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STN Database Summary Sheet

The **GMELIN97** File is a structure and factual database on inorganic and organometallic chemistry. Substance records contain the critically reviewed and evaluated data from the GMELIN Handbook of Inorganic and Organometallic Chemistry issued in 1975 and before, covering the chemical literature for the period 1817 - 1975. Also included are selected data from a pool of the 110 most important journals of inorganic, physical, and organometallic chemistry, and other journals of physics from 1975-1997.

The records contain substance identifying information, e.g., structure image, GMELIN Registry Number, CAS Registry Number, numeric and non-numeric data about chemical and physical properties, and preparation and reaction information. The information is accompanied by a reference to the primary literature. (See database summary sheet GMELIN: Structure Searching for details on the structure-searchable portion of the database).

Subject Coverage

- Identification of Substance
- Chemical Behavior, Reaction, Preparation
- Electrochemical Data
- Multicomponent System Data
- Solid State Data
- Electrical Properties
- Magnetic Properties
- Mechanical Properties
- Molecular Properties
- Optical Properties
- Spectral Data
- Thermodynamic Data
- Quantum Chemical Calculations

Sources

- GMELIN Handbook of Inorganic and Organometallic Chemistry, Main Series and Supplements
- Scientific Publications from 1975 - 1997

File Data

- 1817-1975 for Gmelin Handbook
- 1975-1997 for select journals
- More than 41,800 MSDS sheets on trade name materials (6/06)
- Not presently updated
- Automatic current-awareness searches (SDIs) are not available

User Aids

- Building and Structure Searching on STN
- Online Helps (HELP DIRECTORY lists all help messages available)
- STNGUIDE

Database Producer

Elsevier Information Systems GmbH
Theodor-Heuss-Allee 108
60486 Frankfurt am Main
Germany
Phone: (+49) 69 5050 4252
Fax: (+49) 69 5050 4245
Copyright Holder

In North America

CAS
STN North America
P.O. Box 3012
Columbus, Ohio 43210-0012 U.S.A.

CAS Customer Care:
Phone: 800-753-4227 (North America)
614-447-3700 (worldwide)
Fax: 614-447-3751
E-mail: help@cas.org
Internet: www.cas.org

In Europe

FIZ Karlsruhe
STN Europe
P.O. Box 2465
76012 Karlsruhe
Germany
Phone: +49-7247-808-555
Fax: +49-7247-808-259
E-mail: helpdesk@fiz-karlsruhe.de
Internet: www.stn-international.de

In Japan

JAICI (Japan Association for
International Chemical Information)
STN Japan
Nakai Building
6-25-4 Honkomagome, Bunkyo-ku
Tokyo 113-0021, Japan
Phone: +81-3-5978-3601 (Technical Service)
+81-3-5978-3621 (Customer Service)
Fax: +81-3-5978-3600
E-mail: helpdesk@jaici.or.jp (Technical Service)
cas-stn@jaici.or.jp (Customer Service)
Internet: www.jaici.or.jp

GMELIN97**Search and Display Field Codes**

There are no fields that allow left truncation in this file.

Substance Identifying Information

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index (contains single words from chemical name (CN), chemical name segment (CNS), and controlled term (CT and CTM) fields, as well as molecular formulas (MF), GMELIN Registry Numbers (GRN), and CAS Registry Numbers (RN))	None (or /BI)	S CU2O AND THERMOELECTRIC S RHENOCENE S 50-00-0 S 129948 S METASTABLE PHASE#	CN, CT, GRN, MF, RN
Atom Count (1) Basis Compound CAS Registry Number CAS Registry Number Counter (1) Charge (1) Chemical Name Chemical Name Segment Component Molecular Formula Dopand Element Count (specific) (1) Element Count (total) (1) Element Count Multicomponent Systems (1) Element Formula Element Symbol Element Symbol Multicomponent Systems Family Name Field Availability Formula Weight (Molecular Weight) (1) Fragment Gmelin Registry Number Fragment Molecular Formula (2) Gmelin Registry Number (1) GRN of Revised Substance GRN of Revised Substances Forming a Mixture Isotope Search Data Ligand Linearized Structure Formula (2) Ligand Molecular Formula Linearized Structure Formula (2) Material Composition Atom Percent (3) Unknown Percent (3) Volume Percent (3) Weight Percent (3)	/ATC /MACB /RN /RN.CNT /CHA /CN /CNS /CMF /DOT /Element Symbol,M,X /ELC /ELC.SUB /ELF /ELS /ELS.MCF /FN /FA /FW (or /MW) /FRAGGRN /FRAGMF /GRN /REV.GRN /REV.MGRN /IFOR /LIGLSF /LIGMF /LSF /FA /MAC.A /MAC.X /MAC.V /MAC.W	S 3.55<ATC<3.60 S SI/MACB S 124021-11-0/RN S 2/RN.CNT S -1/CHA S QUARTZ/CN S METHYL/CNS (P) INDANE/CNS S CUO/CMF(L)CU2O/CMF S CU O/CMF (L) CU2 O/CMF S SI/CMF AND GE/DOT S DOT/FA S CO>20 S 3-5/M S 4/ELC S 3/ELC.SUB S AG/ELF S C/ELS AND F/ELS S OS/ELS.MCF S ALLOY/FN S ACEN/FA S 3/FW S 1235/FRAGGRN S "AC(3+)"/FRAGMF S 145-165/GRN S 2510/REV.GRN S 117/REV.MGRN S AS/IFOR S "FE2((8)D)"/LIGLSF S LQ/LIGMF NOT D/LIGMF S Y3AL5O12/LSF S "CAO#C"/LSF S MAC/FA S AU 14-22/MAC.A S PB 49-52/MAC.X S AG 15-17/MAC.V S AG 13/MAC.W	Not displayed Alloy Composition Table RN Not displayed MF CN CN CMF LSF MF Not displayed Not displayed Not displayed Not displayed Not displayed FN Not displayed FW FRAGGRN, FRAGMF FRAGMF GRN REV REV Not displayed LIGLSF LIGMF LSF Alloy Composition Table Alloy Composition Table Alloy Composition Table Alloy Composition Table Alloy Composition Table

Search and Display Field Codes (cont'd)

Search Field Name	Search Code	Search Examples	Display Codes
Modification	/MOD	S ARAGONITE/MOD	MOD
Molecular Formula	/MF	S PUTE/MF S CU2 O/MF S CU2O.O2SN/MF	MF
Number of Components (1)	/NC	S ALLOY/FN AND NC=6	Not displayed
Number of Fragments (1)	/NFRAG	S 6/NFRAG AND H2O/CMF	Not displayed
Number of Structures (1)	/NSTR	S 4/NSTR	Not displayed
Periodic Group	/PG	S B6/PG AND A6/PG	Not displayed
Property Hierarchy	/PH	S MAGNETOSTRICTION/PH	CT
Related Structure	/RSTR	S 260442/RSTR	RSTR
Relative Composition (4)	/RC	S AG.AU. ?/RC	Alloy Composition Table
Atom Percent	/RC.A	S AL.CE.PD/RC.A	Alloy Composition Table
Unknown Percent	/RC.X	S AU.AG/RC.X	Alloy Composition Table
Volume Percent	/RC.V	S BI.AL/RC.V	Alloy Composition Table
Weight Percent	/RC.W	S AG.AU/RC.W	Alloy Composition Table
Revision of Structure or Formula	/FA	S REV/FA	REV
Substance Physical State (5)	/SSTA	S LIQUID/SSTA	SSTA
Trace Compound	/MACT	S FE/MACB AND MN/MACT	Alloy Composition Table

- (1) Numeric search field that may be searched using numeric operators or ranges.
(2) If the formula includes Messenger reserved characters, they must to be masked by quotation marks (" ").
(3) Combined numeric and text field. Composition terms are numeric and may be searched using numeric operators or ranges. Component terms are text terms.
(4) A search in /RC is executed in the /RC.W, /RC.A, /RC.V, and RC.X fields.
(5) Displayed with corresponding properties. SSTA information is available for CP, CTMEC, CTMVOL, CTVP, CV, DEN, DIC, DV, ECND, GFOR, HFOR, KV, RI, SFOR, ST, TCND, TEC, VP.

Referenced Compound

Search Field Name	Search Code	Search Examples	Display Codes
Referenced Compound (contains information about compounds that are not Title Compounds) (1)	/REFCO	S ALBR3/REFCO S 200358/REFCO	AZE, CFS, EREA, FRAGMF, OV, REA, REV, RSTR

- (1) A search in /REFCO is executed in the following fields: Azetrope (/AZE), Compounds Forming System (/CFS), Electrochemical Reaction Starting Material (/EREA.SM), Electrochemical Reaction Product (/EREA.PRO), Fragment Gmelin Registry Number (/FRAGGRN), Overvoltage Gmelin Registry Number of Electrode Material (/OV.GRN), Reaction Catalyst (/REA.CAT), Reaction Intermediate (/REA.INT), Reaction Product (/REA.PRO), Reaction Starting Material (/REA.SM), Gmelin Registry Number of Revised Substance (/REV.GRN), Gmelin Registry Numbers of Substances Forming a Mixture (/REV.MGRN), and Related Structure (/RSTR).

Bibliographic Data (1)

Search Field Name	Search Code	Search Examples	Display Codes
Author	/AU	S SANDERSON, L./AU	References
International Standard (Document) Number (contains CODEN)	/ISN	S WISEAS/ISN	References
Journal Title	/JT	S ACTA CHEM. SCAND./JT	References
Keyword (1)	/ <PROP> .KW	S HANDBOOK/DV.KW	References
Patent Number	/PN	S 167498/PN	References
Publication Year (3)	/PY	S 1882-1890/PY	References

- (1) Bibliographic data presently available are recorded in the property fields. Each property field displays references.
(2) When the reference is a Handbook reference, the flag H for Handbook Data displays in the Footnote(s). If the references are not from the Handbook, no flag is displayed. When the only keyword in the .KW is HANDBOOK, the field is not included in the property table.
(3) Numeric search field that may be searched using numeric operators or ranges.

GMELIN97**Structure Search Terms**

Terms	Search Example
L-number of a structure built using the STRUCTURE command or uploaded from STN Express (Boolean logic allowed between the L-numbers) (1) L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers) (1) L-numbers of structures built using the STRUCTURE command or uploaded from STN Express combined with L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers) (1)	SEARCH L1 CSS FUL S L1 NOT L2 S L3 OR L4 S L1 NOT L3

(1) The L-number answer set from a structure search may be combined with dictionary or factual terms, e.g., S L3 AND POL/FA.

Types of Structure Searching

Type	Definition	Search Code	Search Examples
Substructure (default)	Search for substances that match the query. Substitution is allowed at all open positions.	SSS	SEARCH L1 SSS FUL S L2 OR L3 SSS SAM S L7 SSS RAN
Closed Substructure	Search for substances that match the query exactly. Substitution is allowed at positions opened by CONNECT.	CSS	SEARCH L1 CSS FUL S L2 OR L3 CSS S L4 NOT L5 CSS RAN
Family	Search for substances that match the query exactly. Additional components may be retrieved.	FAM	S L6 FAM FUL
Exact	Search for substances that match the query exactly.	EXA	SEA L5 EXA FUL

Scopes of Structure Searches

To create an L-number answer set containing candidate structures that have passed the screening step of your structure search, enter EXTEND on the search command line or enter SET EXTEND ON or SET EXTEND ON PERM at an arrow prompt (=>). For details, enter HELP SET EXTEND at an arrow prompt.

Scope	Definition	Search Code	Search Examples
Sample (default) (1)	Search a fixed 5% of the file.	SAM	SEARCH L3 EXA SAM S L6 NOT L7 SSS SAM
Full Range	Search 100% of the file. Search a user specified portion of the file.	FUL RAN	S L5 OR L8 SSS FUL S L4 RAN=(72810,) S L3 FAM RAN=(77541, 80001) S L7 CSS SUB=L5 SAM
Subset Sample	Search a fixed sample of an answer set created by a search in GMELIN.	SUB SAM	
Subset Range	Search a user-specified portion of an answer set created by a search in GMELIN.	SUB RAN	S L3 SUB=L2 RAN=(,27505)
Subset Full	Search 100% of an answer set created by a search in GMELIN.	SUB FUL	S L8 SUB=L6 FAM FUL

(1) EXTEND not valid with SAMPLE.

Properties and Property Parameters

Chemical Data

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Controlled Term for General Information and Chemical Behavior	-	/CT	S ECONOMIC DATA/CT S CTGEN/FA	CTGEN
Decomposition Point (1)	Cel	/DP	S DP>2000	DP
Solvent	-	/DP.SOL	S WATER/DP.SOL	DP
Flash Point (1)	Cel	/FP	S FP>500	FP
Reaction (Preparation)	-	/FA	S FP/FA AND P/MF S REA/FA S PRE/FA	REA
Byproduct	-	/REA.BPR (/PRE.BPR)	S ACETIC ACID/REA.BPRO	REA
Catalyst	-	/REA.CAT (/PRE.CAT)	S 485/REA.CAT	REA
Intermediate	-	/REA.INT (/PRE.INT)	S 1378/REA.INT	REA
Keyword	-	/REA.KW (/PRE.KW)	S SURFACE REACTION/REA.KW	REA
Product	-	/REA.PRO (/PRE.PRO)	S 1949/REA.PRO	REA
Reactant	-	/REA.SM (/PRE.SM)	S 12219/REA.SM	REA
Reagent	-	/REA.RGT (/PRE.RGT)	S CLSO2PH/REA.RGT	REA
Solvent	-	/REA.SOL (/PRE.SOL)	S TOLUENE/REA.SOL	REA
Special Condition	-	/REA.CON (/PRE.CON)	S HIGH PRESSU?/REA.CON	REA
Yield	-	/REA.YD (/PRE.YD)	S 20/REA.YD	REA

(1) Numeric search field that may be searched using numeric operators or ranges.

Electrical Data

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Controlled Term for Electric Effects	-	/CT	S (BI AND NB)/ELS AND ANTIFERROELECTRIC?/CT S CTELE/FA	CTELE
Dielectric Constant (1)	none	/DIC	S CR2K2O7/CMF AND DIC/FA S 0.250E1/DIC	DIC
Frequency (1)	Hz	/DIC.FREQ	S QUARTZ/CN AND DIC.FREQ<1E5	DIC
Pressure (1)	Torr	/DIC.P	S 90<DIC.P<110 BAR	DIC
Substance Physical State	none	/DIC.SSTA	S ANTIMONY TRICHLORIDE/CN AND GASEOUS/DIC.SSTA	DIC
Temperature (1)	Cel	/DIC.T	S DIC.T<250 AND CLH/MF	DIC
Electric Conductivity (1)	S/cm	/ECND	S 0.4E3/ECND	ECND
Keyword	-	/ECND.KW	S DIAGRAM/ECND.KW	ECND
Substance Physical State	none	/ECND.SSTA	S WATER/CN AND SOLID/ECND.SSTA	ECND
Temperature	Cel	/ECND.T	S 20/ECND.T	ECND
Superconductivity	-	/FA	S SCND/FA	SCND
Keyword	-	/SCND.KW	S SUPERCON?/SCND.KW	SCND
Temperature (1)	Cel	/SCND.T	S -0.25E3/SCND.T	SCND

(1) Numeric search field that may be searched using numeric operators or ranges.

GMELIN97**Electrochemical Data**

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Controlled Term for Behavior as Electrode	-	/CT	S BEHAVIOR AS ELECTRODE/CT	CTELEC
Controlled Term for Electrolysis	-	/CT	S CTELEC/FA S ELECTROLYSIS/CT	CTELYS
Controlled Term for Transference Number	-	/CT	S CTELYS/FA S INFORMATION ABOUT TRANS?/CT	CTTRAN
Electrochemical Cell Description	-	/ECELL	S CTTRAN/FA S AMALGAM?/ECELL	ECEL
Electrochemical Cell Potential (1)	V	/ECPOT	S ECCELL S ECOT-<0	ECPOT
Temperature (1)	Cel	/ECPOT.T	S ECOT.T<30	ECPOT
Electrochemical Reaction	-	/FA	S EREA/FA	EREA
Description of Electrode	-	/EREA.DES	S GLASS/EREA.DES	EREA
GRN of Reactant	-	/EREA.SM	S 142079/EREA.SM	EREA
GRN of Product	-	/EREA.PRO	S 1574/EREA.PRO	EREA
Keyword	-	/EREA.KW	S POTENTIAL?/EREA.KW	EREA
Kind of Potential	-	/EREA.TYP	S ANODIC?/EREA.TYP	EREA
Method	-	/EREA.MET	S COULOMETRY/EREA.MET	EREA
Number of Transmitted Electrons (1)	none	/EREA.NE	S 2/EREA.NE	EREA
pH (1)	none	/EREA.PH	S 1/EREA.PH	EREA
Potential (1)	V	/EREA.POT	S 4.05/EREA.POT	EREA
Product	-	/EREA.PRO	S 1574/EREA.PRO	EREA
Reactant	-	/EREA.SM	S 142079/EREA.SM	EREA
Solvent	-	/EREA.SOL	S NITROMETHANE/EREA.SOL	EREA
Stoichiometric Factor of Coreactant (1)	none	/EREA.SMSF	S 4/EREA.SMSF	EREA
Stoichiometric Factor of Product (1)	none	/EREA.PROSF	S 4/EREA.PROSF	EREA
Stoichiometric Factor of Title Compound (1)	none	/EREA.SF	S 2/EREA.SF	EREA
Supporting Electrolyte	-	/EREA.NTE	S ACIDIC MEDIUM/EREA.NTE	EREA
Temperature (1)	Cel	/EREA.T	S 25/EREA.T	EREA
Type of Potential	-	/EREA.TYP	S HALF-WAVE?/EREA.TYP	EREA
Electrolysis Decomposition Potential (1)	V	/ELYPOT	S ELYPOT>2	ELYPOT
Electrolytic Conductivity (1)	S*L/cm *mol	/ELYC	S 136/ELYC	ELYC
Solvent	-	/ELYC.SOL	S NITROMETHANE/ELYC.SOL	ELYC
Temperature (1)	Cel	/ELYC.T	S 25/ELYC.T	ELYC
Equivalent Electrolytic Conductivity (1)	S*cm** 2/val	/EQCOND	S 0.58E2/EQCOND	EQCOND
Ionic Mobility (1)	m**2/V *s	/ION	S 1/PB AND 0.258E-2/ION	ION
Temperature (1)	Cel	/ION.T	S 50/ION.T	ION
Overvoltage (1)	V	/OV	S 3.759/OV	OV
GRN of Electrode Material	-	/OV.GRN	S 16236/OV.GRN	OV

(1) Numeric search field that may be searched using numeric operators or ranges.

Information on Condensed Phases

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Controlled Term for Information about Condensed Phases	-	/CT	S CU2MNSN/MF AND SUPERLATTICE/CT S CTCRY/FA	CTCRY
Crystal Lattice Parameter (1)	ang	/CLP	S 0.073/CLP	CLP
Angle (1)	deg	/CLP.ANG	S 0.9062E2/CLP.ANG	CLP
Keyword	-	/CLP.KW	S ATOMIC POSITIONS?/CLP.KW	CLP
Method	-	/CLP.MET	S NEUTRON DIFFRACTION/CLP.MET	CLP
Number of Formula Units (1)	none	/CLP.NFU	S 5/CLP.NFU	CLP
Temperature (1)	Cel	/CLP.T	S -265/CLP.T	CLP
Crystal Property Description	-	/CPD	S GREY/CPD	CPD
Crystal Space Group (1)	none	/CSG	S 62/CSG	CSG
Crystal System	-	/CSYS	S RHOMBIC/CSYS	CSYS
Bravais	-	/CSYS.BRA	S FACE-CENTERED CUBIC/CSYS.BRA	CSYS
Crystal Type	-	/CTYP	S HGSE/MF AND CSCL/CTYP	CTYP

(1) Numeric search field that may be searched using numeric operators or ranges.

Magnetic Data

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Controlled Term for Galvanomagnetic Effects	-	/CT	S GALVANO?/CT S CTGALV/FA	CTGALV
Controlled Term for Magnetic Phenomena	-	/CT	S FERRITE AND THERMOMAG?/CT S CTMAG/FA	CTMAG
Curie Temperature (1)	Cel	/CUT	S NI/MF AND CUT/FA S 0.357E3/CUT	CUT
Curie-Weiss Temperature (1)	Cel	/CWT	S 0.2<NI<0.8 AND CWT/FA S 7/CWT	CWT
Magnetic Moment (1)	A*cm**2	/MM	S 1E-18<MM<1E-17	MM
Molar Magnetic Susceptibility (1)	ml/mol	/MSUS	S 0.33/MSUS	MSUS
Temperature (1)	Cel	/MSUS.T	S MSUS.T<10K	MSUS
Neel Temperature (1)	Cel	/NET	S 520<NET	NET

(1) Numeric search field that may be searched using numeric operators or ranges.

GMELIN97**Mechanical Properties**

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Controlled Term for Mechanical Properties	-	/CT	S COMPRESSIBILITY/CT	CTMEC
Controlled Term for Molar Volume	-	/CT	S INFORMATION ABOUT MOLAR?/CT	CTMVOL
Density (1)	g/ml	/DEN	S CTMVOL/FA S B5H9/LSF AND DEN/FA S 0.61E0/DEN	DEN
Keyword	-	/DEN.KW	S DIAGRAM/DEN.KW	DEN
Pressure (1)	Torr	/DEN.P	S 760/DEN.P AND CLH/MF	DEN
Reference Temperature (1)	Cel	/DEN.RT	S 4/DEN.RT	DEN
Substance Physical State	-	/DEN.SSTA	S ARSINE/CN AND LIQUID/DEN.SSTA	DEN
Temperature (1)	Cel	/DEN.T	S 4/DEN.T	DEN
Hardness (1)	N/mm**2	/HRD	S NI/MF AND HRD/FA S 1/HRD	HRD
Temperature (1)	Cel	/HRD.T	S NI/MF AND 25/HRD.T	HRD
Type	-	/HRD.TYP	S MICRO HARDNESS/HRD.TYP	HRD
Molar Volume (1)	ml/mol	/MVOL	S 20.9/MVOL	MVOL
Strength (1)	N/mm**2	/STRE	S STRE>1E5	STRE
Temperature (1)	Cel	/STRE.T	S 25/STRE.T	STRE
Type	-	/STRE.TYP	S YIELD POINT/STRE.TYP	STRE

(1) Numeric search field that may be searched using numeric operators or ranges.

Molecular Properties

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Controlled Term for Conformation	-	/CT	S CONFORMATION?/CT	CTCFM
Controlled Term for Electronic Energy Levels	-	/CT	S ELECTRONIC ENERGY LEVELS/CT	CTEST
Controlled Term for Information about Molecules	-	/CT	S CTEST/FA S ANHARMONICITY CONSTANTS/CT	CTMOL
Dipole Moment (1)	D	/DM	S CTMOL/FA S H2O/MF AND DM/FA S 0.30E1/DM	DM
Notes	-	/DM.NTE	S METHODS/DM.NTE	DM
Internuclear Distances and Angles	-	/FA	S GEO/FA AND CLO2/MF	GEO
Method	-	/GEO.MET	S NEUTRON DIFFRACTION/GEO.MET	GEO
Ionization Potential (1)	eV	/IP	S BI CS SB2 SN/MF AND IP/FA S 0.7/IP	IP
Keyword	-	/IP.KW	S FORMATION OF IONS/IP.KW	IP
Method of Ionization	-	/IP.MET	S PHOTOIONIZATION/IP.MET	IP
Type of Ionization	-	/IP.TYP	S ADIABATIC/IP.TYP	IP
Molecular Point Group (2)	-	/CPG	S XEF4/LSF AND CPG/FA S C2H/CPG	CPG
Molecular Rotation Constant	-	/FA	S MRC/FA	MRC
CA (1)	Hz	/MRC.CA	S MRC.CA<1E10	MRC
CB (1)	Hz	/MRC.CB	S MRC.CB<1E11	MRC
CC (1)	Hz	/MRC.CC	S MRC.CC<1E10	MRC
Keyword	-	/MRC.KW	S CENTRIFUGAL?/MRC.KW	MRC
Polarizability (1)	ml	/POL	S C O/MF AND POL/FA S POL>=20	POL

(1) Numeric search field that may be searched using numeric operators or ranges.

(2) The CPG search field presently has the property name Crystal Point Group.

Multicomponent System Data

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Azeotrope	-	/AZE	S 133009/AZE	AZE
Components Forming System	-	/CFS	S 3/CFS	CFS
Controlled Term for Multicomponent Systems	-	/CTM	S METASTABLE PHASES/CTM	CTM
Diffusion Coefficient of Title Compound (1)	cm**2/s	/DIF	S 0.38E-4/DIF	DIF
Other Phase	-	/DIF.PHAS	S ACETONITRILE/DIF.PHAS	DIF
Temperature (1)	Cel	/DIF.T	S 25/DIF.T	DIF
Diffusion in Title Compound	-	/FA	S IDIF/FA	IDIF
Phase	-	/IDIF.PHAS	S O2SI/MF AND HG/IDIF.PHAS	IDIF
Distribution Coefficient (1)	none	/DISTR	S 1.7/DISTR	DISTR
Phase	-	/DISTR.PHAS	S CAPRYLIC ACID?/DISTR.PHAS	DISTR
Temperature (1)	Cel	/DISTR.T	S DISTR.T>200K	DISTR
Eutectic Temperature (1)	Cel	/EUT	S 535/EUT	EUT
Peritectic Temperature (1)	Cel	/PET	S CL3EU AND PET/FA S PET>=12	PET
Solubility	-	/SLB	S 1/CO AND SLB/FA S 9.E0?/SLB	SLB
Solvent	-	/SLB.SOL	S ALCOHOL/SLB.SOL	SLB
Temperature (1)	Cel	/SLB.T	S 195.15K/SLB.T	SLB
Solubility Product	-	/SLBP	S 1998/FRAGGRN AND SLBP/FA S 9?/SLBP	SLBP
pL (1)	none	/SLBP.PL	S SLBP.PL>=1.5	SLBP
Solvent	-	/SLBP.SOL	S WATER/SLBP.SOL	SLBP
Temperature (1)	Cel	/SLBP.T	S SLBP.T>100	SLBP
Sorption of Title Compound	-	/FA	S SPOF/FA	SPOF
Adsorbent	-	/SPOF.PHAS	S THO2/SPOF.PHAS	SPOF
Keyword	-	/SPOF.KW	S EQUATION/SPOF.KW	SPOF
Sorption to Title Compound	-	/FA	S SPTO/FA	SPTO
Adsorbate	-	/SPTO.PHAS	S HEXAFLUORO?/SPTO.PHAS	SPTO
Keyword	-	/SPTO.KW	S DIAGRAM/SPTO.KW	SPTO
Surface Tension (1)	erg/cm **2	/ST	S 29/ST	ST
Substance Physical State	-	/ST.SSTA	S COPPER/CN AND LIQUID/ST.SSTA	ST
Temperature (1)	Cel	/ST.T	S FLUORINE AND ST.T<80K	ST

(1) Numeric search field that may be searched using numeric operators or ranges.

Optical Data

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Controlled Term for Optical Effects	-	/CT	S CIRCULAR DICHROI?/CT S CTOPT/FA	CTOPT
Refractive Index (1)	none	/RI	S 2/RI	RI
Keyword	-	/RI.KW	S BIREFRINGENCE?/RI.KW	RI
Substance Physical State	-	/RI.SSTA	S IODINE/CN AND LIQUID/RI.SSTA	RI
Temperature (1)	Cel	/RI.T	S 25/RI.T	RI
Wavelength (1)	nm	/RI.W	S 200<RI.W<400	RI

(1) Numeric search field that may be searched using numeric operators or ranges.

GMELIN97**Quantum Chemical Calculations**

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Quantum Chemical Calculation Method Type	- - -	/FA /QCC.MET /QCC.TYP	S QCC/FA S EMPIRICAL METHODS/QCC.MET S CORIOLIS COUPLING/QCC.TYP	QCC QCC QCC

(1) Numeric search field that may be searched using numeric operators or ranges.

Spectral Data

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Controlled Term for Mass Spectrum	-	/CT	S MASS SPECTRUM/CT S CTMS/FA	CTMS
Controlled Term for Spectra	-	/CT	S AUGER SPECTRUM/CT S CTSPE/FA	CTSPE
ESR Spectrum	-	/FA	S ESR/FA	ESRS
Keyword	-	/ESRS.KW	S G-FACTORS/ESRS.KW	ESRS
Nuclei	-	/ESRS.NUC	S 97 MO/ESRS.NUC	ESRS
Solvent	-	/ESRS.SOL	S METHANOL/ESRS.SOL	ESRS
Temperature (1)	Cel	/ESRS.T	S -269--253/ESRS.T	ESRS
IR Spectrum	-	/FA	S IRS/FA	IRS
Keyword	-	/IRS.KW	S BANDS?/IRS.KW	IRS
Solvent	-	/IRS.SOL	S METHYLENE DICHLORIDE/IRS.SOL	IRS
Spectral Range (1)	cm** ⁻¹	/IRS.W	S 1968-2023/IRS.W	IRS
Temperature (1)	Cel	/IRS.T	S 300K/IRS.T	IRS
Moessbauer Spectrum	-	/FA	S MOS/FA	MOS
Keyword	-	/MOS.KW	S QUADRUPOLE SPLITTING/MOS.KW	MOS
Nuclei	-	/MOS.NUC	S 99 RU/MOS.NUC	MOS
NMR Spectrum	-	/FA	S NMRS/FA	NMRS
Keyword	-	/NMRS.KW	S LINEWIDTH?/NMRS.KW	NMRS
Nuclei	-	/NMRS.NUC	S 95 MO/NMRS.NUC	NMRS
Solvent	-	/NMRS.SOL	S METHYLENE DICHLORIDE/ NMRS.SOL	NMRS
Spin-spin Coupling Atom	-	/NMRS.SSC	S 31 P/NMRS.SSC	NMRS
Temperature (1)	Cel	/NMRS.T	S K/MF AND NMRS.T<10K	NMRS
NQR Spectrum	-	/NQRS	S NQRS/FA	NQRS
Keyword	-	/NQRS.KW	S QUADRUPOLE SPLITTING/NQRS.KW	NQRS
Nuclei	-	/NQRS.NUC	S 37 CL/NQRS.NUC	NQRS
UV and VIS Spectrum	-	/FA	S UVS/FA	UVS
Keyword	-	/UVS.KW	S SPECTRUM DESCRIBED/UVS.KW	UVS
Solvent	-	/UVS.SOL	S WATER/UVS.SOL	UVS
Spectral Range (1)	nm	/UVS.W	S 566-627/UVS.W	UVS

(1) Numeric search field that may be searched using numeric operators or ranges.

State of Aggregation Phase Transition Properties

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Boiling Point (1) Keyword	Cel	/BP	S 300<BP<330	BP
Pressure (1)	-	/BP.KW	S DECOMPOSITION/BP.KW	BP
Controlled Term for Melting Point	Torr	/BP.P	S ZN/CMF AND 760/BP.P	BP
Controlled Term for State of Aggregation	-	/FA	S CTMP/FA	CTMP
Controlled Term for Sublimation Point	-	/CT	S STATE?/CT	CTSSTA
Controlled Term for Vaporization Point	-	/FA	S CTSSTA/FA	CTSP
Controlled Term for Vaporization Point	-	/FA	S CTSP/FA	CTSP
Critical Density (1)	-	/FA	S CTVP/FA	CTVP
Critical Pressure (1)	g/ml	/CRD	S 5<CRD	CRD
Critical Temperature (1)	Torr	/CRP	S 3E6<CRP<4E6	CRP
Critical Volume (1)	Cel	/CRT	S CRT<500	CRT
Crystal Transition Point (1)	ml/mol	/CRV	S 300<CRV	CRV
Pressure (1)	Cel	/CTP	S 1200<CTP	CTP
Enthalpy of Fusion (1)	Torr	/CTP.P	S CTP.P=38000BAR	CTP
Temperature (1)	J/mol	/HFUS	S HFUS=400+-50	HFUS
Enthalpy of Phase Transitions (1)	Cel	/HFUS.T	S 7.57/HFUS.T	HFUS
Temperature (1)	J/mol	/HPT	S 1950/HPT	HPT
Enthalpy of Sublimation (1)	Cel	/HPT.T	S HPT.T<12	HPT
Temperature (1)	J/mol	/HSUB	S 1E3<HSUB<1E4	HSUB
Enthalpy of Vaporization (1)	Cel	/HSUB.T	S 20<HSUB.T<25	HSUB
Temperature (1)	J/mol	/HVAP	S 8E5<HVAP	HVAP
Entropy of Fusion (1)	Cel	/HVAP.T	S HVAP.T>=78	HVAP
Temperature (1)	J/mol*K	/SFUS	S 70<SFUS<80	SFUS
Entropy of Phase Transition (1)	Cel	/SFUS.T	S 10.35/SFUS.T	SFUS
Temperature (1)	J/mol*K	/SPT	S SPT<1	SPT
Entropy of Sublimation (1)	Cel	/SPT.T	S 13/SPT.T	SPT
Temperature (1)	J/mol*K	/SSUB	S SSUB<100	SSUB
Entropy of Vaporization (1)	Cel	/SSUB.T	S 150/SSUB.T	SSUB
Temperature (1)	J/mol*K	/SVAP	S SVAP=240+-10%	SVAP
Gibbs Energy of Fusion (1)	Cel	/SVAP.T	S SVAP.T<=2.2	SVAP
Temperature (1)	J/mol	/GFUS	S 30<GFUS	GFUS
Gibbs Energy of Phase Transition (1)	Cel	/GFUS.T	S 3.84E2/GFUS.T	GFUS
Temperature (1)	J/mol	/GPT	S 1000<GPT<1200	GPT
Gibbs Energy of Sublimation (1)	Cel	/GPT.T	S GPT.T>35	GPT
Temperature (1)	J/mol	/GSUB	S GSUB>1E5	GSUB
Gibbs Energy of Vaporization (1)	Cel	/GSUB.T	S 1753/GSUB.T	GSUB
Temperature (1)	J/mol	/GVAP	S 10200<GVAP<10600	GVAP
Melting Point (1)	Cel	/GVAP.T	S 50-60/GVAP.T	GVAP
Keyword	Cel	/MP	S 100<MP<105	MP
Pressure (1)	-	/MP.KW	S DECOMPOSITION/MP.KW	MP
Solvent	Torr	/MP.P	S MP.P=10+-1%	MP
Specific Enthalpy of Phase Transition (1)	-	/MP.SOL	S METHANOL/MP.SOL	MP
Sublimation Point (1)	J/g	/SPHPT	S SPHPT>15	SPHPT
Keyword	Cel	/SP	S 100/SP	SP
Pressure (1)	-	/SP.KW	S TABLE/SP.KW	SP
Solvent (1)	Torr	/SP.P	S SP.P<1E-4	SP
Triple Point (1)	-	/SP.SOL	S ACETIC ACID/SP.SOL	SP
Phase	Cel	/TP	S TP/FA AND SE/MF	TP
Triple Point Pressure (1)	-	/TP.PHAS	S TP<=25	TP
Vapor Pressure (1)	Torr	/TPP	S GASEOUS/TP.PHAS	TPP
Substance Physical State	Torr	/VP	S TPP>1E4	TPP
Temperature (1)	Torr	/VP	S C7F15P3/MF AND VP/FA	VP
Temperature (1)	-	/VP.SSTA	S VP<=5	VP
Temperature (1)	Cel	/VP.T	S LIQUID/VP.SSTA	VP
Temperature (1)	Cel	/VP.T	S 25/VP.T AND 15/F	VP

(1) Numeric search field that may be searched using numeric operators or ranges.

GMELIN97**Thermal Properties**

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Thermal Conductivity (1) Substance Physical State	cal/m*s*K -	/TCND /TCND.SSTA	S 2000<TCND<3000 S FLUOROTRICHLOROMETHANE/CN AND LIQUID/TCND.SSTA	TCND TCND
Temperature (1) Thermal Expansion (1) Keyword Substance Physical State	Cel 1/K - -	/TCND.T /TEC /TEC.KW /TEC.SSTA	S TCND.T>1000 S TH>=1 AND .99/TEC S CUBIC?/TEC.KW S LIQUID/TEC.SSTA AND TIN/CN	TCND TEC TEC TEC
Temperature (1)	Cel	/TEC.T	S CAF2/MF AND TEC.T>200	TEC

(1) Numeric search field that may be searched using numeric operators or ranges.

Thermodynamic Properties

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Acentric Factor (1) Controlled Term for Equation of State	none -	/ACEN /CT	S ACEN>=0.03 S EQUATION OF STATE/CT	ACEN CTEQST
Enthalpy of Formation (1) Keyword Pressure (1) Substance Physical State	J/mol - Torr -	/HFOR /HFOR.KW /HFOR.P /HFOR.SSTA	S CL2MG/MF AND HFOR/FA S 0.61058E6/HFOR S DIAGRAM/HFOR.KW S 760/HFOR.P S TECHNETIUM/CN AND LIQUID/HFOR.SSTA	HFOR HFOR HFOR HFOR
Temperature (1) Entropy of Formation (1) Keyword Pressure (1) Substance Physical State Temperature (1)	Cel J/mol*K - Torr -	/HFOR.T /SFOR /SFOR.KW /SFOR.P /SFOR.SSTA	S HFOR.T>1000K S O2TI AND SFOR/FA S 0.3508E3/SFOR S EQUATION/SFOR.KW S 760/SFOR.P S 59212/GRN AND SOLID/SFOR.SSTA	HFOR SFOR SFOR SFOR SFOR
Temperature (1) Gibbs Enthalpy of Formation (1) Keyword Pressure (1) Substance Physical State Temperature (1)	Cel J/mol - Torr -	/SFOR.T /GFOR /GFOR.KW /GFOR.P /GFOR.SSTA	S SFOR.T>1000K S GFOR=1E6+-2E5 S TABLE/GFOR.KW S 760/GFOR.P S 378595/GRN AND SOLID/GFOR.SSTA	SFOR GFOR GFOR GFOR GFOR
Temperature (1) Heat Capacity at Constant Pressure (1) Keyword Pressure (1) Substance Physical State	Cel J/mol*K - Torr -	/GFOR.T /CP /CP.KW /CP.P /CP.SSTA	S 25/GFOR.T S 6E4<CP<8E4 S TABLE/CP.KW S 760/CP.P S PHOSPHINE/CN AND LIQUID/CP.SSTA	GFOR GFOR CP CP CP
Temperature (1) Heat Capacity at Constant Volume (1) Keyword Pressure (1) Substance Physical State Temperature (1)	Cel J/mol*K - Torr -	/CP.T /CV /CV.KW /CV.P /CV.SSTA	S 25/CP.T S CLH/MF AND CV/FA S 0.2080E2/CV S EQUATION/CV.KW S CV.P>100 S MERCURY/CN AND SOLID/CV.SSTA	CP CV CV CV CV
Temperature (1)	Cel	/CV.T	S CV.T=<25	CV

Thermodynamic Properties (cont'd)

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Specific Enthalpy of Formation (1) Keyword Pressure (1) Temperature (1)	J/g - Torr Cel	/SPHFOR /SPHFOR.KW /SPHFOR.P /SPHFOR.T	S SPHFOR>0 S DIAGRAM/SPHFOR.KW S SPHFOR.P=760 S SPHFOR.T=15	HFOR, SPHFOR HFOR, SPHFOR HFOR, SPHFOR HFOR, SPHFOR
Specific Heat Capacity at Constant Pressure (1) Keyword Pressure (1) Temperature (1)	J/g*K - Torr Cel	/SPCP /SPCP.KW /SPCP.P /SPCP.T	S SPCP>3 S DIAGRAM/SPCP.KW S SPCP.P>10 S SPCP.T=500+-10CEL	CP, SPCP CP, SPCP CP, SPCP CP, SPCP
Specific Heat Capacity at Constant Volume (1) Keyword Pressure (1) Temperature (1)	J/g*K - Torr Cel	/SPCV /SPCV.KW /SPCV.P /SPCV.T	S SPCV>0.17 S EQUATION/SPCV.KW S SPCV.P>=760TORR S SPCV.T>4500	CV, SPCV CV, SPCV CV, SPCV CV, SPCV

(1) Numeric search field that may be searched using numeric operators or ranges.

Transport Phenomena

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Dynamic Viscosity (1) Temperature (1)	P Cel	/DV /DV.T	S 40<DV<50 S CLH/MF AND DV.T>200	DV DV
Kinematic Viscosity (1)	St	/KV	S HNAO/CMF AND KV/FA S 0.4251E-1/KV	KV
Substance Physical State	-	/KV.SSTA	S 939985/GRN AND LIQUID/KV.SSTA	KV
Temperature (1)	Cel	/KV.T	S 25/KV.T AND HNAO/CMF	KV

(1) Numeric search field that may be searched using numeric operators or ranges.

DISPLAY and PRINT Formats

Any combination of display fields and formats may be used to display or print answer. Multiple codes must be separated by commas or spaces. The fields are displayed or printed in the order requested.

The default format in the GMELIN97 database is the dynamic display format QRD (Query Related Data) providing information on identification of substance (IDE) plus those display fields in which your search term appears (HIT).

All predefined formats are listed in an hierarchical order with the indented subformats included in the previous format.

Hit-term highlighting is available for the following display fields: GRN, CMF, CN, FN, FRAGMF, FW, LIGLSF, LIGMF, LSF, REV, MOD, RN. Highlighting must be on during search in order to use the HIT, OCC, and QRD (default). If highlighting is set OFF, the default changes to IDE.

Two display formats are available for entries of a certain property of a compound:

```
display : only the first 20 entries are displayed
          e.g.: => D EREA
display F: maximum of 500 entries are displayed
          e.g.: => D FEREA
```

GMELIN97**Substance Identification Formats**

Format	Content	Examples
CMF	Component Molecular Formula	D CMF
CN	Chemical Name	D CN
FA	Field Availability	D 1-4 FA
FN	Family Name	D FN
FRAGMF	Fragment Molecular Formula (includes Fragment Gmelin Registry Number)	D FRAGMF
FW	Formula Weight	D FW
GRN	GMELIN Registry Number	D L5 1-5 GRN
LIGLSF	Ligand Linearized Structure Formula	D LIGLSF
LIGMF	Ligand Molecular Formula	D L5 2 LIGMF
LSF	Linearized Structure Formula	D L4 1-5 LSF
MAC	Alloy Composition Table	D MAC
MF	Molecular Formula	D 3-6 MF
MOD	Modification	D MOD
REV	Revision of Structure	D REV
RN	CAS Registry Number	D RN
RSTR	Related Structure	D RSTR
STR	Structure Image	D STR

Property Formats

Format	Content	Examples
<prop>	First 20 values of a property (molar unit)	D BP
F<prop>	All values of a property (molar unit)	D FCV
FSP<prop>	All values of a property (mass unit) (includes CV, CP, HFOR, HPT)	D FSPCV
SP<prop>	First 20 values of a property (mass unit)	D SPCV
ACEN	Acentric Factor	D ACEN
BP	Boiling Point	D BP
CFS	Components Forming System	D CFS
CPP	Crystal Lattice Parameter	D CLP
CP	Heat Capacity at Constant Pressure	D CP
CPD	Crystal Property Description	D CPD
CPG	Molecular Point Group	D CPG
CRD	Critical Density	D CRD
CRP	Critical Pressure	D CRP
CRT	Critical Temperature	D CRT
CRV	Critical Volume	D CRV
CSG	Crystal Space Group	D CSG
CSYS	Crystal System	D CSYS
CTP	Crystal Transition Point	D CTP
CTYP	Crystal Type	D CTYP
CUT	Curie Temperature	D CUT
CV	Heat Capacity at Constant Volume	D CV
CWT	Curie-Weiss Temperature	D CWT
DEN	Density	D DEN
DIC	Dielectric Constant	D DIC
DIF	Diffusion	D DIF
DISTR	Distribution	D DISTR
DM	Dipole Moment	D DM
DP	Decomposition Point	D DP
DV	Dynamic Viscosity	D DV
ECELL	Electrochemical Cell	D ECELL
ECND	Electric Conductivity	D ECND
ECPOT	Electrochemical Cell Potential	D ECPOT
ELYC	Electrolytic Conductivity	D ELYC

Property Formats (cont'd)

Format	Content	Examples
ELYPOT	Electrolysis Decomposition Potential	D ELYPOT
EQCOND	Equivalent Electrolytic Conductivity	D EQCOND
EREA	Electrochemical Reaction	D EREA
EUT	Eutectic Temperature	D EUT
FP	Flash Point	D FP
GEO	Internuclear Distances and Angles	D GEO
GFOR	Gibbs Enthalpy of Formation	D GFOR
GFUS	Gibbs Energy of Fusion	D GFUS
GPT	Gibbs Energy of Phase Transition	D GPT
GSUB	Gibbs Energy of Sublimation	D GSUB
GVAP	Gibbs Energy of Vaporization	D GVAP
HFOR	Enthalpy of Formation	D HFOR
HFUS	Enthalpy of Fusion	D HFUS
HPT	Enthalpy of Phase Transition	D HPT
HRD	Hardness	D HRD
HSUB	Enthalpy of Sublimation	D HSUB
HVAP	Enthalpy of Vaporization	D HVAP
IDIF	Diffusion in Title Compound	D IDIF
ION	Ionic Mobility	D ION
IP	Ionization Potential	D IP
KV	Kinematic Viscosity	D KV
MM	Magnetic Moment	D MM
MP	Melting Point	D MP
MRC	Molecular Rotation Constant	D MRC
MSUS	Magnetic Susceptibility	D MSUS
MVOL	Molar Volume	D MVOL
NET	Neel Temperature	D NET
PET	Peritectic Temperature	D PET
POL	Polarizability	D POL
QCC	Quantum Chemical Calculation	D QCC
REA (PRE)	Reaction Information	D REA
RI	Refractive Index	D RI
SCND	Superconductivity	D SCND
SFOR	Entropy of Formation	D SFOR
SFUS	Entropy of Fusion	D SFUS
SLB	Solubility	D SLB
SLBP	Solubility Product	D SLBP
SP	Sublimation Point	D SP
SPOF	Sorption of Title Compound	D SPOF
SPT	Entropy of Phase Transition	D SPT
SPTO	Sorption to Title Compound	D SPTO
SSUB	Entropy of Sublimation	D SSUB
ST	Surface Tension	D ST
STRE	Strength	D STRE
SVAP	Entropy of Vaporization	D SVAP
TP	Triple Point Phase	D TP
TPP	Triple Point Pressure	D TPP
VP	Vapor Pressure	D VP
<prop>COM	Several properties belonging together	D BPCOM
BPCOM	BP, HVAP, SVAP, GVAP	D BPCOM 1-3
CLPCOM	CSG, CLP, CTYP, CSYS	D CLPCOM
CRPCOM	CRP, CRT, CRV, CRD	D L5 1-4 CRPCOM
CTPCOM	CTP, GPT, HPT, SPT	D 5 CTPCOM
MPCOM	MP, HFUS, SFUS, GFUS	D L7 1-2 MPCOM
MSUSCOM	MSUS, CUT, CWT, NET	D MSUSCOM 1-7
MULTCOM	EUT, PET	D MULTCOM

GMELIN97**Property Formats (cont'd)**

Format	Content	Examples
SLBCOM	SLB, SLBP	D SLBCOM
SPCOM	SP, HSUB, SSUB, GSUB	D SPCOM
TPCOM	TP, TPP	D TPCOM
CTCFM	Controlled Term for Conformation	D CTCFM
CTCRY	Controlled Term for Information about Condensed Phases	D CTCRY
CTELE	Controlled Term for Electric Effects	D CTELE
CTELEC	Controlled Term for Behavior as Electrode	D CTELEC
CTELYS	Controlled Term for Electrolysis	D CTELYS
CTEQST	Controlled Term for Equation of State	D CTEQST
CTEST	Controlled Term for Electronic Energy Levels	D CTEST
CTGALV	Controlled Term for Galvanomagnetic Effects	D CTGALV
CTGEN	Controlled Term for General Information and Chemical Behavior	D CTGEN
CTMAG	Controlled Term for Magnetic Effects	D CTMAG
CTMEC	Controlled Term for Mechanical Properties	D CTMEC
CTMOL	Controlled Term for Information about Molecules	D CTMOL
CTMP	Controlled Term for Melting Point	D CTMP
CTMS	Controlled Term for Mass Spectrum	D CTMS
CTMVOL	Controlled Term for Molar Volume	D CTMVOL
CTOPT	Controlled Term for Optical Effects	D CTOPT
CTSP	Controlled Term for Sublimation Point	D CTSP
CTSPE	Controlled Term for Spectra	D CTSPE
CTSSTA	Controlled Term for State of Aggregation	D CTSSTA
CTTRAN	Controlled Term for Transference Number	D CTTRAN
CTVP	Controlled Term for Vaporization Point	D CTVP

Tabular Formats

Format	Content	Examples
IDETAB	Table containing GRN, LSF, and CN for a single answer or for several records in a single table	D IDETAB 1-12
MACTAB	Table of alloy compositions containing GRN, component, weight %, atom % for a single answer or for several records in a single table	C 1-3 MACTAB
RNTAB	Table containing GRN and RN for a single answer or several records in a single table	D 2,10 RNTAB D RNTAB
<prop>TAB	Table containing GRN and first 20 values of a property (molar unit) for a single answer or for several records in a single table	D DENTAB
SP<prop>TAB	Table containing GRN and first 20 values of a property (mass unit) for a single answer or for several records in a single table	D SPCVTAB

Predefined Formats

Format	Content	Examples
ALL	All display fields (IDE, PHY, QCC, CHE)	D ALL
IDE	Identification of substance (GRN, RN, MF, CMF, FRAGMF, LIGLSF, LIGMF, CN, FN, FW, LSF, MOD, REV, RSTR, FRAGGRN, MAC, STR)	D L1 IDE
CHE	Chemical Behavior (CTGEN, FP, REA, DP)	D CHE L7 1-3
PHY	Structure and Physical Properties (MOL, PHT, CRY, MEC, THA, TRA, THE, ELE, MAG, OPT, SPE, MCS, ECH)	D PHY L3 1-2
CRY	Information about Condensed Phases (CLP, CPD, CSG, CSYS, CTCRY, CTYP)	D CRY L3
ECH	Electrochemistry (EREA, ECELL, OV, ELYC, CTTRAN, ION, ELYPOT, ECPO, CTELEC, EQCOND, CTELYS)	D ECH L1 1-4
ELE	Electrical Properties (CTELE, DIC, ECND, SCND)	D DIC L10 1-6
MAG	Magnetic Properties (CTMAG, CUT, CWT, MSUS, NET, MM, CTGALV)	D MAG L7 3
MCS	Properties of Multicomponent Systems (AZE, CTM, DIF, DISTR, EUT, PET, IDIF, SLB, SLBP, SPOF, SPTO, ST, CFS)	D MCS L3 1-7
MEC	Mechanical Properties (CTMEC, DEN, HRD, CTMVOL, STRE, MVOL)	D MEC
MOL	Molecular Properties (CPG, CTCFM, CTEST, CTMOL, DM, GEO, IP, MRC, POL)	D MOL L3 1-6
OPT	Optical Properties (CTOPT, RI)	D OPT L1 1-5
PHT (SAG)	Information on Phase Transition ((BP, CTMP, CTSP, CTVP, CRD, CRP, CRT, CRV, CTP, GFUS, GPT, GSUB, GVAP, HFUS, HPT, SPHPT, HSUB, HVAP, MP, SFUS, SP, SPT, CTSSTA, SSUB, SVAP, TP, TPP, VP)	D PHT L2 1-2
THA	Thermal Properties (TCND, TEC)	D THA L1 1-3
TRA	Transport Phenomena (DV, KV)	D TRA L4 1-2
THE	Thermodynamic Data (ACEN, CP, CV, GFOR, HFOR, SPHFOR, SFOR, CTEQST, SPCP, SPCV)	D THE L3 1-4
SPE	Spectroscopic Information (CTSPE, ESRS, IRS, MOS, CTMS, NMRS, NQRS, UVS)	D SPE L3 1-5
QRD	Query Related Data (default) (IDE HIT)	D 5
TRIAL	GRN, MF, CMF, FRAGMF, LIGLSF, LIGMF, CN, FN, FW, LSF, FA	D L3 1-3 TRI
HIT	All fields containing hit terms	D HIT 4
OCC	Fields that contain hit terms and number of times they occur	D L3 4 OCC

GMELIN97**SELECT, ANALYZE, and SORT Fields**

The SELECT command is used to create E-numbers or an L-number containing terms taken from the specified field in an answer set.

The ANALYZE command is used to create an L-number containing terms taken from the specified field in an answer set.

The SORT command is not valid in this file.

Field Name	Field Code	ANALYZE/ SELECT (1)
Azetrope	AZE	Y (2)
CAS Registry Number	RN	Y
Chemical Name	CN	Y
Component Formed in Systema	CFS	Y (2)
Component Molecular Formula	CMF	Y (3)
Electrochemical Reaction	EREA	Y (2)
Family Name	FN	Y
Formula Weight	FW	Y
Fragment Molecular Formula	FRAGMF	Y (4)
GMELIN Registry Number	GRN	Y
Ligand Linearized Structure Formula	LIGLSF	Y
Ligand Molecular Formula	LIGMF	Y
Linearized Structure Formula	LSF	Y
Molecular Formula	MF	Y (default)
Modification	MOD	Y
Preparation	PRE	Y (2,5)
Reaction	REA	Y (2,6)
Related Structure	RSTR	Y (2)
Revision of Structure	REV	Y

- (1) HIT may be used to restrict terms extracted to terms that match the search expression used to create the answer set, e.g., SEL HIT RN.
 (2) SELECT HIT and ANALYZE HIT are not valid with this field.
 (3) Appends /COMP to the terms created by SELECT.
 (4) Appends /FRAG to the terms created by SELECT.
 (5) Selects or analyzes reactants and products with /PRE appended to the terms created by SELECT.
 (6) Selects or analyzes reactants and products with /REA appended to the terms created by SELECT.

GMELIN97**DISPLAY FA**

Field Availability:

Code	Field Name	Occur.
RN	CAS Registry Number	1
MF	Molecular Formula	1
CMF	Component Molecular Formula	1
LIGLSF	Ligand Linearized Structure Formula	1
LIGMF	Ligand Molecular Formula	2
CN	Chemical Name	1
FN	Family Name	1
FW	Formula Weight	1
LSF	Linearized Structure Formula	1
CTCFM	Conformation and Bonding Models/Description of Struc	1
GEO	Information about Internuclear Distances and Angles	1
CPD	Crystal Property Description	1
CLP	Fundamental Crystal Structure Data	1
DEN	Density	2
IRS	Infrared Spectrum	1
UVS	UV and Visible Spectrum	1
REA	Reaction	1
CSYS	Crystal System	1
CSG	Space Group	1