HA		C H	*1C	-1C	*1N	6.44
1112	AA		C	*1C	-1C	*2N	3.47
1113	AA		C	*1C	-2C	*1N	0.48
1114	AA		C	*2C	-1C	*1N	6.96
1115	AA	2	C	*2C	-1C	*1N	1.52
1116	AA		C	*4C	*4C	*1N	10.82
1117	AA	2	C	*4C	*4C	*1N	3.71
1118	AA		C	*4C	*4C	*4N	3.24
1119	AA	2	C	*4C	*4C	*4N	1.15
1120	AA		C	*4C	*4C	-1N	23.48
1121	AA	2	C	*4C	*4C	-1N	8.53
1122	AA		C	*4C	-1C	*4N	3.89
1123	AA		C	- C	- C	- N	13.50
1124	AA	2	C	- C	- C	- N	5.13
1125	AA	3	C	- C	- C	- N	3.46
1126	HA		C H	-1C	-1C	-1N	10.60
1127	HA	2	C H	-1C	-1C	-1N	4.59
1128	AA		C	-1C	-1C	-2N	1.48
1129	AA		C	-1C	-2C	-1N	0.47
1130	AA		C	C	C	N N	0.19

Screen Number		Screen Number Order					Fragment Definition		Frequency Percent
1131	AA		C	- C	- C	* N	* N		1.00
	AA		C	- C	- C	* N	* O		
	AA		C	- C	- C	* N	* S		
	AA		C	- C	- C	* O	* O		
	AA		C	- C	- C	* O	* S		
	AA		C	- C	- C	* S	* S		
1132	AA		C	C	C	N	O		0.46
	AA		C	C	C	N	S		
1133	AA		C	* C	* C	* O			8.35
1134	AA	2	C	* C	* C	* O			4.34
1135	AA		C	* C	* C	- O			35.34
1136	AA	2	C	* C	* C	- O			17.07
1137	AA		C	*1C	*1C	*10			3.06
1138	AA		C	*1C	*1C	-10			8.84
1139	AA		C	*1C	*1C	-20			5.34
1140	AA	2	C	*1C	*1C	-20			1.31
1141	AA		C	*1C	*2C	*10			0.47
1142	AA		C	*1C	*2C	-10			1.32
1143	AA		C	*1C	-1C	*10			7.20
1144	AA		C	*1C	-2C	*10			0.14
1145	AA		C	*2C	-1C	*10			2.75
1146	AA		C	- C	- C	- O			16.97
1147	AA	2	C	- C	- C	- O			3.76
1148	AA	3	C	- C	- C	- O			1.06
1149	HA		C H	-1C	-1C	-10			8.63
1150	HA	2	C H	-1C	-1C	-10			2.01
1151	AA		C	-1C	-1C	-20			5.56
1152	AA	2	C	-1C	-1C	-20			0.49
1153	AA		C	-1C	-2C	-10			0.34
1154	AA		C	C	C	P			2.04
1155	AA		C	- C	- C	- P			0.26

		Screen Number Order					Frequency Percent
Screen Number				Fragment Definition			
1156	AA		C	* C	* C	* S	3.07
1157	AA	2	C	* C	* C	* S	0.72
1158	AA		C	* C	* C	- S	7.91
1159	AA	2	C	* C	* C	- S	1.93
1160	AA		C	* C	- C	* S	3.95
1161	AA		C	*1C	*1C	-1S	0.51
1162	AA		C	*1C	*1C	-2S	0.44
	AA		C	*1C	*2C	-1S	
1163	AA		C	-1C	-1C	-1S	0.85
1164	HA		C H	-1C	-1C	-1S	0.62
1165	AA		C	-1C	-1C	-2S	0.15
	AA		C	-1C	-2C	-1S	
1166	HA		C H	*1C	*1C	-1O	7.88
	HA		C H	*1C	*1C	-1S	
1167	HA		C H	*1C	-1C	*1O	6.41
	HA		C H	*1C	-1C	*1S	
1168	AA		C	C	C	O O	1.94
	AA		C	C	C	O S	
	AA		C	C	C	S S	
1169	AA		C	* C	* C	- O - O	0.10
	AA		C	* C	* C	- O - S	
	AA		C	* C	* C	- S - S	
1170	AA		C	* C	- C1		11.60
1171	AA	2	C	* C	- C1		3.88
1172	AA	3	C	* C	- C1		0.86
1173	AA	4	C	* C	- C1		0.39
1174	AA		C	* C	- F		5.23
1175	AA	2	C	* C	- F		1.54
1176	AA		C	* C	- X		19.40
1177	AA	2	C	* C	- X		7.30
1178	AA	3	C	* C	- X		2.13
1179	AA		C	*1C	-1X		1.94

		Screen Number Order						
Screen Number			Fragment Definition				Frequency Percent	
1180	AA		C	*2C	-1X			1.34
1181	AA		C	*4C	-1X			17.48
1182	AA		C	- C	- X			7.92
1183	AA	2	C	- C	- X			2.18
1184	AA	3	C	- C	- X			0.81
1185	AA		C	-1C	-1X			7.60
1186	HA		C	H2-1C	-1X			1.70
1187	HA	2	C	H2-1C	-1X			0.26
1188	AA		C	-2C	-1X			0.69
1189	HA		C	H -2C	-1X			0.15
1190	AA		C	-1As	-3C			0.20
	AA		C	-1B	-3C			
	AA		C	-3C	-1N			
	AA		C	-3C	-1O			
	AA		C	-3C	-1P			
	AA		C	-3C	-1S			
	AA		C	-3C	-1Se			
	AA		C	-3C	-1Si			
	AA		C	-3C	-1Te			
	AA		C	-3C	-1X			
1191	AA		C	-1C	-1X	-1X		4.83
1192	HA		C	H -1C	-2N			5.19
	HA		C	H -1C	-1N	-1N		
	HA		C	H -1C	-1N	-1O		
	HA		C	H -1C	-1N	-1S		
	HA		C	H -1C	-1N	-1X		
	HA		C	H -1C	-2O			
	HA		C	H -1C	-1O	-1O		
	HA		C	H -1C	-1O	-1S		
	HA		C	H -1C	-1O	-1X		
	HA		C	H -1C	-2S			
	HA		C	H -1C	-1S	-1S		
	HA		C	H -1C	-1S	-1X		
	HA		C	H -1C	-1X	-1X		
	1193	AA		C	-2C	-1N	-1X	
AA			C	-2C	-1O	-1X		
AA			C	-2C	-1S	-1X		
AA			C	-2C	-1X	-1X		
1194	AA		C	C	X	X	X	4.37

Screen Number	Fragment Definition						Frequency Percent
1195	AA	C	C	N	N	N	0.40
	AA	C	C	N	N	O	
	AA	C	C	N	N	S	
	AA	C	C	N	N	X	
	AA	C	C	N	O	O	
	AA	C	C	N	O	S	
	AA	C	C	N	O	X	
	AA	C	C	N	S	S	
	AA	C	C	N	S	X	
	AA	C	C	N	X	X	
	AA	C	C	O	O	O	
	AA	C	C	O	O	S	
	AA	C	C	O	O	X	
	AA	C	C	O	S	S	
	AA	C	C	O	S	X	
	AA	C	C	S	S	S	
	AA	C	C	S	S	X	
	AA	C	C	S	X	X	
	1196	HA	C H	-1N	-1N	-1N	
HA		C H	-1N	-1N	-1O		
HA		C H	-1N	-1N	-1S		
HA		C H	-1N	-1N	-1X		
HA		C H	-1N	-1O	-1O		
HA		C H	-1N	-1O	-1S		
HA		C H	-1N	-1O	-1X		
HA		C H	-1N	-1S	-1S		
HA		C H	-1N	-1S	-1X		
HA		C H	-1N	-1X	-1X		
HA		C H	-1O	-1O	-1O		
HA		C H	-1O	-1O	-1S		
HA		C H	-1O	-1O	-1X		
HA		C H	-1O	-1S	-1S		
HA		C H	-1O	-1S	-1X		
HA		C H	-1O	-1X	-1X		
HA		C H	-1S	-1S	-1S		
HA		C H	-1S	-1S	-1X		
HA		C H	-1S	-1X	-1X		
AA		C	-1C	-1N	-1N	-1N	
AA		C	-1C	-1N	-1N	-1O	
AA		C	-1C	-1N	-1N	-1S	
AA		C	-1C	-1N	-1N	-1X	
AA		C	-1C	-1N	-1O	-1O	
AA		C	-1C	-1N	-1O	-1S	
AA		C	-1C	-1N	-1O	-1X	
AA		C	-1C	-1N	-1S	-1S	
AA		C	-1C	-1N	-1S	-1X	
AA		C	-1C	-1N	-1X	-1X	
AA		C	-1C	-1O	-1O	-1O	
AA		C	-1C	-1O	-1O	-1S	
AA		C	-1C	-1O	-1O	-1X	
AA		C	-1C	-1O	-1S	-1S	
AA	C	-1C	-1O	-1S	-1X		
AA	C	-1C	-1O	-1X	-1X		
AA	C	-1C	-1O	-1X	-1X		
AA	C	-1C	-1O	-1O	-1O		
AA	C	-1C	-1O	-1O	-1S		
AA	C	-1C	-1O	-1O	-1X		
AA	C	-1C	-1O	-1S	-1S		
AA	C	-1C	-1O	-1S	-1X		
AA	C	-1C	-1O	-1X	-1X		

Screen Number Order								
Screen Number	Fragment Definition						Frequency Percent	
1196	AA	C	-1C	-1S	-1S	-1S	0.97	(continued)
	AA	C	-1C	-1S	-1S	-1X		
	AA	C	-1C	-1S	-1X	-1X		
	AA	C	-1N	-1N	-1N	-1N		
	AA	C	-1N	-1N	-1N	-1O		
	AA	C	-1N	-1N	-1N	-1S		
	AA	C	-1N	-1N	-1N	-1X		
	AA	C	-1N	-1N	-1O	-1O		
	AA	C	-1N	-1N	-1O	-1S		
	AA	C	-1N	-1N	-1O	-1X		
	AA	C	-1N	-1N	-1S	-1S		
	AA	C	-1N	-1N	-1S	-1X		
	AA	C	-1N	-1N	-1X	-1X		
	AA	C	-1N	-1O	-1O	-1O		
	AA	C	-1N	-1O	-1O	-1S		
	AA	C	-1N	-1O	-1O	-1X		
	AA	C	-1N	-1O	-1S	-1S		
	AA	C	-1N	-1O	-1S	-1X		
	AA	C	-1N	-1O	-1X	-1X		
	AA	C	-1N	-1S	-1S	-1S		
	AA	C	-1N	-1S	-1S	-1X		
	AA	C	-1N	-1S	-1X	-1X		
	AA	C	-1N	-1X	-1X	-1X		
	AA	C	-1O	-1O	-1O	-1O		
	AA	C	-1O	-1O	-1O	-1S		
	AA	C	-1O	-1O	-1O	-1X		
	AA	C	-1O	-1O	-1O	-1S		
	AA	C	-1O	-1O	-1S	-1X		
	AA	C	-1O	-1O	-1X	-1X		
	AA	C	-1O	-1S	-1S	-1S		
	AA	C	-1O	-1S	-1S	-1X		
	AA	C	-1O	-1S	-1X	-1X		
	AA	C	-1O	-1X	-1X	-1X		
	AA	C	-1S	-1S	-1S	-1S		
	AA	C	-1S	-1S	-1S	-1X		
	AA	C	-1S	-1S	-1X	-1X		
	AA	C	-1S	-1X	-1X	-1X		
1197	AA	C	* C	* N	- X		0.81	
1198	HA	C H	*1C	*1N	-1X		0.05	
	HA	C H	*1C	*1O	-1X			
	HA	C H	*1C	*1S	-1X			
	HA	C H	*1N	*1N	-1X			
	HA	C H	*1N	*1O	-1X			
	HA	C H	*1N	*1S	-1X			
	HA	C H	*1O	*1O	-1X			
	HA	C H	*1O	*1S	-1X			
	HA	C H	*1S	*1S	-1X			
1199	AA	C	-1C	-1N	-2N		43.86	
	AA	C	-1C	-4N	-4N			
	AA	C	-1C	-1N	-2O			
	AA	C	-1C	-2N	-1O			
	AA	C	-1C	-4N	-4O			



Screen Number Order							
Screen Number	Fragment Definition					Frequency Percent	
1199	AA	C	-1C	-1N	-2S	43.86 (continued)	
	AA	C	-1C	-2N	-1S		
	AA	C	-1C	-4N	-4S		
	AA	C	-1C	-2N	-1X		
	AA	C	-1C	-1O	-2O		
	AA	C	-1C	-4O	-4O		
	AA	C	-1C	-1O	-2S		
	AA	C	-1C	-2O	-1S		
	AA	C	-1C	-4O	-4S		
	AA	C	-1C	-2O	-1X		
	AA	C	-1C	-1S	-2S		
	AA	C	-1C	-4S	-4S		
	AA	C	-1C	-2S	-1X		
	1200	AA	C	- C	* N		* N
AA		C	- C	* N	* N	- O	
AA		C	- C	* N	- N	* O	
AA		C	- C	* N	* N	- S	
AA		C	- C	* N	- N	* S	
AA		C	- C	* N	* N	- X	
AA		C	- C	* N	* O	- O	
AA		C	- C	- N	* O	* O	
AA		C	- C	* N	* O	- S	
AA		C	- C	* N	- O	* S	
AA		C	- C	- N	* O	* S	
AA		C	- C	* N	* O	- X	
AA		C	- C	* N	* S	- S	
AA		C	- C	- N	* S	* S	
AA		C	- C	* N	* S	- X	
AA		C	- C	* O	* O	- O	
AA		C	- C	* O	* O	- S	
AA		C	- C	* O	- O	* S	
AA		C	- C	* O	* O	- X	
AA		C	- C	* O	* S	- S	
AA		C	- C	- O	* S	* S	
AA		C	- C	* O	* S	- X	
AA		C	- C	* S	* S	- S	
AA		C	- C	* S	* S	- X	
AA		C	* N	* N	- N	- N	
AA		C	* N	* N	- N	- O	
AA		C	* N	- N	- N	* O	
AA		C	* N	* N	- N	- S	
AA		C	* N	- N	- N	* S	
AA		C	* N	* N	- N	- X	
AA		C	* N	* N	- O	- O	
AA		C	* N	- N	* O	- O	
AA		C	- N	- N	* O	* O	
AA		C	* N	* N	- O	- S	
AA		C	* N	- N	* O	- S	
AA		C	* N	- N	- O	* S	
AA		C	- N	- N	* O	* S	
AA		C	* N	* N	- O	- X	
AA		C	* N	- N	* O	- X	
AA		C	* N	* N	- S	- S	
AA		C	* N	- N	* S	- S	

Screen Number Order									
Screen Number		Fragment Definition						Frequency Percent	
1200	AA		C	- N	- N	* S	* S	0.05	(continued)
	AA		C	* N	* N	- S	- X		
	AA		C	* N	- N	* S	- X		
	AA		C	* N	* N	- X	- X		
	AA		C	* N	* O	- O	- O		
	AA		C	* N	* O	- O	- S		
	AA		C	* N	- O	- O	* S		
	AA		C	* N	* O	- O	- X		
	AA		C	- N	* O	* O	- X		
	AA		C	* N	* O	- S	- S		
	AA		C	* N	- O	* S	- S		
	AA		C	* N	* O	- S	- X		
	AA		C	* N	- O	* S	- X		
	AA		C	- N	* O	* S	- X		
	AA		C	* N	* O	- X	- X		
	AA		C	* N	* S	- S	- S		
	AA		C	* N	* S	- S	- X		
	AA		C	- N	* S	* S	- X		
	AA		C	* N	* S	- X	- X		
	AA		C	* O	* O	- O	- O		
	AA		C	* O	* O	- O	- S		
	AA		C	* O	- O	- O	* S		
	AA		C	* O	* O	- O	- X		
	AA		C	* O	* O	- S	- S		
	AA		C	* O	- O	* S	- S		
	AA		C	- O	- O	* S	* S		
	AA		C	* O	* O	- S	- X		
	AA		C	* O	- O	* S	- X		
	AA		C	* O	* O	- X	- X		
	AA		C	* O	* S	- S	- S		
	AA		C	- O	* S	* S	- S		
	AA		C	* O	* S	- S	- X		
	AA		C	- O	* S	* S	- X		
	AA		C	* O	* S	- X	- X		
	AA		C	* S	* S	- S	- S		
	AA		C	* S	* S	- S	- X		
AA		C	* S	* S	- X	- X			
1201	AA		C	* C	- I			0.76	
1202	AA	2	C	* C	- I			0.16	
1203	AA		C	* C	- N			32.73	
1204	AA	2	C	* C	- N			13.07	
1205	AA	3	C	* C	- N			4.45	
1206	AA	5	C	* C	- N			0.92	
1207	AA	7	C	* C	- N			0.38	
1208	AA		C	*1C	*1N			27.22	
1209	AA	2	C	*1C	*1N			20.48	

Screen Number Order						Frequency Percent
Screen Number	Fragment Definition					
1210	HA		C	H2*1C	*1N	16.15
1211	HA	2	C	H2*1C	*1N	11.14
1212	AA		C	*1C	*2N	6.60
1213	AA	2	C	*1C	*2N	1.69
1214	HA		C	H *1C	*2N	14.42
	HA		C	H *2C	*1N	
	HA		C	H *4C	*4N	
1215	AA		C	*1C	*4N	4.72
1216	AA		C	*1C	-1N	8.08
1217	AA		C	*1C	-2N	1.15
1218	AA		C	*1C	-4N	0.66
1219	AA		C	*2C	*1N	14.18
1220	AA	2	C	*2C	*1N	5.96
1221	AA		C	*2C	-1N	2.66
1222	AA		C	*4C	*1N	11.39
1223	AA		C	*4C	*4N	13.12
1224	AA	3	C	*4C	*4N	3.41
1225	AA		C	*4C	-1N	24.08
1226	AA		C	*4C	-4N	1.99
1227	AA		C	- C	* N	24.24
1228	AA	2	C	- C	* N	9.01
1229	AA	3	C	- C	* N	2.39
1230	AA		C	-1C	*1N	16.13
1231	AA		C	-1C	*2N	7.86
1232	AA		C	-1C	*4N	5.34
1233	AA		C	-1C	-1N	35.46
1234	AA	2	C	-1C	-1N	18.10
1235	HA		C	H2-1C	-1N	26.67
1236	HA	2	C	H2-1C	-1N	11.86

Screen Number Order						
Screen Number	Fragment Definition					Frequency Percent
1237	HA	3	C	H2-1C	-1N	4.79
1238	HA	4	C	H2-1C	-1N	2.51
1239	HA	5	C	H2-1C	-1N	1.08
1240	AA		C	-1C	-2N	4.59
1241	HA		C	H -1C	-2N	2.80
1242	AA		C	-1C	-4N	20.28
1243	AA		C	-1C	-3N	4.12
1244	AA		C	-2C	*1N	0.78
1245	AA		C	-2C	-1N	1.05
1246	HA		C	H -2C	-1N	0.53
1247	AA		C	* C	* N * N	3.51
1248	AA	2	C	* C	* N * N	0.68
1249	AA		C	* C	* N - N	4.43
1250	AA		C	*1C	*1N *1N	0.15
1251	HA		C	H *1C	*1N *1N	1.12
	HA		C	H *1C	*1N *1O	
	HA		C	H *1C	*1N *1S	
	HA		C	H *1C	*1O *1O	
	HA		C	H *1C	*1O *1S	
	HA		C	H *1C	*1S *1S	
	HA		C	H *1N	*1N *1N	
	HA		C	H *1N	*1N *1O	
	HA		C	H *1N	*1N *1S	
	HA		C	H *1N	*1O *1O	
	HA		C	H *1N	*1O *1S	
	HA		C	H *1N	*1S *1S	
	HA		C	H *1O	*1O *1O	
	HA		C	H *1O	*1O *1S	
	HA		C	H *1O	*1S *1S	
	HA		C	H *1S	*1S *1S	
1252	AA		C	*1C	*1N *2N	3.36
	AA		C	*1C	*4N *4N	
	AA		C	*2C	*1N *1N	
	AA		C	*4C	*1N *4N	
	AA		C	*4C	*4N *4N	
1253	AA		C	*1C	*1N -1N	0.45
	AA		C	*1C	*1N -1O	
	AA		C	*1C	*1N -1S	

Screen Number Order					
Screen Number			Fragment Definition		Frequency Percent
1254	HA		C H *1C	*1N -1N	1.20
	HA		C H *1C	-1N *1O	
	HA		C H *1C	-1N *1S	
	HA		C H *1N	*1N -1N	
	HA		C H *1N	-1N *1O	
	HA		C H *1N	-1N *1S	
	HA		C H -1N	*1O *1O	
	HA		C H -1N	*1O *1S	
	HA		C H -1N	*1S *1S	
1255	AA		C *1C	*1N -2N	4.33
	AA		C *1C	*2N -1N	
	AA		C *1C	*4N -4N	
	AA		C *2C	*1N -1N	
	AA		C *4C	*4N -1N	
	AA		C *4C	*4N -4N	
1256	AA		C - C	* N * N	4.52
1257	AA		C - C	- N - N	0.76
1258	AA		C -1C	*1N *1N	0.25
1259	HA		C H -1C	*1N *1N	0.85
	HA		C H -1C	*1N *1O	
	HA		C H -1C	*1N *1S	
	HA		C H -1C	*1O *1O	
	HA		C H -1C	*1O *1S	
	HA		C H -1C	*1S *1S	
1260	HA		C H -1C	-1N -1N	0.96
	HA		C H -1C	-1N -1O	
	HA		C H -1C	-1N -1S	
	HA		C H -1C	-1O -1O	
	HA		C H -1C	-1O -1S	
	HA		C H -1C	-1S -1S	
1261	AA		C -1C	-1N -2N	0.63
	AA		C -1C	-4N -4N	
	AA		C -2C	-1N -1N	
1262	AA		C * C	* N * O	0.53
1263	AA		C * C	* N - O	12.82
1264	AA	2	C * C	* N - O	3.42
1265	AA		C * C	- N * O	1.51
1266	AA		C - C	* N * O	1.53
1267	AA		C - C	- N - O	24.08
1268	AA	2	C - C	- N - O	8.22

		Screen Number Order				
Screen Number				Fragment Definition		Frequency Percent
1269	AA		C	* C	* N   * S	1.27
1270	AA		C	* C	* N   - S	0.84
1271	AA		C	* C	- N   * S	0.68
1272	AA		C	- C	* N   * S	1.39
1273	AA		C	- C	- N   - S	0.29
1274	HA		C H	*1C	*1N   -1O	2.43
	HA		C H	*1C	*1N   -1S	
	HA		C H	*1C	*1O   -1O	
	HA		C H	*1C	*1O   -1S	
	HA		C H	*1C	-1O   *1S	
	HA		C H	*1C	*1S   -1S	
	HA		C H	*1N	*1N   -1O	
	HA		C H	*1N	*1N   -1S	
	HA		C H	*1N	*1O   -1O	
	HA		C H	*1N	*1O   -1S	
	HA		C H	*1N	-1O   *1S	
	HA		C H	*1N	*1S   -1S	
	HA		C H	*1O	*1O   -1O	
	HA		C H	*1O	*1O   -1S	
	HA		C H	*1O	-1O   *1S	
	HA		C H	*1O	*1S   -1S	
	HA		C H	-1O	*1S   *1S	
	HA		C H	*1S	*1S   -1S	
1275	AA		C	* C	- O	45.33
1276	AA	2	C	* C	- O	23.50
1277	AA		C	*1C	*1O	14.92
1278	AA	2	C	*1C	*1O	11.83
1279	AA		C	*1C	-1O	10.84
1280	AA	2	C	*1C	-1O	4.74
1281	AA	3	C	*1C	-1O	2.71
1282	AA	4	C	*1C	-1O	1.93
1283	AA		C	*1C	-2O	16.45
1284	AA		C	*1C	-4O	2.70
1285	AA		C	*2C	*1O	3.96
1286	AA		C	*2C	-1O	1.67
1287	AA		C	*4C	*1O	5.34

Screen Number Order						
Screen Number	Fragment Definition					Frequency Percent
1288	AA	2	C	*4C	*10	2.39
1289	AA	3	C	*4C	*10	0.48
1290	AA		C	*4C	-10	25.19
1291	AA	2	C	*4C	-10	10.71
1292	AA	3	C	*4C	-10	3.45
1293	AA	4	C	*4C	-10	1.58
1294	AA		C	*4C	-40	1.10
1295	AA		C	-1C	*10	11.58
1296	AA		C	-1C	-10	40.88
1297	HA		C	H2-1C	-10	28.13
1298	HA	2	C	H2-1C	-10	10.61
1299	HA	3	C	H2-1C	-10	4.00
1300	HA	4	C	H2-1C	-10	2.34
1301	HA	5	C	H2-1C	-10	1.26
1302	AA		C	-1C	-20	28.91
1303	AA	2	C	-1C	-20	8.29
1304	HA		C	H -1C	-20	1.12
1305	HA	2	C	H -1C	-20	0.08
1306	AA		C	-1C	-40	26.47
1307	AA		C	-2C	*10	0.20
1308	AA		C	-2C	-10	0.80
1309	AA		C	* C	* O * O	0.90
1310	AA		C	* C	* O - O	5.39
1311	AA		C	- C	* O * O	1.47
1312	AA		C	- C	- O - O	28.04
1313	AA	2	C	- C	- O - O	8.84
1314	AA		C	C	O S	0.64
1315	AA		C	- C	- P	1.30

Screen Number Order						
Screen Number	Fragment Definition					Frequency Percent
1316	AA		C	-2C	-1P	0.11
1317	AA		C	* C	- S	8.93
1318	AA	2	C	* C	- S	2.23
1319	AA	3	C	* C	- S	0.54
1320	AA		C	*1C	*1S	4.10
1321	AA	2	C	*1C	*1S	1.72
1322	AA		C	*1C	-1S	1.16
1323	AA		C	*1C	-2S	1.03
	AA		C	*1C	-4S	
	AA		C	*2C	-1S	
	AA		C	*4C	-4S	
1324	AA		C	*2C	*1S	5.45
1325	AA		C	*4C	*1S	2.38
1326	AA	2	C	*4C	*1S	0.58
1327	AA		C	*4C	-1S	7.63
1328	AA		C	-1C	*1S	4.50
1329	AA		C	-1C	-1S	7.34
1330	AA	2	C	-1C	-1S	1.98
1331	AA	3	C	-1C	-1S	0.43
1332	HA		C	H2-1C	-1S	6.20
1333	AA		C	-1C	-2S	0.25
	AA		C	-1C	-4S	
1334	HA		C	H -1C	-2S	0.00
1335	AA		C	-2C	*1S	0.91
1336	AA		C	-2C	-1S	0.40
1337	AA		C	C	S S	0.74
1338	HA		C	H2*1C	*1O	8.20
	HA		C	H2*1C	*1S	
1339	HA	2	C	H2*1C	*1O	3.90
	HA	2	C	H2*1C	*1S	



Screen Number		Screen Number Order				Fragment Definition		Frequency Percent	
1340	HA		C H	*2C		*1O		4.19	
	HA		C H	*2C		*1S			
1341	HA	2	C H	*2C		*1O		0.63	
	HA	2	C H	*2C		*1S			
1342	HA		C H	-2C		-1O		0.59	
	HA		C H	-2C		-1S			
1343	HA		C H	*1C		*1O	*1O	0.36	
	HA		C H	*1C		*1O	*1S		
	HA		C H	*1C		*1S	*1S		
1344	AA		C	- As		* C		2.97	
	AA		C	- B		* C			
	AA		C	* C		- P			
	AA		C	* C		- Se			
	AA		C	* C		- Si			
	AA		C	* C		- Te			
1345	AA		C	-1As		*1C		0.47	
	AA		C	-1As		*2C			
	AA		C	-1B		*1C			
	AA		C	-1B		*2C			
	AA		C	*1C		-1P			
	AA		C	*2C		-1P			
	AA		C	*1C		-1Se			
	AA		C	*2C		-1Se			
	AA		C	*1C		-1Si			
	AA		C	*2C		-1Si			
	AA		C	*1C		-1Te			
	AA		C	*2C		-1Te			
1346	AA		C	-1As		*4C		2.63	
	AA		C	-1B		*4C			
	AA		C	*4C		-1P			
	AA		C	*4C		-1Se			
	AA		C	*4C		-1Si			
	AA		C	*4C		-1Te			
1347	AA		C		C1			14.11	
	AA		C1		C				
1348	AA	2	C		C1			4.63	
1349	AA	3	C		C1			1.04	
1350	AA		C		C1	C1		0.77	
1351	AA		C		C1	C1	C1	0.35	
1352	AA		C	- C1		* N		0.85	
1353	AA		C		F			10.12	
	AA		F		C				

Screen Number Order								
Screen Number	Fragment Definition						Frequency Percent	
1354	AA	2	C	F			3.32	
1355	AA	3	C	F			1.39	
1356	AA		C	F	F		5.18	
1357	AA		C	F	F	F	4.49	
1358	AA	2	C	F	F	F	0.88	
1359	AA		C	- F	* N		0.11	
1360	AA		C	X			26.42	
	AA		X	C				
1361	AA		C	X	X		6.02	
1362	AA	2	C	X	X		1.63	
1363	HA		C	H2-2N			1.18	
	HA		C	H2-1N	-1N			
	HA		C	H2-1N	-1O			
	HA		C	H2-1N	-1S			
	HA		C	H2-1N	-1X			
	HA		C	H2-2O				
	HA		C	H2-1O	-1O			
	HA		C	H2-1O	-1S			
	HA		C	H2-1O	-1X			
	HA		C	H2-2S				
	HA		C	H2-1S	-1S			
	HA		C	H2-1S	-1X			
	HA		C	H2-1X	-1X			
1364	AA		C	X	X	X	4.93	
1365	AA		C	N	N	N	N	0.59
	AA		C	N	N	N	O	
	AA		C	N	N	N	S	
	AA		C	N	N	N	X	
	AA		C	N	N	O	O	
	AA		C	N	N	O	X	
	AA		C	N	N	S	S	
	AA		C	N	N	S	X	
	AA		C	N	N	X	X	
	AA		C	N	N	O	S	
	AA		C	N	O	O	O	
	AA		C	N	O	O	S	
	AA		C	N	O	O	X	
	AA		C	N	O	S	S	
	AA		C	N	O	S	X	
	AA		C	N	O	X	X	
	AA		C	N	S	S	S	
	AA		C	N	S	S	X	
	AA		C	N	S	X	X	
	AA		C	N	X	X	X	

Screen Number Order								
Screen Number				Fragment Definition			Frequency Percent	
1365	AA	C	O	O	O	O	0.59	(continued)
	AA	C	O	O	O	S		
	AA	C	O	O	O	X		
	AA	C	O	O	S	S		
	AA	C	O	O	S	X		
	AA	C	O	O	X	X		
	AA	C	O	S	S	S		
	AA	C	O	S	S	X		
	AA	C	O	S	X	X		
	AA	C	O	X	X	X		
	AA	C	S	S	S	S		
	AA	C	S	S	S	X		
	AA	C	S	S	X	X		
	AA	C	S	X	X	X		
	AA	C	X	X	X	X		
1366	AA	C	N	X	X		0.99	
	AA	C	O	X	X			
	AA	C	S	X	X			
1367	AA	C	-4N	-4O	-1X		9.76	
	AA	C	-1N	-1N	-2N			
	AA	C	-1N	-4N	-4N			
	AA	C	-4N	-4N	-4N			
	AA	C	-1N	-2N	-1O			
	AA	C	-1N	-4N	-4O			
	AA	C	-4N	-4N	-1O			
	AA	C	-4N	-4N	-4O			
	AA	C	-1N	-1N	-2S			
	AA	C	-1N	-2N	-1S			
	AA	C	-1N	-4N	-4S			
	AA	C	-4N	-4N	-1S			
	AA	C	-4N	-4N	-4S			
	AA	C	-1N	-2N	-1X			
	AA	C	-4N	-4N	-1X			
	AA	C	-1N	-1N	-2O			
	AA	C	-1N	-1O	-2O			
	AA	C	-1N	-4O	-4O			
	AA	C	-2N	-1O	-1O			
	AA	C	-4N	-1O	-4O			
	AA	C	-4N	-4O	-4O			
	AA	C	-1N	-1O	-2S			
	AA	C	-1N	-2O	-1S			
	AA	C	-1N	-4O	-4S			
	AA	C	-2N	-1O	-1S			
	AA	C	-4N	-1O	-4S			
	AA	C	-4N	-4O	-1S			
	AA	C	-4N	-4O	-4S			
	AA	C	-1N	-2O	-1X			
	AA	C	-2N	-1O	-1X			
	AA	C	-1N	-1S	-2S			
	AA	C	-1N	-4S	-4S			
	AA	C	-2N	-1S	-1S			
	AA	C	-4N	-1S	-4S			
	AA	C	-4N	-4S	-4S			

Screen Number Order							
Screen Number	Fragment Definition					Frequency Percent	
1367	AA	C	-1N	-2S	-1X	9.76	(continued)
	AA	C	-2N	-1S	-1X		
	AA	C	-4N	-4S	-1X		
	AA	C	-2N	-1X	-1X		
	AA	C	-1O	-1O	-2O		
	AA	C	-1O	-4O	-4O		
	AA	C	-4O	-4O	-4O		
	AA	C	-1O	-1O	-2S		
	AA	C	-1O	-2O	-1S		
	AA	C	-1O	-4O	-4S		
	AA	C	-4O	-4O	-1S		
	AA	C	-4O	-4O	-4S		
	AA	C	-1O	-2O	-1X		
	AA	C	-4O	-4O	-1X		
	AA	C	-1O	-1S	-2S		
	AA	C	-1O	-4S	-4S		
	AA	C	-2O	-1S	-1S		
	AA	C	-4O	-1S	-4S		
	AA	C	-4O	-4S	-4S		
	AA	C	-1O	-2S	-1X		
	AA	C	-2O	-1S	-1X		
	AA	C	-4O	-4S	-1X		
	AA	C	-2O	-1X	-1X		
	AA	C	-1S	-1S	-2S		
	AA	C	-1S	-4S	-4S		
	AA	C	-4S	-4S	-4S		
	AA	C	-1S	-2S	-1X		
	AA	C	-4S	-4S	-1X		
	AA	C	-2S	-1X	-1X		
	1368	AA	C	N	X		
1369	AA	C	* N	- X		1.09	
1370	AA	2	C	* N	- X	0.18	
1371	AA	3	C	* N	- X	0.02	
1372	AA		C	*1N	-1X	0.25	
1373	AA		C	*2N	-1X	0.14	
1374	AA		C	*4N	-1X	0.75	
1375	AA		C	-1N	-1X	0.14	
1376	AA		C	-2N	-1X	0.06	
1377	HA		C H	-1N	-2N	0.47	
	HA		C H	-4N	-4N		
	HA		C H	-1N	-2O		
	HA		C H	-2N	-1O		
	HA		C H	-4N	-4O		
	HA		C H	-1N	-2S		
	HA		C H	-2N	-1S		

		Screen Number Order					
Screen Number				Fragment Definition		Frequency Percent	
1377	HA		C H	-4N	-4S	0.47	(continued)
	HA		C H	-2N	-1X		
	HA		C H	-1O	-2O		
	HA		C H	-4O	-4O		
	HA		C H	-1O	-2S		
	HA		C H	-2O	-1S		
	HA		C H	-4O	-4S		
	HA		C H	-2O	-1X		
	HA		C H	-1S	-2S		
	HA		C H	-4S	-4S		
	HA		C H	-2S	-1X		
	1378	AA		C	N		
AA			C	N	O X		
AA			C	N	S X		
AA			C	O	O X		
AA			C	O	S X		
AA			C	S	S X		
1379	AA		C	* N	* N - X	0.29	
1380	AA		C	O	X	1.00	
1381	AA		C	P	X	0.08	
1382	AA		C	S	X	0.74	
1383	AA		C	* O	- X	0.37	
	AA		C	* S	- X		
1384	AA		C	-1O	-1X	1.03	
	AA		C	-1S	-1X		
1385	AA		C	-2O	-1X	0.34	
	AA		C	-2S	-1X		
1386	AA		C	I		1.01	
	AA		I	C			
1387	AA	2	C	I		0.19	
1388	AA		C	I	I	0.01	
1389	AA		C	- I	* N	0.02	
1390	AA		C	M		3.55	
	AA		M	C			
1391	AA		As	* M		6.30	
	AA		B	* M			
	AA		C	* M			
	AA		M	* As			
	AA		M	* B			
	AA		M	* C			
	AA		M	* N			

Screen Number Order				Frequency Percent				
Screen Number		Fragment Definition						
1391	AA	M	* O	6.30	(continued)			
	AA	M	* P					
	AA	M	* S					
	AA	M	* Se					
	AA	M	* Si					
	AA	M	* Te					
	AA	M	* X					
	AA	N	* M					
	AA	O	* M					
	AA	P	* M					
	AA	S	* M					
	AA	Se	* M					
	AA	Si	* M					
	AA	Te	* M					
	AA	X	* M					
	1392	AA	As			- M	6.25	
		AA	B			- M		
AA		C	- M					
AA		M	- As					
AA		M	- B					
AA		M	- C					
AA		M	- N					
AA		M	- O					
AA		M	- P					
AA		M	- S					
AA		M	- Se					
AA		M	- Si					
AA		M	- Te					
AA		M	- X					
AA		N	- M					
AA		O	- M					
AA		P	- M					
AA		S	- M					
AA		Se	- M					
AA		Si	- M					
AA		Te	- M					
AA		X	- M					
1393	AA	C	* N	49.27				
	AA	N	* C					
1394	AA	C	*1N	40.50				
	AA	N	*1C					
1395	AA	C	*2N	14.45				
	AA	N	*2C					
1396	AA	C	*4N	20.41				
	AA	N	*4C					
1397	AA	C	-1N	58.10				
	AA	N	-1C					
1398	HA	C	H3-1N	10.55				

Screen Number Order						Frequency Percent
Screen Number	Fragment Definition					
1399	HA	2	C	H3-1N		4.78
1400	HA	3	C	H3-1N		1.35
1401	HA	4	C	H3-1N		0.74
1402	AA		C	-2N		6.98
1402	AA		N	-2C		
1403	AA		C	-4N		27.74
	AA		N	-4C		
1404	AA		C	-3N		4.65
	AA		N	-3C		
1405	AA	2	C	-3N		0.94
1406	AA		C	* N	* N	15.53
1407	AA	2	C	* N	* N	5.53
1408	AA	3	C	* N	* N	2.43
1409	AA		C	* N	- N	8.70
1410	AA	2	C	* N	- N	1.83
1411	AA	3	C	* N	- N	0.54
1412	AA		C	*1N	*1N	2.53
1413	HA		C	H2*1N	*1N	0.31
	HA		C	H2*1N	*1O	
	HA		C	H2*1N	*1S	
1414	AA		C	*1N	*2N	6.52
1415	HA		C	H *1N	*2N	3.87
	HA		C	H *4N	*4N	
	HA		C	H *2N	*1O	
	HA		C	H *2N	*1S	
1416	AA		C	*1N	*4N	3.07
1417	AA		C	*1N	-1N	1.07
1418	AA		C	*1N	-2N	0.86
1419	AA		C	*1N	-4N	0.32
1420	AA		C	*2N	-1N	0.82
1421	AA		C	*4N	*4N	6.90
1422	AA		C	*4N	-1N	1.30

Screen Number Order						
Screen Number	Fragment Definition					Frequency Percent
1423	AA		C	* 4N	- 4N	5.40
1424	AA		C	- N	- N	6.63
1425	AA	2	C	- N	- N	1.16
1426	AA	3	C	- N	- N	0.31
1427	AA		C	-1N	-1N	0.60
1428	AA		C	-1N	-2N	0.29
1429	AA		C	-1N	-4N	1.22
1430	AA		C	-1N	-3N	0.14
1431	AA		C	-2N	-2N	0.02
1432	AA		C	-4N	-4N	4.68
1433	AA		C	N	N N	5.10
1434	AA	2	C	N	N N	1.41
1435	AA	3	C	N	N N	0.56
1436	AA		C	* N	* N * N	0.88
	AA		C	* N	* N * O	
	AA		C	* N	* N * S	
	AA		C	* N	* O * O	
	AA		C	* N	* O * S	
	AA		C	* N	* S * S	
	AA		C	* O	* O * O	
	AA		C	* O	* O * S	
	AA		C	* O	* S * S	
	AA		C	* S	* S * S	
1437	AA		C	* N	* N - N	2.57
1438	AA		C	- N	- N - N	2.24
1439	AA		C	-1N	-1N -1N	0.04
	AA		C	-1N	-1N -1O	
	AA		C	-1N	-1N -1S	
	AA		C	-1N	-1O -1O	
	AA		C	-1N	-1O -1S	
	AA		C	-1N	-1S -1S	
	AA		C	-1O	-1O -1O	
	AA		C	-1O	-1O -1S	
	AA		C	-1O	-1S -1S	
	AA		C	-1S	-1S -1S	
1440	AA		C	* N	* N - O	2.77
1441	AA	2	C	* N	* N - O	0.47



Screen Number		Screen Number Order				Fragment Definition		Frequency Percent
1442	AA		C	* N	- N	* O		0.15
1443	AA		C	- N	- N	- O		2.24
1444	AA	2	C	- N	- N	- O		0.14
1445	AA		C	* N	* N	- S		1.97
1446	AA	2	C	* N	* N	- S		0.07
1447	AA		C	* N	- N	* S		2.29
1448	AA	2	C	* N	- N	* S		0.12
1449	AA		C	- N	- N	- S		1.12
1450	AA	2	C	- N	- N	- S		0.08
1451	AA		C	-1N	-1N	-2O		0.21
	AA		C	-1N	-1N	-2S		
1452	AA		C	-1N	-2N	-1O		0.18
	AA		C	-4N	-4N	-1O		
	AA		C	-1N	-2N	-1S		
	AA		C	-4N	-4N	-1S		
1453	AA		C	-1N	-4N	-4O		1.09
	AA		C	-1N	-4N	-4S		
1454	AA		C	-4N	-4N	-4O		1.91
	AA		C	-4N	-4N	-4S		
1455	AA		C	* N	* O			2.73
1456	AA	2	C	* N	* O			0.63
1457	AA		C	* N	- O			14.41
1458	AA	2	C	* N	- O			5.00
1459	AA	3	C	* N	- O			1.38
1460	AA		C	*1N	*1O			0.99
1461	AA		C	*1N	-1O			0.63
1462	AA		C	*1N	-2O			9.29
1463	AA		C	*1N	-4O			1.16
1464	AA		C	*2N	*1O			1.38
1465	AA		C	*2N	-1O			0.30
1466	AA		C	*4N	*1O			0.25

Screen Number Order						
Screen Number	Fragment Definition					Frequency Percent
1467	AA		C	*4N	-1O	0.95
1468	AA		C	*4N	-4O	4.42
1469	AA		C	- N	* O	1.68
1470	AA		C	- N	- O	28.84
1471	AA	2	C	- N	- O	10.44
1472	AA	3	C	- N	- O	4.87
1473	AA	4	C	- N	- O	3.68
1474	AA		C	-1N	-1O	1.75
1475	AA		C	-1N	-2O	8.11
1476	AA		C	-2N	-1O	0.13
1477	AA		C	-2N	-2O	0.39
1478	AA		C	-4N	-4O	23.05
1479	AA		C	N	O O	4.22
1480	AA	2	C	N	O O	0.55
1481	AA		C	* N	* O - O	0.46
1482	AA		C	- N	- O - O	3.78
1483	AA		C	N	O S	0.54
1484	AA		C	N	P	0.29
1485	AA		C	* N	* S	5.70
1486	AA	2	C	* N	* S	1.19
1487	AA		C	* N	- S	3.57
1488	AA	2	C	* N	- S	0.25
1489	AA		C	*1N	*1S	2.72
1490	AA		C	*2N	*1S	2.26
1491	AA		C	*4N	*1S	1.62
1492	AA		C	- N	- S	2.05
1493	AA	2	C	- N	- S	0.27
1494	AA		C	-1N	-1S	0.29

		Screen Number Order					
Screen Number				Fragment Definition			Frequency Percent
1495	AA	C	-1N	-2S			0.18
1496	AA	C	-2N	-1S			0.11
1497	AA	C	-2N	-2S			0.16
1498	AA	C	-4N	-4S			1.15
1499	AA	C	N	S	S		0.92
1500	AA	C	-1N	*1O			2.47
	AA	C	-1N	*1S			
1501	AA	C	-2N	*1O			1.94
	AA	C	-4N	*1O			
	AA	C	-2N	*1S			
	AA	C	-4N	*1S			
1502	AA	C	-3N	-1O			0.12
	AA	C	-3N	-1S			
1503	AA	C	-1N	-1O	-2O		3.82
	AA	C	-4N	-1O	-4O		
	AA	C	-1N	-1O	-2S		
	AA	C	-1N	-2O	-1S		
	AA	C	-4N	-1O	-4S		
	AA	C	-4N	-4O	-1S		
	AA	C	-1N	-1S	-2S		
	AA	C	-4N	-1S	-4S		
1504	AA	C	- N	* O	* O	- O	0.00
	AA	C	- N	* O	* O	- S	
	AA	C	- N	* O	- O	* S	
	AA	C	- N	* O	* S	- S	
	AA	C	- N	- O	* S	* S	
	AA	C	- N	* S	* S	- S	
1505	AA	C	* O				20.22
	AA	O	* C				
1506	HA	C	H3-1O				17.33
1507	HA	2	C	H3-1O			5.70
1508	HA	3	C	H3-1O			1.69
1509	HA	4	C	H3-1O			0.67
1510	AA	C	-2O				41.18
	AA	O	-2C				
1511	AA	C	-4O				31.52
	AA	O	-4C				
1512	AA	C	* O	* O			2.94

Screen Number Order						
Screen Number	Fragment Definition					Frequency Percent
1513	AA	2	C	* O	* O	0.67
1514	AA		C	* O	- O	5.68
1515	AA	2	C	* O	- O	1.92
1516	AA		C	*10	-10	2.36
1517	AA		C	*10	-20	3.54
1518	AA		C	- O	- O	29.91
1519	AA	2	C	- O	- O	10.19
1520	AA	3	C	- O	- O	3.17
1521	AA	4	C	- O	- O	1.56
1522	AA		C	-10	-10	1.52
1523	AA		C	-10	-20	18.25
1524	AA	2	C	-10	-20	4.97
1525	AA		C	-10	-40	2.49
1526	AA		C	-40	-40	11.09
1527	AA	2	C	-40	-40	3.39
1528	AA		C	O	P	0.20
1529	AA		C	* O	* S	0.08
1530	AA		C	* O	- S	0.29
1531	AA		C	- O	* S	0.37
1532	AA		C	- O	- S	0.55
1533	AA		C	- P		2.98
	AA		P	- C		
1534	AA		C	-2P		0.07
	AA		C	-3P		
	AA		C	-4P		
	AA		P	-2C		
	AA		P	-3C		
	AA		P	-4C		
1535	AA		C	P	P	0.19
1536	AA		C	P	S	0.04

Screen Number		Screen Number Order				Fragment Definition		Frequency Percent	
1537	AA		C	*	S			10.23	
	AA		S	*	C				
1538	AA		C	-	S			17.07	
	AA		S	-	C				
1539	AA		C	-1	S			14.89	
	AA		S	-1	C				
1540	HA		C	H3-1	S			2.72	
1541	HA	2	C	H3-1	S			0.39	
1542	AA		C	-2	S			2.60	
	AA		C	-4	S				
	AA		S	-2	C				
	AA		S	-4	C				
1543	AA		C	*	S	*	S	0.47	
1544	AA		C	*	S	-	S	0.96	
1545	AA		C	-	S	-	S	0.38	
1546	AA	2	C		Si			2.69	
1547	AA	3	C		Si			2.51	
1548	AA	4	C		Si			1.43	
1549	AA		C	-	Si			2.84	
	AA		Si	-	C				
1550	HA		C	H2*10		*10		0.80	
	HA		C	H2*10		*1S			
	HA		C	H2*1S		*1S			
1551	AA		C		O	O	O	0.63	
	AA		C		O	O	S		
	AA		C		O	S	S		
	AA		C		S	S	S		
1552	AA		As	*	C			1.15	
	AA		B	*	C				
	AA		C	*	As				
	AA		C	*	B				
	AA		C	*	P				
	AA		C	*	Se				
	AA		C	*	Si				
	AA		C	*	Te				
	AA		P	*	C				
	AA		Se	*	C				
	AA		Si	*	C				
	AA		Te	*	C				

Screen Number Order					Frequency Percent
Screen Number	Fragment Definition				
1553	AA	Cl	P		0.13
	AA	P	Cl		
1554	AA	Cl	S		0.08
	AA	S	Cl		
1555	AA	F	P		0.27
	AA	P	F		
1556	AA	F	S		0.06
	AA	S	F		
1557	AA	X	X		0.06
1558	AA	As	M		3.13
	AA	B	M		
	AA	M	As		
	AA	M	B		
	AA	M	P		
	AA	M	Se		
	AA	M	Si		
	AA	M	Te		
	AA	M	X		
	AA	P	M		
	AA	Se	M		
	AA	Si	M		
	AA	Te	M		
	AA	X	M		
1559	AA	N	X		0.06
	AA	X	N		
1560	AA	O	X		0.51
	AA	X	O		
1561	AA	P	X		0.42
	AA	X	P		
1562	AA	S	X		0.14
	AA	X	S		
1563	AA	M	N		4.05
	AA	N	M		
1564	AA	M	O		4.03
	AA	M	S		
	AA	O	M		
	AA	S	M		
1565	AA	4	N	* C	8.42
1566	AA	5	N	* C	3.53
1567	AA	6	N	* C	2.31

Screen Number Order					
Screen Number	Fragment Definition				Frequency Percent
1568	HA		N H2-1C		7.57
1569	HA	2	N H2-1C		2.12
1570	HA	3	N H2-1C		0.62
1571	HA		N H -2C		0.34
1572	HA		N H -2As		0.36
	HA		N H -2B		
	HA		N H -2C		
	HA		N H -2N		
	HA		N H -2O		
	HA		N H -2P		
	HA		N H -2S		
	HA		N H -2Se		
	HA		N H -2Si		
	HA		N H -2Te		
1573	AA		N	* C * C	43.08
1574	AA	2	N	* C * C	23.90
1575	AA	3	N	* C * C	10.35
1576	AA	4	N	* C * C	5.64
1577	AA		N	* C - C	26.04
1578	AA	2	N	* C - C	7.82
1579	AA	3	N	* C - C	1.99
1580	AA		N	*1C *1C	30.13
1581	AA	2	N	*1C *1C	10.29
1582	AA	3	N	*1C *1C	2.86
1583	HA		N H	*1C *1C	4.55
1584	HA	2	N H	*1C *1C	0.72
1585	AA		N	*1C *2C	8.37
1586	AA	2	N	*1C *2C	1.31
1587	AA		N	*2C -1C	0.65
1588	AA		N	*4C *4C	14.32
1589	AA	2	N	*4C *4C	6.63
1590	AA	3	N	*4C *4C	2.11

Screen Number		Screen Number Order					Frequency Percent	
Screen Number				Fragment Definition				
1591	AA		N	*4C	-1C			0.87
1592	AA		N	- C	- C			35.21
1593	AA	2	N	- C	- C			13.94
1594	AA	3	N	- C	- C			5.73
1595	AA		N	-1C	-1C			14.72
1596	AA	2	N	-1C	-1C			2.46
1597	HA		N H	-1C	-1C			4.20
1598	HA	2	N H	-1C	-1C			0.48
1599	AA		N	-1C	-2C			2.33
1600	AA		N	-1C	-4C			21.05
1601	AA		N	-4C	-4C			1.92
1602	AA		N	C	C	C		31.96
1603	AA	2	N	C	C	C		10.54
1604	AA	3	N	C	C	C		2.71
1605	AA		N	* C	* C	* C		3.71
1606	AA	2	N	* C	* C	* C		0.51
1607	AA		N	* C	* C	- C		22.55
1608	AA		N	*1C	*1C	-1C		21.59
1609	AA		N	- C	- C	- C		8.91
1610	AA	2	N	- C	- C	- C		1.24
1611	AA		N	C	C	C	C	1.17
1612	AA	2	N	C	C	C	C	0.16
1613	AA		N	* C	* C	* C	* C	0.35
	AA		N	* C	* C	* C	- C	
	AA		N	* C	* C	- C	- C	
1614	AA		N	- C	- C	- C	- C	0.83
1615	AA		N	C	C	C	N	0.08
	AA		N	C	C	C	O	
	AA		N	C	C	C	S	
1616	AA		N	C	C	N		5.31



Screen Number		Screen Number Order				Fragment Definition		Frequency Percent	
1617	AA		N	* C	* C	* N		0.97	
	AA		N	* C	* C	* O			
	AA		N	* C	* C	* S			
1618	AA		N	- C	- C	- N		0.41	
1619	AA		N	C	C	O		0.98	
1620	AA		N	* C	* C	- O		0.53	
1621	AA		N	- C	- C	- O		0.27	
1622	AA		N	C	C	P		0.32	
1623	AA		N	C	C	S		2.00	
1624	AA		N	- C	- C	- S		0.90	
1625	AA		N	* C	- N			0.76	
1626	AA		N	*1C	*1N			5.00	
1627	HA		N H	*1C	*1N			0.67	
	HA		N H	*1C	*1O				
	HA		N H	*1C	*1S				
1628	AA		N	*2C	*1N			5.47	
1629	AA	2	N	*2C	*1N			1.61	
1630	AA		N	- C	* N			3.78	
1631	AA	2	N	- C	* N			0.54	
1632	AA		N	-1C	-1N			1.19	
1633	HA		N H	-1C	-1N			0.77	
1634	AA		N	-2C	-1N			2.84	
1635	AA		N	-4C	-1N			2.74	
1636	AA		N	* C	* O			1.22	
1637	AA		N	* C	- O			0.71	
1638	AA		N	*4C	-2O			0.19	
1639	AA		N	- C	* O			0.15	
1640	AA		N	- C	- O			6.80	
1641	AA		N	-1C	-1O			0.30	
1642	AA		N	-1C	-2O			5.21	

Screen Number Order					
Screen Number				Fragment Definition	Frequency Percent
1643	AA		N	-2C -1O	1.03
1644	AA		N	C P	0.62
1645	AA		N	C S	4.46
1646	AA		N	* C - S	0.98
1647	AA		N	- C * S	0.19
1648	AA		N	- C - S	3.03
1649	AA		N	-1C -1S	0.97
1650	AA		N	-1C -4S	1.46
1651	AA		N	-4C -4S	0.57
1652	HA		N H	-1C -1O	0.08
	HA		N H	-1C -1S	
1653	AA		N	- As * N	0.13
	AA		N	- B * N	
	AA		N	* N - N	
	AA		N	* N - O	
	AA		N	* N - P	
	AA		N	* N - S	
	AA		N	* N - Se	
	AA		N	* N - Si	
	AA		N	* N - Te	
	AA		N	* N - X	
1654	AA		N	As P	0.20
	AA		N	B P	
	AA		N	N P	
	AA		N	O P	
	AA		N	P P	
	AA		N	P S	
	AA		N	P Se	
	AA		N	P Si	
	AA		N	P Te	
1655	AA		N	N	13.07
1656	AA	3	N	N	3.57
1657	AA	5	N	N	0.66
1658	AA	7	N	N	0.24
1659	AA		N	*1N	6.78
1660	AA		N	*2N	0.99

Screen Number		Screen Number Order			Fragment Definition	Frequency Percent
1661	AA		N		*4N	0.64
1662	AA		N		- N	6.18
1663	AA		N		-1N	4.36
1664	HA		N		H2-1N	0.41
1665	AA		N		-2N	1.77
1666	AA	3	N		-2N	0.78
1667	AA		As		-4N	2.86
	AA		B		-4N	
	AA		N		-4As	
	AA		N		-4B	
	AA		N		-4N	
	AA		N		-4O	
	AA		N		-4P	
	AA		N		-4S	
	AA		N		-4Se	
	AA		N		-4Si	
	AA		N		-4Te	
	AA		O		-4N	
	AA		P		-4N	
	AA		S		-4N	
	AA		Se		-4N	
	AA		Si		-4N	
	AA		Te		-4N	
1668	AA		N		-3N	0.08
1669	AA		N	*	N * N	1.06
1670	AA		N	-	N - N	0.43
1671	AA		N		N O	0.28
1672	AA		N		N S	0.22
1673	AA	2	N		O	1.99
1674	AA	3	N		O	0.63
1675	AA	5	N		O	0.07
1676	AA		N	*	O	1.31
	AA		O	*	N	
1677	AA		N	-	O	8.04
	AA		O	-	N	
1678	AA		N		-1O	2.25
	AA		O		-1N	

Screen Number		Screen Number Order				Fragment Definition		Frequency Percent	
1679	AA		N	-2O				5.78	
	AA		O	-2N					
1680	AA		N	O	O			5.54	
1681	AA	2	N	O	O			1.28	
1682	AA	3	N	O	O			0.42	
1683	AA	5	N	O	O			0.03	
1684	AA		N	O	O	O		0.29	
1685	AA		N	* P				0.20	
	AA		P	* N					
1686	AA		N	- P				0.60	
	AA		P	- N					
1687	AA		N	-1P				0.36	
	AA		P	-1N					
1688	AA		N	-2P				0.09	
	AA		P	-2N					
1689	AA		N	-4P				0.21	
	AA		P	-4N					
1690	AA	2	N	S				0.62	
1691	AA		N	* S				0.62	
	AA		S	* N					
1692	AA		N	*2S				2.59	
	AA		N	*4S					
	AA		N	-2S					
	AA		N	-4S					
	AA		S	*2N					
	AA		S	*4N					
	AA		S	-2N					
	AA		S	-4N					
1693	AA		N	- S				4.40	
	AA		S	- N					
1694	AA		N	O	S			0.10	
	AA		N	S	S				
1695	AA		N	Si				0.24	
	AA		Si	N					

Screen Number		Screen Number Order				Fragment Definition	Frequency Percent
1696	HA					N H2-1As	0.03
	HA					N H2-1B	
	HA					N H2-1O	
	HA					N H2-1P	
	HA					N H2-1S	
	HA					N H2-1Se	
	HA					N H2-1Si	
	HA					N H2-1Te	
1697	AA	2	O	*	C		8.15
1698	AA	3	O	*	C		3.30
1699	AA	4	O	*	C		2.15
1700	HA		O	H	-1C		20.14
1701	HA	2	O	H	-1C		7.80
1702	HA	3	O	H	-1C		3.33
1703	HA	4	O	H	-1C		1.93
1704	HA	5	O	H	-1C		1.15
1705	HA	6	O	H	-1C		0.81
1706	AA		O	*	C	* C	17.14
1707	AA		O	-	C	- C	38.39
1708	AA	2	O	-	C	- C	17.09
1709	AA	3	O	-	C	- C	6.63
1710	AA	4	O	-	C	- C	3.26
1711	AA		O	*	C	* N	1.07
1712	AA		O	-	C	- N	1.20
1713	AA		O		C	P	2.32
1714	AA	2	O		C	P	1.72
1715	AA	3	O		C	P	0.73
1716	AA		O		C	S	0.97
1717	AA	2	O		C	S	0.15

Screen Number Order					Frequency Percent
Screen Number	Fragment Definition				
1718	AA	O	As	As	0.63
	AA	O	As	B	
	AA	O	As	N	
	AA	O	As	O	
	AA	O	As	P	
	AA	O	As	S	
	AA	O	As	Se	
	AA	O	As	Si	
	AA	O	As	Te	
	AA	O	As	X	
	AA	O	B	B	
	AA	O	B	N	
	AA	O	B	O	
	AA	O	B	P	
	AA	O	B	S	
	AA	O	B	Se	
	AA	O	B	Si	
	AA	O	B	Te	
	AA	O	B	X	
	AA	O	N	N	
	AA	O	N	O	
	AA	O	N	P	
	AA	O	N	S	
	AA	O	N	Se	
	AA	O	N	Si	
	AA	O	N	Te	
	AA	O	N	X	
	AA	O	O	O	
	AA	O	O	P	
	AA	O	O	S	
	AA	O	O	Se	
	AA	O	O	Si	
	AA	O	O	Te	
	AA	O	O	X	
	AA	O	P	P	
	AA	O	P	S	
	AA	O	P	Se	
	AA	O	P	Si	
	AA	O	P	Te	
	AA	O	P	X	
	AA	O	S	S	
	AA	O	S	Se	
	AA	O	S	Si	
	AA	O	S	Te	
	AA	O	S	X	
	AA	O	Se	Se	
	AA	O	Se	Si	
	AA	O	Se	Te	
	AA	O	Se	X	
	AA	O	Si	Si	
	AA	O	Si	Te	
	AA	O	Si	X	
	AA	O	Te	Te	
	AA	O	Te	X	
	AA	O	X	X	

Screen Number		Screen Number Order		Fragment Definition	Frequency Percent
1719	HA			O H -1N	0.80
1720	AA			O O	0.23
1721	AA			O * P	0.36
	AA			P * O	
1722	AA			O -1P	2.22
	AA			P -1O	
1723	AA			O -2P	1.11
	AA			P -2O	
1724	AA			O -4P	1.35
	AA			P -4O	
1725	AA	2		O -4P	1.20
1726	AA	3		O -4P	0.83
1727	AA			O * S	0.09
	AA			S * O	
1728	AA			O -1S	1.03
	AA			S -1O	
1729	AA			O -2S	4.78
	AA			S -2O	
1730	AA			O -4S	4.43
	AA			S -4O	
1731	AA	2		O -4S	4.41
1732	AA	3		O -4S	2.17
1733	AA	2		O Si	0.86
1734	AA			O * Si	0.15
	AA			Si * O	
1735	AA			O - Si	1.82
	AA			Si - O	
1736	HA			O H -1O	0.06
	HA			O H -1S	
1737	HA			O H -1As	0.16
	HA			O H -1B	
	HA			O H -1P	
	HA			O H -1Se	
	HA			O H -1Si	
	HA			O H -1Te	
1738	AA	2		P C	1.26

Screen Number		Screen Number Order						Frequency Percent
		Fragment Definition						
1739	AA		P	C	C			2.11
1740	AA		P	- C	- C			1.95
1741	AA		P	C	C	C		1.75
1742	AA		P	C	C	O		0.37
1743	AA		P	C	N			0.29
1744	AA		P	C	O			1.25
1745	AA		P	C	O	O		0.94
1746	AA		P	C	O	O	O	0.69
1747	AA		P	C	S			0.17
1748	AA		P	C	O	O	O	0.75
	AA		P	C	O	O	S	
	AA		P	C	O	S	S	
	AA		P	C	S	S	S	
1749	AA		P	X	X			0.32
1750	AA	2	P	N				0.18
1751	AA		P	N	N			0.27
1752	AA		P	N	O			0.49
1753	AA		P	N	O	O		0.33
1754	AA		P	N	S			0.13
1755	AA		P	N	O	O	O	0.19
	AA		P	N	O	O	S	
	AA		P	N	O	S	S	
	AA		P	N	S	S	S	
1756	AA	2	P	O				0.77
1757	AA		P	O	O			2.69
1758	AA		P	O	O	O		2.16
1759	AA		P	O	O	O	O	1.06
1760	AA		P	O	S			0.41
1761	AA		P	S				0.53
	AA		S	P				
1762	AA		P	* S				0.06
	AA		S	* P				



Screen Number		Screen Number Order						Fragment Definition		Frequency Percent	
1763	AA		P	-1S						0.22	
	AA		S	-1P							
1764	AA		P	-2S						0.25	
	AA		S	-2P							
1765	AA		P	-4S						0.11	
	AA		S	-4P							
1766	AA		P	S		S				0.18	
1767	AA	2	P	-4O						0.41	
	AA	2	P	-4S							
1768	AA	3	P	-4O						0.23	
	AA	3	P	-4S							
1769	AA		P	O	O	O	O			1.29	
	AA		P	O	O	O	S				
	AA		P	O	O	S	S				
	AA		P	O	S	S	S				
	AA		P	S	S	S	S				
1770	AA	2	S	- C						3.55	
1771	HA		S H	-1C						0.85	
1772	AA		S	* C	* C					9.14	
1773	AA	2	S	* C	* C					1.52	
1774	AA		S	- C	- C					7.80	
1775	AA	2	S	- C	- C					0.91	
1776	AA		S	C	C	N				0.05	
1777	AA		S	C	C	O				1.96	
1778	AA	2	S	C	C	O				0.18	
1779	AA		S	* C	* C	- O				0.35	
1780	AA		S	- C	- C	- O				1.61	
1781	AA		S	* C	* C	- O	- O			0.25	
1782	AA		S	- C	- C	- O	- O			1.23	
1783	AA		S	* C	* N					0.48	
1784	AA		S	- C	- N					4.15	
1785	AA	2	S	- C	- N					0.34	

		Screen Number Order					Frequency Percent
Screen Number			Fragment Definition				
1786	AA		S	C	N	O O	4.19
1787	AA		S	* C	* N	- O - O	0.19
1788	AA		S	- C	- N	- O - O	4.02
1789	AA		S	* C	* O		0.04
1790	AA		S	* C	- O		0.59
1791	AA		S	- C	- O		7.61
1792	AA	2	S	- C	- O		1.22
1793	AA	3	S	- C	- O		0.38
1794	AA		S	* C	- O	- O	0.47
1795	AA		S	- C	- O	- O	7.20
1796	AA		S	C	O	O O	2.09
1797	AA	2	S	C	O	O O	0.65
1798	AA		S	C	P		0.21
1799	AA	2	S	C	P		0.04
1800	AA		S	X	X		0.02
1801	AA	2	S	N			0.47
1802	AA		S	N	N		0.25
1803	AA		S	N	O		4.51
1804	AA	2	S	N	O		0.39
1805	AA	3	S	N	O		0.04
1806	AA		S	* N	- O		0.26
1807	AA		S	N	O	O O	0.09
1808	AA		S	N	P		0.00
1809	AA	2	S	O			1.44
1810	AA	3	S	O			0.45
1811	AA		S	O	O		8.41
1812	AA		S	O	O	O	2.72
1813	AA		S	O	O	O O	0.47

		Screen Number Order				
Screen Number				Fragment Definition		Frequency Percent
1814	AA	S	O	P		0.00
1815	AA	S	* S			0.21
1816	AA	S	- S			0.24
1817	AA AA	Si X	X Si			0.15
1818	AA AA	O S	* C * C	- C - C		0.15
1819	AA AA	O S	C C	C C	C C	0.46
1820	AA 					

Screen Number Order							
Screen Number	Fragment Definition						Frequency Percent
1823	TW		C	*1C	*2C	-1C H3	2.48
1824	TW		C	*4C	*4C	-1C H3	9.55
1825	TW	2	C	*4C	*4C	-1C H3	3.33
1826	TW		C	-1C	-1C	-1C -1O H	0.83
	TW		C	-1C	-1C	-1C -1S H	
1827	TW		C	*1C	*1C	-1N H2	0.63
	TW		C	*1C	*2C	-1N H2	
	TW		C H	*1C	*1C	-1N H2	
1828	TW		C	*4C	*4C	-1N H2	1.65
1829	TW	2	C	*4C	*4C	-1N H2	0.46
1830	TW		C H	-1C	-1C	-1N H2	3.13
1831	TW		C	*1C	*1C	-1O H	5.45
	TW		C	*1C	*1C	-1S H	
	TW		C	*1C	*2C	-1O H	
	TW		C	*1C	*2C	-1S H	
	TW		C H	*1C	*1C	-1O H	
	TW		C H	*1C	*1C	-1S H	
1832	TW		C	*4C	*4C	-1O H	6.53
	TW		C	*4C	*4C	-1S H	
1833	TW	2	C	*4C	*4C	-1O H	1.82
	TW	2	C	*4C	*4C	-1S H	
1834	TW		C H	-1C	-1C	-1O H	5.02
	TW		C H	-1C	-1C	-1S H	
1835	TW		C	H2-1C	-1N H2		2.72
1836	TW		C	H2-1C	-1O H		6.73
	TW		C	H2-1C	-1S H		
1837	TW	2	C	H2-1C	-1O H		2.13
	TW	2	C	H2-1C	-1S H		
1838	RC	1					86.17
1839	RC	2					72.82
1840	RC	3					53.05
1841	RC	4					33.05
1842	RC	5					17.59
1843	RC	6					10.11

Screen Number Order				Frequency Percent
Screen Number			Fragment Definition	
1844	RC	7		6.54
1845	RC	8		5.01
1846	RC	10		3.12
1847	RC	15		1.13
1848	TR		DDD	2.06
1849	TR	2	DDD	0.21
1850	TR		DDT	0.26
1851	TR		DTT	2.46
	TR		TTT	
1852	TR		DDDD	0.97
1853	TR		DDDT	2.17
	TR		DDTT	
	TR		DTDT	
	TR		DTTT	
	TR		TTTT	
1854	TR	2	DDTT	0.04
1855	TR		DDDDD	21.27
1856	TR	2	DDDDD	4.03
1857	TR	3	DDDDD	0.93
1858	TR		DDDDT	1.30
1859	TR		DDDTT	17.81
1860	TR	2	DDDTT	3.68
1861	TR	3	DDDTT	0.68
1862	TR		DDTDT	1.60
1863	TR		DDTTT	2.02
1864	TR		DTDTT	0.62
1865	TR		DTTTT	3.57
1866	TR		TTTTT	1.04
1867	TR		DDDDDD	64.12
1868	TR	2	DDDDDD	36.55

Screen Number Order				Frequency Percent
Screen Number	Fragment Definition			
1869	TR	3	DDDDDD	15.00
1870	TR	4	DDDDDD	5.96
1871	TR	5	DDDDDD	2.30
1872	TR	6	DDDDDD	1.49
1873	TR		DDDDDT	1.07
1874	TR		DDDDTT	31.00
1875	TR	2	DDDDTT	16.61
1876	TR	3	DDDDTT	2.91
1877	TR	4	DDDDTT	1.76
1878	TR		DDDTDT	1.04
1879	TR	2	DDDTDT	0.34
1880	TR		DDDTTT	2.10
1881	TR	2	DDDTTT	1.32
1882	TR	3	DDDTTT	0.53
1883	TR		DDTDDT	0.66
1884	TR		DDTDTT	0.64
1885	TR		DDTTTT	4.57
1886	TR	2	DDTTTT	2.20
1887	TR		DTDTDT	0.53
1888	TR		DTDTTT	0.35
1889	TR		DTTDTT	3.09
1890	TR	2	DTTDTT	0.66
1891	TR		DTTTTT	1.26
1892	TR		TTTTTT	0.59
1893	TR		DDDDDDD	0.67
1894	TR	2	DDDDDDD	0.03

Screen Number Order			
Screen Number		Fragment Definition	Frequency Percent
1895	TR	DDDDDDT	0.49
	TR	DDDDTDT	
	TR	DDDDTTT	
	TR	DDDTDDT	
	TR	DDDTDTT	
	TR	DDTDDTT	
	TR	DDTDTDT	
	TR	DDTDTTT	
	TR	DDTTTTT	
	TR	DTDTDTT	
	TR	DTDTTTT	
	TR	DTTDTTT	
	TR	DTTTTTT	
	TR	TTTTTTT	
1896	TR	DDDDDTT	0.94
1897	TR	DDDTTTT	0.64
	TR	DDTTDTT	
1898	TR	8-membered ring or larger	2.61
1899	AC	1	98.15
1900	AC	6	92.64
1901	AC	8	91.95
1902	AC	10	90.59
1903	AC	12	88.21
1904	AC	14	84.50
1905	AC	16	79.75
1906	AC	18	73.85
1907	AC	20	67.45
1908	AC	22	60.62
1909	AC	24	53.61
1910	AC	26	46.59
1911	AC	28	40.01
1912	AC	30	33.97
1913	AC	35	21.92
1914	AC	40	14.78
1915	AC	50	8.50

Screen Number Order			
Screen Number		Fragment Definition	Frequency Percent
1916	AC	70	4.27
1917	AC	90	2.45
1918	EC	Ac	14.84
	EC	Ag	
	EC	Al	
	EC	Am	
	EC	Au	
	EC	Ba	
	EC	Be	
	EC	Bi	
	EC	Bk	
	EC	Ca	
	EC	Cd	
	EC	Ce	
	EC	Cf	
	EC	Cm	
	EC	Co	
	EC	Cr	
	EC	Cu	
	EC	Dy	
	EC	Er	
	EC	Es	
	EC	Eu	
	EC	Fe	
	EC	Fm	
	EC	Fr	
	EC	Ga	
	EC	Gd	
	EC	Ge	
	EC	Hf	
	EC	Hg	
	EC	Ho	
	EC	In	
	EC	Ir	
	EC	K	
	EC	La	
	EC	Li	
	EC	Lr	
	EC	Lu	
	EC	Md	
	EC	Mg	
	EC	Mn	
	EC	Mo	
	EC	Na	
	EC	Nb	
	EC	Nd	
	EC	Ni	
	EC	No	
	EC	Np	
	EC	Os	
	EC	Pa	
	EC	Pb	
	EC	Pd	



Screen Number Order				
Screen Number		Fragment Definition	Frequency Percent	
1918	EC	Pm	14.84	(continued)
	EC	Po		
	EC	Pr		
	EC	Pt		
	EC	Pu		
	EC	Ra		
	EC	Rb		
	EC	Re		
	EC	Rh		
	EC	Ru		
	EC	Sb		
	EC	Sc		
	EC	Sm		
	EC	Sn		
	EC	Sr		
	EC	Ta		
	EC	Tb		
	EC	Tc		
	EC	Th		
	EC	Ti		
	EC	Tl		
	EC	Tm		
	EC	U		
	EC	V		
	EC	W		
	EC	Y		
	EC	Yb		
	EC	Zn		
	EC	Zr		
	GM	E Ac		
	GM	E Ag		
	GM	E Al		
	GM	E Am		
	GM	E Au		
	GM	E Ba		
	GM	E Be		
	GM	E Bi		
	GM	E Bk		
	GM	E Ca		
	GM	E Cd		
	GM	E Ce		
	GM	E Cf		
	GM	E Cm		
	GM	E Co		
	GM	E Cr		
	GM	E Cu		
	GM	E Dy		
	GM	E Er		
	GM	E Es		
	GM	E Eu		
GM	E Fe			
GM	E Fm			
GM	E Fr			
GM	E Ga			
GM	E Gd			

Screen Number Order				
Screen Number	Fragment Definition		Frequency Percent	
1918	GM	E Ge	14.84	(continued)
	GM	E Hf		
	GM	E Hg		
	GM	E Ho		
	GM	E In		
	GM	E Ir		
	GM	E K		
	GM	E La		
	GM	E Li		
	GM	E Lr		
	GM	E Lu		
	GM	E Md		
	GM	E Mg		
	GM	E Mn		
	GM	E Mo		
	GM	E Na		
	GM	E Nb		
	GM	E Nd		
	GM	E Ni		
	GM	E No		
	GM	E Np		
	GM	E Os		
	GM	E Pa		
	GM	E Pb		
	GM	E Pd		
	GM	E Pm		
	GM	E Po		
	GM	E Pr		
	GM	E Pt		
	GM	E Pu		
	GM	E Ra		
	GM	E Rb		
	GM	E Re		
	GM	E Rh		
	GM	E Ru		
	GM	E Sb		
	GM	E Sc		
	GM	E Sm		
	GM	E Sn		
	GM	E Sr		
	GM	E Ta		
	GM	E Tb		
	GM	E Tc		
	GM	E Th		
	GM	E Ti		
	GM	E Tl		
	GM	E Tm		
	GM	E U		
	GM	E V		
	GM	E W		
	GM	E Y		
	GM	E Yb		
	GM	E Zn		
	GM	E Zr		

Screen Number Order			
Screen Number	Fragment Definition		Frequency Percent
1919	EC	Ac	0.19
	EC	Am	
	EC	Bk	
	EC	Cf	
	EC	Cm	
	EC	Es	
	EC	Fm	
	EC	Lr	
	EC	Md	
	EC	No	
	EC	Np	
	EC	Pa	
	EC	Pu	
	EC	Th	
	EC	U	
	GM	E Ac	
	GM	E Am	
	GM	E Bk	
	GM	E Cf	
	GM	E Cm	
	GM	E Es	
	GM	E Fm	
	GM	E Lr	
	GM	E Md	
	GM	E No	
	GM	E Np	
	GM	E Pa	
	GM	E Pu	
	GM	E Th	
	GM	E U	
1920	EC	Ag	2.10
	EC	Au	
	EC	Cu	
	GM	E Ag	
	GM	E Au	
	GM	E Cu	
1921	EC	Ag	3.35
	EC	Mo	
	EC	Nb	
	EC	Pd	
	EC	Rh	
	EC	Ru	
	EC	Tc	
	EC	Zr	
	GM	E Ag	
	GM	E Mo	
	GM	E Nb	
	GM	E Pd	
	GM	E Rh	
	GM	E Ru	
	GM	E Tc	
	GM	E Zr	

Screen Number Order			
Screen Number		Fragment Definition	Frequency Percent
1922	EC	Al	1.27
	GM	E Al	
1923	EC	Al	2.93
	EC	B	
	EC	Ga	
	EC	In	
	EC	Ti	
	GM	E Al	
	GM	E B	
	GM	E Ga	
	GM	E In	
	GM	E Ti	
1924	EC	Ar	0.03
	EC	He	
	EC	Kr	
	EC	Ne	
	EC	Rn	
	EC	Xe	
	GM	E Ar	
	GM	E He	
	GM	E Kr	
	GM	E Ne	
	GM	E Rn	
	GM	E Xe	
1925	EC	As	6.12
	EC	Bi	
	EC	P	
	EC	Sb	
	GM	E As	
	GM	E Bi	
	GM	E P	
	GM	E Sb	
1926	EC	As	2.27
	EC	Ga	
	EC	Ge	
	EC	Kr	
	EC	Rb	
	EC	Se	
	EC	Sr	
	EC	Y	
	EC	Zn	
	GM	E As	
	GM	E Ga	
	GM	E Ge	
	GM	E Kr	
	GM	E Rb	
	GM	E Se	
	GM	E Sr	
	GM	E Y	
	GM	E Zn	

Screen Number Order				
Screen Number	Fragment Definition			Frequency Percent
1927	EC	As		0.28
	GM	E As		
1928	EC	2 As		
1929	EC	At		31.99
	EC	Br		
	EC	Cl		
	EC	F		
	EC	I		
	GM	E At		
	GM	E Br		
	GM	E Cl		
	GM	E F		
	GM	E I		
	1930	EC	At	
EC		Bi		
EC		Fr		
EC		Hg		
EC		Pb		
EC		Po		
EC		Ra		
EC		Rn		
EC		Tl		
GM		E At		
GM		E Bi		
GM		E Fr		
GM		E Hg		
GM		E Pb		
GM		E Po		
GM		E Ra		
GM		E Rn		
GM		E Tl		
1931		EC	Au	
	EC	Hf		
	EC	Ir		
	EC	Os		
	EC	Pt		
	EC	Re		
	EC	Ta		
	EC	W		
	GM	E Au		
	GM	E Hf		
	GM	E Ir		
	GM	E Os		
	GM	E Pt		
	GM	E Re		
	GM	E Ta		
GM	E W			
1932	EC	B		1.36
	GM	E B		

Screen Number Order				
Screen Number	Fragment Definition			Frequency Percent
1933	EC	2	B	0.26
1934	EC	3	B	0.17
1935	EC		Ba	2.27
	EC		Cd	
	EC		Cs	
	EC		In	
	EC		Sb	
	EC		Sn	
	EC		Te	
	EC		Xe	
	GM	E	Ba	
	GM	E	Cd	
	GM	E	Cs	
	GM	E	In	
	GM	E	Sb	
	GM	E	Sn	
	GM	E	Te	
	GM	E	Xe	
1936	EC		Ba	1.24
	EC		Be	
	EC		Ca	
	EC		Mg	
	EC		Ra	
	EC		Sr	
	GM	E	Ba	
	GM	E	Be	
	GM	E	Ca	
	GM	E	Mg	
	GM	E	Ra	
	GM	E	Sr	
1937	EC		Be	0.05
	GM	E	Be	
1938	EC		Br	5.30
	GM	E	Br	
1939	EC	2	Br	1.12
1940	EC	3	Br	0.30
1941	EC	4	Br	0.18
1942	EC	4	C	91.88
1943	EC	6	C	90.62
1944	EC	8	C	87.91
1945	EC	10	C	83.53
1946	EC	12	C	77.56

Screen Number Order				Screen Number	Fragment Definition	Frequency Percent
1947	EC	14	C			70.23
1948	EC	16	C			61.95
1949	EC	18	C			53.38
1950	EC	20	C			44.93
1951	EC	25	C			26.45
1952	EC	30	C			15.81
1953	EC	35	C			10.30
1954	EC	49	C			7.56
1955	EC		Ca			0.34
	GM		E Ca			
1956	EC		Cd			1.03
	EC		Hg			
	EC		Zn			
	GM		E Cd			
	GM		E Hg			
	GM		E Zn			
1957	EC		Ce			1.31
	EC		Dy			
	EC		Er			
	EC		Eu			
	EC		Gd			
	EC		Ho			
	EC		La			
	EC		Lu			
	EC		Nd			
	EC		Pm			
	EC		Pr			
	EC		Sm			
	EC		Tb			
	EC		Tm			
	EC		Yb			
	GM		E Ce			
	GM		E Dy			
	GM		E Er			
	GM		E Eu			
	GM		E Gd			
	GM		E Ho			
	GM		E La			
	GM		E Lu			
	GM		E Nd			
	GM		E Pm			
	GM		E Pr			
	GM		E Sm			
	GM		E Tb			
	GM		E Tm			
	GM		E Yb			

Screen Number Order				
Screen Number	Fragment Definition			Frequency Percent
1958	EC		Cl	18.33
	GM		E Cl	
1959	EC	2	Cl	6.14
1960	EC	3	Cl	1.93
1961	EC	4	Cl	0.93
1962	EC	5	Cl	0.39
1963	EC		Co	1.32
	GM		E Co	
1964	EC		Co	7.39
	EC		Cr	
	EC		Cu	
	EC		Fe	
	EC		Mn	
	EC		Ni	
	EC		Ti	
	EC		V	
	GM		E Co	
	GM		E Cr	
	GM		E Cu	
	GM		E Fe	
	GM		E Mn	
	GM		E Ni	
	GM		E Ti	
	GM		E V	
1965	EC		Co	6.72
	EC		Fe	
	EC		Ni	
	EC		Os	
	EC		Pd	
	EC		Pt	
	EC		Rh	
	EC		Ru	
	GM		E Co	
	GM		E Fe	
	GM		E Ni	
	GM		E Os	
	GM		E Pd	
	GM		E Pt	
	GM		E Rh	
	GM		E Ru	
1966	EC		Cr	2.44
	EC		Mo	
	EC		W	
	GM		E Cr	
	GM		E Mo	
	GM		E W	



Screen Number Order				
Screen Number	Fragment Definition			Frequency Percent
1967	EC		Cs	2.00
	EC		Fr	
	EC		K	
	EC		Li	
	EC		Na	
	EC		Rb	
	GM		E Cs	
	GM		E Fr	
	GM		E K	
	GM		E Li	
	GM		E Na	
	GM		E Rb	
1968	EC		F	10.62
	GM		E F	
1969	EC	2	F	6.99
1970	EC	3	F	5.71
1971	EC	4	F	2.67
1972	EC	5	F	1.96
1973	EC	6	F	1.70
1974	EC	7	F	0.85
1975	EC		Fe	2.96
	GM		E Fe	
1976	EC	2	X	15.15
1977	EC	3	X	8.64
1978	EC	4	X	4.76
1979	EC	5	X	2.84
1980	EC	6	X	2.22
1981	EC	8	X	0.95
1982	EC	10	X	0.64
1983	EC		Ge	5.61
	EC		Pb	
	EC		Si	
	EC		Sn	
	GM		E Ge	
	GM		E Pb	
	GM		E Si	
	GM		E Sn	

Screen Number Order				
Screen Number			Fragment Definition	Frequency Percent
1984	EC		Hf	1.39
	EC		Ti	
	EC		Zr	
	GM		E Hf	
	GM		E Ti	
	GM		E Zr	
1985	EC		I	1.71
	GM		E I	
1986	EC	2	I	0.33
1987	EC		K	0.42
	GM		E K	
1988	EC		La	0.53
	EC		Sc	
	EC		Y	
	GM		E La	
	GM		E Sc	
	GM		E Y	
1989	EC		Li	0.40
	GM		E Li	
1990	EC		Mg	0.52
	GM		E Mg	
1991	EC		Mn	1.96
	EC		Re	
	EC		Tc	
	GM		E Mn	
	GM		E Re	
	GM		E Tc	
1992	EC		N	71.10
	GM		E N	
1993	EC	2	N	53.96
1994	EC	3	N	35.41
1995	EC	4	N	23.08
1996	EC	6	N	9.30
1997	EC	8	N	5.03
1998	EC	10	N	3.47
1999	EC	14	N	2.13
2000	EC		Na	1.11
	GM		E Na	

Screen Number Order				
Screen Number	Fragment Definition			Frequency Percent
2001	EC	Nb		1.12
	EC	Ta		
	EC	V		
	GM	E Nb		
	GM	E Ta		
	GM	E V		
2002	EC	Ni		1.81
	GM	E Ni		
2003	EC	O		86.62
	EC	S		
	GM	E O		
	GM	E S		
2004	EC	O		83.63
	GM	E O		
2005	EC	2	O	70.64
2006	EC	3	O	53.74
2007	EC	4	O	39.45
2008	EC	5	O	25.77
2009	EC	6	O	18.58
2010	EC	7	O	12.97
2011	EC	8	O	10.08
2012	EC	10	O	6.70
2013	EC	12	O	5.07
2014	EC	15	O	3.37
2015	EC	18	O	2.40
2016	EC	P		5.44
	GM	E P		
2017	EC	2	P	1.90
2018	EC	3	P	0.76
2019	EC	Po		0.66
	EC	Se		
	EC	Te		
	GM	E Po		
	GM	E Se		
	GM	E Te		

Screen Number Order				
Screen Number	Fragment Definition			Frequency Percent
2020	EC		Pt	0.50
	GM		E Pt	
2021	EC		S	26.05
	GM		E S	
2022	EC	2	S	7.69
2023	EC	3	S	2.16
2024	EC	4	S	1.14
2025	EC	5	S	0.44
2026	EC		Si	4.55
	GM		E Si	
2027	EC	2	Si	0.96
2028	EC	3	Si	0.39
2029	GM		E Ac	0.61
	GM		E Ag	
	GM		E Al	
	GM		E Am	
	GM		E Ar	
	GM		E As	
	GM		E At	
	GM		E Au	
	GM		E B	
	GM		E Ba	
	GM		E Be	
	GM		E Bi	
	GM		E Bk	
	GM		E C	
	GM		E Cd	
	GM		E Ce	
	GM		E Cf	
	GM		E Cm	
	GM		E Co	
	GM		E Cr	
	GM		E Cs	
	GM		E Cu	
	GM		E Dy	
	GM		E Er	
	GM		E Es	
	GM		E Eu	
	GM		E F	
	GM		E Fe	
	GM		E Fm	
	GM		E Fr	
	GM		E Ga	
	GM		E Gd	
	GM		E Ge	
	GM		E He	

Screen Number Order				
Screen Number	Fragment Definition		Frequency Percent	
2029	GM	E Hf	0.61	(continued)
	GM	E Hg		
	GM	E Ho		
	GM	E In		
	GM	E Ir		
	GM	E Kr		
	GM	E La		
	GM	E Li		
	GM	E Lr		
	GM	E Lu		
	GM	E Md		
	GM	E Mg		
	GM	E Mn		
	GM	E Mo		
	GM	E Nb		
	GM	E Nd		
	GM	E Ne		
	GM	E Ni		
	GM	E No		
	GM	E Np		
	GM	E Os		
	GM	E P		
	GM	E Pa		
	GM	E Pb		
	GM	E Pd		
	GM	E Pm		
	GM	E Po		
	GM	E Pr		
	GM	E Pt		
	GM	E Pu		
	GM	E Ra		
	GM	E Rb		
	GM	E Re		
	GM	E Rh		
	GM	E Rn		
	GM	E Ru		
	GM	E S		
	GM	E Sb		
	GM	E Sc		
	GM	E Se		
	GM	E Sm		
	GM	E Sn		
	GM	E Sr		
	GM	E Ta		
	GM	E Tb		
	GM	E Tc		
	GM	E Te		
	GM	E Th		
	GM	E Ti		
	GM	E Tl		
	GM	E Tm		
	GM	E U		
	GM	E V		
	GM	E W		
	GM	E Xe		

Screen Number Order			Frequency	
Screen Number		Fragment Definition	Percent	
2029	GM	E Y	0.61	(continued)
	GM	E Yb		
	GM	E Zn		
	GM	E Zr		
2030	GM	E Br	0.55	
2031	GM	E Ca	0.06	
2032	GM	E Cl	2.95	
2033	GM	E H	3.85	
2034	GM	E I	0.45	
2035	GM	E K	0.30	
2036	GM	E N	0.15	
2037	GM	E Na	0.95	
2038	GM	E O	0.50	
2039	GM	abnormal mass -- all isotopic specifications	0.97	
2040	GM	charge -- all charges: fixed, tautomeric	12.50	
2041	GM	abnormal valence	32.34	
2042	GM	delocalized charge only	0.10	
2043	GM	polymer (general category)	4.18	
2044		Not used		
2045	GM	deuterium isotope	0.49	
2046	GM	tritium and higher H isotopes (e.g., 4H, 5H, etc.)	0.06	
2047	GM	isotope at unknown location (IUL)	0.05	
2048	GM	incompletely defined (ID) substance	1.43	
2049	GM	coordination compound	8.16	
2050	GM	alloy	3.22	
2051	GM	mixture (substance named as "mixt. with" in CA and CApplus)	0.29	
2052	GM	mineral	0.05	
2053	GM	manual registration	221.62	

Screen Number Order			
Screen Number		Fragment Definition	Frequency Percent
2054	GM	radical ion	0.23
2055		Not Used	
2056		Not Used	
2057		Not Used	
2058		Not Used	
2059		Not Used	
2060		Not Used	
2061		Not Used	
2062		Not Used	
2063		Not Used	
2064		Not Used	
2065		Not Used	
2066		Not Used	
2067	GM	homopolymers and copolymers [ (A) <sub>x</sub> , (A.B) <sub>x</sub> , etc.]	3.20
2068	GM	polymers defined as structural repeating units(SRUs)	1.48
2069	GM	SRU with end groups [ X-(-Y-) <sub>n</sub> -Z]	0.52
2070	GM	SRU without end groups [ -(-Y-) <sub>n</sub> -]	1.00
2071	GM	ID - unknown structure (ID molform)	0.21
2072	GM	ID - unknown point of attachment	0.99
2073	GM	ID - ester	0.14
2074	GM	ID - hydrogen (bond)	0.10
2075		Not Used	
2076	GM	tautomer	39.88
2077	GM	3 or more components	7.24
2078	GM	4 or more components	4.55
2079	GM	single atom fragment (SAF)	6.69

Screen Number Order						Frequency Percent
Screen Number	Fragment Definition					
2080	AS	C	C	C	N	67.06
	AS	N	C	C	C	
2081	AS	C	C	C	O	76.51
	AS	C	C	C	S	
	AS	O	C	C	C	
	AS	S	C	C	C	
2082	CASREACT compound					14.04
2083	AS	C	C	N	C	61.18
	AS	C	N	C	C	
2084	AS	C	C	O	C	55.24
	AS	C	C	S	C	
	AS	C	O	C	C	
	AS	C	S	C	C	
2085	AS	C	C	N	N	26.07
	AS	C	C	N	O	
	AS	C	C	N	S	
	AS	C	C	O	N	
	AS	C	C	O	O	
	AS	C	C	O	S	
	AS	C	C	S	N	
	AS	C	C	S	O	
	AS	C	C	S	S	
	AS	N	N	C	C	
	AS	N	O	C	C	
	AS	N	S	C	C	
	AS	O	N	C	C	
	AS	O	O	C	C	
	AS	O	S	C	C	
	AS	S	N	C	C	
	AS	S	O	C	C	
	AS	S	S	C	C	
2086	AS	C	N	C	N	30.95
	AS	C	O	C	N	
	AS	C	S	C	N	
	AS	N	C	N	C	
	AS	N	C	O	C	
	AS	N	C	S	C	
2087	AS	C	N	C	O	39.80
	AS	C	N	C	S	
	AS	O	C	N	C	
	AS	S	C	N	C	



Screen Number Order						
Screen Number				Fragment Definition		Frequency Percent
2088	AS	C	O	C	O	27.26
	AS	C	O	C	S	
	AS	C	S	C	O	
	AS	C	S	C	S	
	AS	O	C	O	C	
	AS	O	C	S	C	
	AS	S	C	O	C	
	AS	S	C	S	C	
2089	AS	N	C	C	N	23.97
2090	AS	N	C	C	O	35.39
	AS	N	C	C	S	
	AS	O	C	C	N	
	AS	S	C	C	N	
2091	AS	O	C	C	O	24.29
	AS	O	C	C	S	
	AS	S	C	C	O	
	AS	S	C	C	S	
2092	AS	C	N	O	C	13.08
2092	AS	C	N	O	O	13.08
	AS	C	N	O	S	
	AS	C	N	S	C	
	AS	C	N	S	O	
	AS	C	N	S	S	
	AS	C	O	N	C	
	AS	C	O	O	C	
	AS	C	O	S	C	
	AS	C	S	N	C	
	AS	C	S	O	C	
	AS	C	S	S	C	
	AS	N	C	N	N	
	AS	N	C	O	N	
	AS	N	C	S	N	
	AS	N	N	C	N	
	AS	N	O	C	N	
	AS	N	S	C	N	
	AS	O	C	N	O	
	AS	O	C	N	S	
	AS	O	N	C	O	
	AS	O	O	N	C	
	AS	O	S	N	C	
	AS	S	C	N	S	
	AS	S	N	C	O	
	AS	S	N	C	S	
	AS	S	O	N	C	
	AS	S	S	N	C	

Screen Number		Screen Number Order					Frequency Percent	
Screen Number		Fragment Definition						
2093	AS	C	N	N	C		24.67	
	AS	C	O	C	N			
	AS	C	O	O	C			
	AS	C	O	S	C			
	AS	C	S	C	N			
	AS	C	S	O	C			
	AS	C	S	S	C			
	AS	N	C	O	C			
	AS	N	C	S	C			
2094	AS	C	O	C	O		27.26	
	AS	C	O	C	S			
	AS	C	S	C	O			
	AS	C	S	C	S			
	AS	O	C	O	C			
	AS	O	C	S	C			
	AS	S	C	O	C			
	AS	S	C	S	C			
2095		Not used						
2096	AS	O	C	C	C	O	20.23	
	AS	S	C	C	C	S		
2097		Not used						
2098	AS	N	C	C	C	N	22.43	
2099	AA	C		C	N		69.37	
2100	AA	2	C	C	N		62.62	
2101	AA		C	C	O		75.88	
2102	AA	2	C	C	O		60.80	
2103	AA		N	C	C		61.82	
2104	AA		O	C	C		47.10	
2105	AA		C	C	M		31.14	
	AA		C	C	S			
	AA		N	C	X			
	AA		O	C	M			
	AA		O	C	N			
	AA		O	C	O			
	AA		O	C	P			
	AA		P	C	C			
	AA		S	C	S			
2106	AA		C	C	P		36.37	
	AA		C	N	N			
	AA		C	O	S			
	AA		C	S	S			
	AA		N	N	N			
	AA		S	C	C			

Screen Number Order					Frequency Percent
Screen Number	Fragment Definition				
2107	AA	C	N	S	42.77
	AA	C	O	O	
2108	AA	C	N	O	44.41
	AA	N	C	N	
2109	AA	C	C	X	33.25
	AA	N	C	O	
2109	AA	S	C	N	33.25
2111	DC	3			92.87
2112	DC	3	3		87.28
2113	DC	5	3		75.61
2114	DC	7	3		59.22
2115	DC	9	3		41.91
2116	DC	12	3		21.66
2117	DC	14	3		13.95
2118	DC	16	3		9.96
2119	DC	20	3		6.39
2120	DC		4		42.03
2121	DC	2	4		17.53
2122	DC	3	4		8.61
2123	DC	4	4		4.94
2124	DC	5	4		3.04
2125	DC	6	4		2.10
2126	DC		6		4.73
2127	2 or more components				18.61

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