CrossFire Gmelin™ Database Reference Guide

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Introduction

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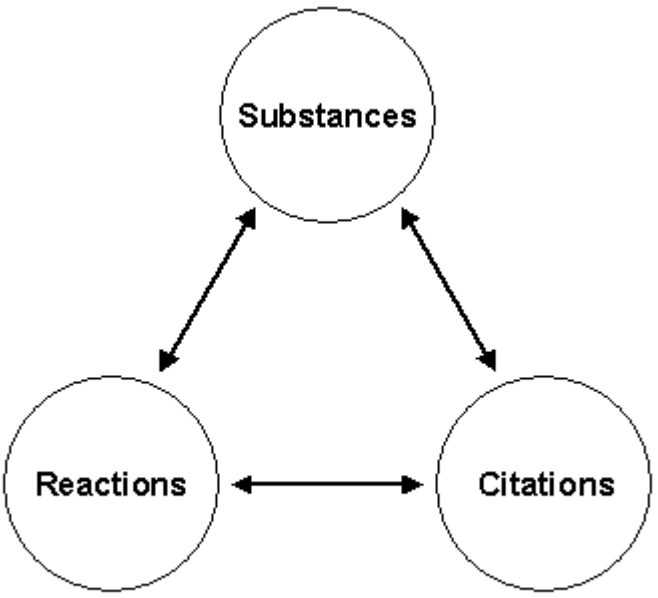
Introduction

The GMELIN File is a database, which contains information about structural, chemical, and physical information on inorganic and organometallic compounds.

This is an implementation under CrossFire. The MDL CrossFire system is a complete chemical information system comprising of the Gmelin Database, the CrossFire search and retrieval server software, and the Commander client.

When using CrossFire, the Commander is configured with a Structure and Reaction editor, a Fact editor and the Display Hits module. These are all linked together through the Commander to give one coherent interface. The Commander provides the means to access the CrossFire databases; allowing searches to be carried out, results displayed, and the database to be browsed - thus giving you the ability to navigate through the world of inorganic and organometallic chemistry.

The CrossFire system provides a new way of handling chemical information. The emphasis is on content, not on form. There are no artificial barriers between the different forms of viewing information. CrossFire allows you to search and display chemical information as you prefer, whether in terms of Substances (structures and properties), Reactions, or Citations and provides hyperlinks between the different forms.



Substances. The database contains a broad variety of chemical and physical parameters for approximately 1.6 million inorganic and organometallic compounds. You can access structures and their associated chemical, physical, and bibliographic information. A specified substance is directly accessible via its unique GMELIN Registry Number, which is assigned during registration of new input. Hyperlinks are available to reactions and literature references, as well as, to other referenced compounds such as precursors or components.

Reactions. The database contains over 1.3 million reactions, which are searchable with CrossFire as reaction substructures. You define the role of a structure or substructure in the reaction mode. Furthermore it is possible to do a factual reaction search or a search combining structural and factual information. Hyperlinks are provided to substances and to literature references.

Properties. The database contains a very broad variety of chemical and physical parameters. The facts of a substance are shown in the field availability list. Hyperlinks are provided to the fact details. You can search for the properties using predefined forms or tabular queries.

Citations. These are stored in a separate domain of the database. This facilitates citation searching and a citation orientated display. It is also possible to search for titles and abstracts. You can display, in one document, all of the compounds and reactions that have been abstracted from the original reference. Hyperlinks are provided to substances, components and reactions.

Hyperlinks. These are provided for substances, reactions and citations. Thus, for example, when you are viewing a reaction one click of the hyperlink calls up the substance record for one of the reaction partners. Similarly, when viewing some properties, simply click the citation hyperlink to call up the citation record showing all the compounds and reactions abstracted from that reference.

Display Context. You can carry out structure searches (on the whole database or on subsets), factual searches, and combined searches. The Display Context of the search, which is usually automatically set at search time (a search for reactions will result in a display in reaction context), can be subsequently changed for either single compound, lists of compounds (or reactions or citations) or for the whole hit set. By using combinations of searches, changes of context and hyperlinks, navigation through the database results in not only solutions to inorganic chemistry problems but can also lead to discoveries by "chance".

Database Contents

There are two different sources for the Gmelin database:

1. The first source of information is the Gmelin Handbook of Inorganic and Organometallic Chemistry, from 1817 to 1975, including all main volumes and supplements. It presents critically evaluated facts based on original literature and systematically arranges for a given substance.

2. The second source of information is a series of 110 scientific journals dealing with inorganic, organometallic, and physical chemistry, as well as, with physics. From these journals inorganic and organometallic compounds, together with their relevant facts, are extracted. Information from this source is from 1975 to the present.

This data source is continuously evaluated and updated to provide data for all data fields.

Acceptance Criteria for Substances

The GMELIN database is a factual database on inorganic and organometallic compounds.

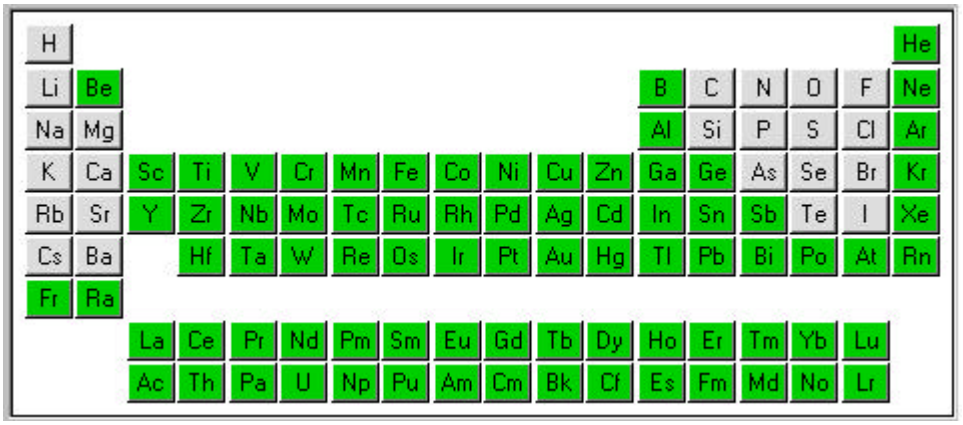
Each substance abstracted (together with its possible components) is assigned a unique number, the GMELIN Registry Number (GRN), during registration procedure. This registry number is the link between structure and data.

The following substances are designated as Gmelin substances:

- all compounds without carbon
- compounds, which contain carbon, containing at least one 'Gmelin element'
- all elements, including carbon (including all modifications and fullerenes)
- alloys and multi-components with carbon components
- carbides and carbideoxides
- carbonic acids and the thio- and seleno-analoges as well as their salts with 'Gmelin cations'

- compounds, in which carbon is present exclusively in the form of cyanide or isocyanide, e.g. HCN, HOCN, HSCN, their isoacids and salts, dicyan, polycyan, cyanamide
- and small molecules like CO, CS, CO2, CS2, COS, or phosgene.

"Gmelin" elements are shaded dark in the periodic table:



All further substances belong to the "organic" domain and can be found in CrossFire Beilstein.

Reference compounds:

If references are made in the preparation or the chemical behavior to starting materials or products, which are defined as Beilstein compounds, and which are necessary for the correct description of the reaction (e.g. iron(III) chloride with pyridine) then the formula and structure of the Beilstein compound is abstracted. However their properties are included in the Beilstein database.

The Gmelin database distinguishes between single - and multi-component compounds.

Single-Component Compounds

These are "classical" compounds having a stoichiometric formula. Substances of this type may consist of one (e.g. oxygen, ferrocene) or more fragments (e.g. salts, adducts).

Substances of this type are:

elements	e.g. H2, Fe, Cu
simple molecules	e.g. H2O, CO2, HCl
inorganic salts	e.g. NaCl, Na2SO4, KMnO4, KOH, CaTiO3
adducts	e.g. Na2SO4*10H2O, CoCl2*4NH3
coordination compounds	e.g. Fe(C5H5)2, Mo(CO)6, [Co(NH3)6]Cl3, [Co(NH3)5(SCN)]Cl2
polymers	e.g. (HF)n, {Pt(CO)2}n, {Fe(C5H4)2}n
solid solutions (exact formula)	e.g. Na0.5K0.5Cl, Ca0.2Y0.8Ba2Cu3O6.78
minerals	e.g. dolomite CaMg(CO3)2, pyrite FeS2
alloys (as formula)	e.g. Fe0.66Pd0.34, Ni45Zr55, Cu2TiAl
glasses / ceramic materials (as formula)	e.g. BaTiO3, SiO2, YBa2Cu3O(x)

Single-component compounds are divided into fragments, if they consist of discrete polyatomic ions or molecules. The individual fragments are separated from one another by asterisks (*) in a linearized molecular formula.

Rules on whether a compound is fragmented or not are as follows.

1. Solid state structures, ionic compounds:
   - Substances are divided into formal fragments if the compounds contain at least one discrete polyatomic ion or molecule in the crystal, the gas phase, the liquid phase, or in solution. The structures of these discrete ions or molecules are available.
     e.g. 2Na(1+)*SO4(2-)=Na2SO4
     e.g. K(1+)*MnO4(1-)=KMnO4
     e.g. 2Na(1+)*SO4(2-)*10H2O=Na2SO4*10H2O
     e.g. Ca(2+)*Mg(2+)*2CO3=CaMg(CO3)2

- Substances are not divided into fragments, if the compounds consist exclusively of single-atomic ions (including OH-, SH-, SeH-, and TeH-), e.g. NaCl, KOH,
  or have no discrete polyatomic ion or molecule, e.g. CaTiO3

2. Organometallic and coordination compounds:

- Organometallic compounds and coordination compounds with known manner of ligand coordination are stored with the complete formula and structure.
  e.g. Fe(C5H5)2

- Organometallic salts and ionic coordination compounds with known manner of ligand coordination are divided into cations and anions. The complete structures of the ions are available.
  e.g. [Co(NH3)6](3+)*3Cl(1-)=[Co(NH3)6]Cl3

- Organometallic compounds and coordination compounds with unknown manner of ligand coordination are divided into fragments by separating all ligands from the metal center.
  e.g. If there is an unknown coordination of thiocyanate to Co(3+) in [Co(NH3)5(SCN)]Cl2 (coordination by N or S atom possible), the formula is given as Co(3+)*5NH3*SCN(1-)*2Cl(1-)
  =[Co(NH3)5 (SCN)]Cl2.

Multi-Component Compounds

Multi-component compounds consists of two or more single-component compounds having no stoichiometrical relationship to each other. Each single-component compound may consist of one or more fragments. For multi-component compounds the linearized formulas of individual compounds are separated from one another by a hush (#).

Substances of this type are:

Description	Gmelin formula	components
(multi-component) systems		
e.g. zinc oxide and titanium oxide	ZnO#TiO2	ZnO and TiO2
e.g. lead sulfate, lead oxide and silicium dioxide	PbSO4#PbO#SiO2	PbSO4 and PbO and SiO2
Solutions		
aqueous solution of sodium chloride	NaCl#H2O	NaCl and H2O
aqueous solution of lithium nitrate	LiNO3#H2O	LiNO3 and H2O
solution of aluminium chloride in phosgene	AlCl3#COCl2	AlCl3 and COCl2
doped compounds		
silicon doped with boron nitride	Si#dotBN	Si and BN
Tin-doped indium(III) oxide	In2O3#dotSn	In2O3 and Sn
Cadmium titaniumhexafluoride hexahydrate doped with manganese(2+)	CdTiF6*6H2O#dotMn(2+)	CdTiF6*6H2O and Mn(2+)
solid solutions (with formula range or undefined formula)		
solid solution of zinc sulfide (range x=0-015) and zinc selenide	ZnS(x)Se(1-x) x=0-0.15	ZnSe and ZnS0.15Se0.85
solid solution of sodium sulfate and cesium sulfate	Na2SO4#Cs2SO4	Na2SO4 and Cs2SO4
solid solution of potassium chloride and potassium bromide	K(Cl,Br)	KCl and KBr

note: the description of solid solutions is dependent on the author's declaration

alloys (in percentage)

iron alloy containing 30 weight% molybdenum and 5 weight% nickel	Fe(75)Mo(20),Ni(5) (W)	Fe and Mo and Ni

glasses / ceramic materials (in percentage)

silicium dioxide glass containing 10-15 weight% aluminium oxide and 10-15 weight% boron oxide	Al2O3(10-15),B2O3(10-15), O2Si (W)	Al2O3 and B2O3 and SiO2

According to the fragmentation rules of single-component compounds, the following examples mentioned in the table are divided into fragments. Each single-component compound is viewed isolated on fragmentation:

Pb(2+)*SO4(2-)=PbSO4#PbO#SiO2

Li(1+)*NO3(1-)=LiNO3#H2O

Cd(2+)*TiF6(2-)*6H2O=CdTiF6*6H2O#dotMn(2+)

2Na(1+)*SO4(2-)=Na2SO4#2Cs(1+)*SO4(2-)=Cs2SO4

Note:

Multi-component compounds have no overall molecular formulas, because there is no stoichiometric relationship between the single components.

Registry Criteria

There can be more than one GMELIN Registry Number for the same Molecular Formula.

The following critera are used to assign a compound its own GMELIN Registry Number:

- Molecular Formula MF
- Structure STR

  comprising the connectivity of atoms, total charge of fragments or compounds, and stereo descriptors
- The types of substance TYPE
- glasses or ceramic materials
- isomorphous or diadochous compounds,

  solid solutions isotopes or isotope containing compounds, minerals, polymers

  Note: The family names alloys and coordination compounds are not criteria for registration
- Modification MODTXT

The chemical name of a substance is not a criterion for registration

The substance physical state is only displayed within the relevant facts:
DIC, ELCO, ST, COM, MVOL, DEN, RI, VP, VPFI, TCND, TEC, CV, CVFI, CP,CPFI GFOR, GFFI, HFOR, HFFI, SFOR, SFFI, DYVI, and KIVI.

Acceptance Criteria for Attributes

Acceptable data for the Gmelin database falls into the following categories:

1. Characterization / Identification
2. General Information
3. Physical Properties
4. Properties of / in Systems
5. Quantum Chemical Calculations
6. Electrochemistry
7. Chemical Properties
8. Bibliographic Information

The general rules for accepted data will be discussed in the relevant chapters. Subjects are sorted in hierarchical order. To find information for a specific topic, use the Help index or the Help Find function.

Database Searching

CrossFire Gmelin offers you different ways of searching:

- searching for compounds either via characterization criteria or via structure
- searching for reactions either via factual fields or via structure
- searching for physical and chemical properties
- searching for bibliographic information

All of these topics can be combined with each other.

Structures:

Full structures, substructures, generic structures, and stereoisomers can be searched for. You can use global query options such as "Free Sites on All Atoms", or set options on specific atoms and bonds. Query atom types such as "X", to designate any halogen can be set as well as Atom lists (e.g. A1= Fe, Co, Ni). Predefined generic groups, e.g. ALK (alkyl), and user defined generic groups are easily attached.

Note:

You should be aware that only compounds or compound parts, which are formed by discrete molecules or ions, have a structure. Compounds with a solid-state structure will not have a structure in the Gmelin database.

Reactions: The role of a substance (reactant or product) can be defined in the reaction mode of the structure editor.

Thus you can search for the following reaction types:

? => B	"how do I make this type of compound"
A => ?	"what do these starting materials give"
A => B	"general or specific transformations".

Properties: A very broad variety of chemical and physical data can be searched for as numeric values and ranges, strings, and keywords. The CrossFire database contains more than 6 million reports on chemical and physical properties. You can search for molecular formulas, reaction conditions, electric, or magnetic data. All of these are stored in discrete fields.

Searching for Facts

The database contains numerical and textual data in more than 800 searchable fields. Searching is carried out using the **Fact Editor**, where the matrix form, field name lists, and index expand buttons make the query formulation straightforward. High flexibility is given by option to carry out numerical, text, field availability, and hierarchical searching. A successful search retrieves records, each of which contain all the information of a particular substance, reaction, or citation in the database. For information on structure and reaction searching, and displaying hit lists, see the relevant chapters.

- Substance Factual Search
- Reaction Factual Search
- Citation Factual Search
- Numerical Search
- Text Searching
- Keyword Searching
- Truncation
- Operators
- Field Availability Search
- Hierarchical Group Code Search

Substance Factual Search

This is a search specific for substance related facts in the database. Whether numeric, numeric range, string, or keywords, you will retrieve all substances in the database which contain the matching terms. The display context is automatically set to Substance. This type of search applies to most of the fields in the database, with the exceptions of reactions and citations.

See also: Basic Index for Substances

Reaction Factual Search

This is a search specific for graphical reaction related facts. The display context will automatically be set to Reactions.

See also: Basic Index for Reactions.

Citation Factual Search

This is a search specific to citation related fields. The display context will automatically be set to Citation.

See also: Basic Index for Citations

Numerical Search

The GMELIN file contains more than 100 search fields with numeric data for chemical and physical properties of substances.

In numerical fields searching can be carried out for single value or ranges, as well as, greater than/less than a certain value. The values of physical properties and parameters are stored in the units and dimensions of the CrossFire Database, these are the units and dimensions most commonly used in inorganic chemistry and are, therefore, not necessarily SI units.

For searching a single value, e.g. a melting point (field code mp) at 223°C, the following values and ranges may be employed:

- the exact temperature 223°C
- the range from e.g. 220 - 225°C (temperature is within the range)
- the ranges from e.g. 220 - 223°C and 223 - 225°C (temperature is either upper or lower limit of the range)

When searching for a range, e.g. melting point mp=220-225, all records will be retrieved where the value falls within this range, no matter whether they are derived from a single value or a range.

Numerical values are also present in some string fields, where they are searchable as strings.

Scientific Notation

Numeric values of physical properties may cover a large range of numbers, for example, from 1.88E-53 mol**2/l**2 for the solubility product of the alpha modification of mercury(II) sulfide in water at 25 °C to 5.309E13 Hz for the molecular rotation constant about a particular axis of the Ar*HCONH2 molecule. For this reason the scientific notation for numbers is used throughout to display numerical values.

Text Searching

Searching for strings or partial strings can be carried out in text fields. To search for a partial string use the (Sprung) wild card symbols. It is highly recommendrd to look in the index and use "Expand Field", to check the spelling of terms before carrying out a search. Index terms can be directly copied into the Fact Editor for searching.

The text fields are indexed in several ways:

String (Phrase)

The complete string is indexed without splitting:

e.g. Molecular Formula, Keyword Fields

String (Wordwise)

The entry is split into words using the following symbols:

. , ; : ( ) < > [ ] { } / = ? * + - # ! $ % space

These symbols will not be found in the index, and should therefore not be searched for.

Keyword Searching

Many topics in the Gmelin database have fields of the type Description. These fields contain entries, which usually derive from a controlled vocabulary. These keywords are indexed as phrases and can be searched as a typical text field.

It is recommended always to use the expand function of the CrossFire system before starting a search. The keywords can be copied out of the list into the edit mask for searching.

Truncation

All text fields can be searched by using truncation (wild card) symbols.

*	any number of characters (including no character)
?	any single character
??	any two characters

Both right, left, and middle truncation are allowed.

Left truncation is useful for phrase fields where the searched for term occurs within the phrase.

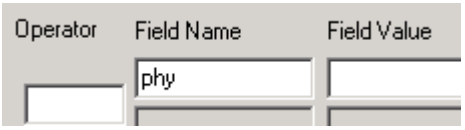
Right truncation is useful for free text fields, e.g. Abstracts, to make sure that all occurrences of a term are found. Thus, to retrieve the records with both photochemistry and photochemical the following should be input:

ab=photochem*

It is also particularly useful for the Authors fields, due to the different rules used by journals. Author's first names are often written differently in various journals. Right truncation can be used to ensure that all articles of a particular author are found.

Field Availability Search

This is a search for the occurrence of a fact in the database. Thus you can search for all compounds with physiological information by entering PHY in the Field Name column and leaving the Value column empty.



Hierarchical Group Code Search

This is a search for the presence of data in any specified group of fields. Data fields are grouped together according to the hierarchy of the Gmelin Database. The group fields, e.g. Spectral Information (SPE) (which identifies all particular data fields concerned with spectral data information) are searchable using their group codes.

Thus you can carry out a search for compounds for which at least one piece of information from any type of spectral data, e.g. NMR, IR, etc., is available by entering SPE in the field name column.

Operators

In the operator column of the Commander Fact Editor and in the Fact Query Window, the Boolean operators AND, NOT, OR, and PROXIMITY can be input. For search in text fields the two additional operators NEAR and NEXT are also available:

AND Operator

OR Operator

NOT Operator

PROXIMITY Operator

NEAR Operator

NEXT Operator

AND Operator

With this Boolean operator the two connected search terms will only be retrieved as a hit if they are present in the same record.

e.g. mp > 1000 AND tec < 0

This search will result in a list of compounds, where the compounds melt above 1000°C and have negative expansion coefficients.

When using this operator with hit lists, e.g. from structure searches, the resulting list will only contain those records present in both original lists.

e.g. .q1 AND .q2

OR Operator

This Boolean operator retrieves only hit lists in which the individual records contain at least one of the search terms.

e.g. mp > 1000 OR tec < 0

This search will result in a list of compounds, where either the compounds melt above 1000°C or have negative expansion coefficients (including records with both properties).

When using this operator with hit lists, e.g. from structure searches, the resulting list will contain all records from both original lists.

e.g. .q1 OR .q2

NOT Operator

This Boolean operator retrieves only those records from the first hit set not present in the second hit set.

e.g. type = "alloy" NOT (elc = "Fe" OR elc = "Ni")

This example will retrieve all alloys without the elements iron or nickel.

When using this operator with hit lists, e.g. from structure searches, the resulting list will contain all records from the first list minus all records from the second list.

e.g. .q1 NOT .q2

PROXIMITY Operator

This operator is a version of the AND operator, whereby the two connected search terms will only be retrieved as a hit if they are present in the same occurrence of a fact. This operator is very important when searching for facts that contain sub-fields or parameter fields.

Thus when searching for a boiling point measured at a particular pressure, the PROXIMITY operator should be used to ensure that both retrieved terms come from the same occurrence of the Boiling Point fact.

e.g. bp = 120 PROXIMITY bp.p = 750-760

This example will retrieve all compounds having a boiling point of 120 ° C measured in the pressure range of 750 to 760 Torr.

NEAR Operator

This operator retrieves hit lists in which the individual records always contain both of the search terms and are adjacent to each other.

e.g. ab=crystal* NEAR ab=structure*

NEXT Operator

This operator retrieves hit lists in which the individual records always contain both of the search terms and where the first search term will appear before the second search term.

e.g. ab=solid* NEXT ab=state*

Description of Data Fields

The description of data fields will be illustrated using the field MSUS as an example:

Description:

The volumetric magnetic susceptibility is the difference in the magnetic permeability of a substance and of vacuum, divided by the permeability of vacuum. The specific (or mass) magnetic susceptibility of a substance is the quotient of its volumetric susceptibility and its density. The molar magnetic susceptibility of a substance is the product of its volumetric susceptibility and its molar volume. The Magnetic Susceptibility (specific: MSUS.VALA, molar: MSUS.VALO) field contains the values for a given substance in the literature**.** The search field is a numerical range search field and is linked to the associated temperature MSUS.T. Further information about the magnetic susceptibility is given as diagram or equation using the parameter field codes MSUS.DGM and MSUS.EQN respectively. Information about pretreatment of samples, or concentration of solutions, is given in the field remarks MSUS.MR.

Note:

Searching for magnetic susceptibility diagrams or equation field codes requires the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing	Unit
MSUS.VALO	Molar Magnetic Susceptibility	numerical	ml/mol
MSUS.VALA	Specific Magnetic Susceptibility	numerical	l/kg
MSUS.T	Temperature	numerical	°C
MSUS.DGM	Diagram	string (phrase)	
MSUS.EQN	Equation	string (phrase)	
MSUS.MR	Remarks	string (phrase)	

The GMELIN File offers approximately 800 textual, numeric, and flag fields. In general, flag fields can be searched by their group codes. However, if the flag field is part of further data fields of a group code, it is indexed as a string with a controlled term. The corresponding field value is given in the note. For an easy search you can generally use wildcards ("*").

Physical properties can appear as molar or specific and are stored in individual fields with the extension property.valo (molar) and property.vala (specific).

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Data Fields

Data Fields

Data Fields

The GMELIN Database is organized hierarchially. The following is the top level of the hierarchy:

BI	Basic Indexes
CHAR	Characterization
GEN	General Information
PHY	Physical Properties
MCS	Properties of / in Systems
EC	Electrochemistry
CHE	Chemical Properties
QCC	Quantum Chemical Calculations
BIB	Bibliographic Information

Basic Indexes (BI)

Basic Indexes are collective indexes, which allow convenient searching without thinking about field codes. The Gmelin database offers the following Basic Indexes.

Search Fields:

BISUB	Substance Basic Index
BIREA	Reaction Basic Index
BICIT	Citation Basic Index
AGRN	All GRN References

Substance Basic Index (BISUB)

Description:

This is the basic index for substances. If a user enters keywords and operators, such as "and", "or" or "not", in the fact window of the Commander, without specifying a field name and with staying in the substance context, the keywords will automatically be searched in this index.

The Substance Basic Index contains the following fields:

Field Code	Field Name
RN	CAS Registry Number
CN / .EDN / .PRO	Substance Names
.PA / .PHAS*	Chemical Partners
.TYP	Specification to Facts
.MET	Methods
.MR	Remarks

The substance basic index belongs to the substance context and a search will result in a substance/structure hitset.

Type of Indexing:

string (wordwise)

except: CAS Registry Number – string (phrase)

Example:

Search for all substances with the information "triphos":

Field Name	Field Value
BISUB	triphos

The hits show the ligand itself, as well as, compounds containing the ligand.

You should be aware that only those substances are retrieved having a name assigned.

Example:

Search for all substances with the information "pressure":

Field Name	Field Value
BISUB	pressure

Substances are retrieved having properties depending on pressure.

Reaction Basic Index (BIREA)

Description:

This is the basic index for reactions. If a user enters keywords and operators, such as "and", "or" or "not", in the fact window of the CrossFire Commander without specifying a field name and with staying in the reaction context the keywords will automatically be searched in this index.

The Reaction Basic Index contains the following fields:

Field Code	Field Name
RX.RCT	Reactant (name)
RX.PRO	Product (name)
RX.RGT	Reagent
RX.BPRO	Byproduct
RX.INT	Intermediate (name)
RX.CAT	Catalyst
RX.SOL	Solvents
RX.SCON	Special Conditions
RX.GCON	General Conditions
RX.ISOL	Purification, Isolation

The reaction basic index belongs to the reaction context and a search will result in a reaction hitset.

Type of Indexing:

string (wordwise)

Example:

Search for irradiation reactions:

Field Name	Field Value
BIREA	irradiation

Example:

Search for all reactions with the information "mechanism":

Field Name	Field Value
BIREA	mechanism

The hits show reactions with descriptions of reaction mechanism in the articles.

Citation Basic Index (BICIT)

Description:

This is the basic index for citations. If a user enters keywords and operators, such as "and", "or" or "not", in the fact window of the Commander without specifying a field name and with staying in the citation context the keywords will automatically be searched in this index.

The Citation Basic Index contains the following fields:

Field Code	Field Name
AU	Author
JT	Journal Title
JTT	Journal Title (Translation)
TI	Article Title
AB	Article Abstract
AB.KW	Article Abstract Keywords

The citation basic index belongs to the citation context and a search will result in a citation hitset (reference list).

Type of Indexing:

string (phrase)

except: title, abstract – string (wordwise)

Example:

Search for all documents with the information "enzym*":

Field Name	**Field Value**
BICIT	enzym*

The hits show documents containing phrases like enzymes, enzymatic activity, enzymatic methods, and enzymatic reactions in titles, keywords, and abstracts.

Example:

Search for all documents with the information "industr*":

Field Name	Field Value
BICIT	industr*

Documents are retrieved containing phrases like chemical industry, industrial processes, industrial applications, and industrial tools in titles, keywords, and abstracts.

All GRN's (AGRN)

Description:

This is the basic index for Gmelin Registry Numbers (GRN's).

This basic index belongs to the substance context and a search will result in a substance/structure hitset.

The basic index contains the following fields:

Field Code	Field Name
GRN	Gmelin Registry Number
FRAGRN	Fragment Gmelin Registry Number
CGRN	Component Gmelin Registry Number
MULT.GRN	System Component Registry Number
AZE.PG	Azeotropes (GRN)
POT.EGRN	Electrochemical Coreactant(s) (Registry Number)
POT.PGRN	Electrochemical Product(s) (Registry Number)

Notes:

It is especially useful where referenced compounds need to be found.

Type of Indexing:

numerical

Example:

Search for all substances containing GRN 171518 (= KH(HCO2)2):

Field Name	Field Value
AGRN	171518

The first hits show the single-component compound KH(HCO2)2. The second hit is a multi-component compound, the solution of KH(HCO2)2 in HCO2H having KH(HCO2)2 as component.

Example:

Search for all substances containing GRN 8908 (= BaTiO3):

Field Name	Field Value
AGRN	8908

The hits show all substances having BaTiO3 as component, e.g. doped compounds, ceramic materials, or systems. Furthermore, hits are retrieved with BaTiO3 as system component.

Characterization (CHAR)

Search Fields:

IDE	Identification of Substance
FOR	Formula Search Data
CMPS	Composition
LIG	Ligands around Metals

Identification of Substance (IDE)

Search Fields:

GRN	GMELIN Registry Number
MOFO	Search MF Range
ALLOY	Alloy Search Field
LSF	Linearized Structure Formula
MF	Molecular Formula
FRAGMF	Fragment Molecular Formula
FRAGRN	Fragment GMELIN Registry Number
LIGMF	Ligand Molecular Formula
LIGFO	Ligand Formulas
LIGFC	Ligand Formula Count
NC	Number of Components
NFRAG	Number of Fragments
NSTRUC	Number of Structures
MW	Molecular Weight

RN	CAS Registry Number
CN	Chemical Name
CNS	Chemical Name Segment
TYPE	Type of Substance
MODTXT	Modification
ED	Entry Date
UPD	Update Date

See also:

LIG	Ligands around Metals
FOR	Formula Search Data
CMPS	Composition

GMELIN Registry Number (GRN)
Description:

The numerical search field GMELIN Registry Number contains the accession number, which is assigned at the registration of a substance. This number is unique for a given substance and depends on the formula, structure, modification, and the family names isotope or isotope containing compounds, mineral, polymer, isomorphous or diadochous compound, solid solution, and glass or ceramic material.

Note:

The chemical name of a substance is not used as a criterion for the assignment of the GMELIN Registry Number.

Type of Indexing:

numerical

Related Information:

AGRN

Example:

Search for	Field Name	Field Value
substance with the Gmelin Registry Number 3385	GRN	3385

Search MF Range (MOFO)

Description:

The MOFO field is a non-display field that allows the search of compounds by normal chemical formula using chemical symbols in capital and small letters as well as the search of ranges with molecular formula. It is not possible to have a look at this field via the expand command, because it is calculated "on the fly" during the search.

Tips and Hints:

1. If you want to restrict searches to compounds with a specific number of components or fragments it is necessary to combine the query with restrictions in the field NC or NFRAG, respectively. Otherwise, multi-component compounds with a spread combination of the entered elements will also be found.
   For example, to search for a one-component compound, NC = 1 has to be set additionally.
   This is a powerful search code for formulas, especially when searching for inorganic compounds without molecular structures.
2. You can search for molecular formulas with stoichiometric range (see example (e)).

3. The symbols greater than/less than (<>) are not allowed, instead you must enter a large range; for example, more than three Oxygen atoms can be input as in (f).

4. You can search for certain molecular formulas by typing an asterisk at the end of a value (see example (g)).

Type of Indexing:

string (phrase)

Examples:

	Search for	Field Name	Field Value
(a)	sodium chloride	MOFO	NaCl
(b)	sodium sulfate	MOFO	Na2SO4
(c)	iron(III) chloride with 6 ammonia	MOFO	FeCl3*6 NH3
(d)	tris(tetrabutylammonium) hexakis-(thiocyanato) osmate(III)	MOFO	(N(C4H9)4)3[Os(SCN)6]
(e)	zirconium oxides with defined zirconium and oxygen range Zr: 1-3, O: 1-5	MOFO	Zr(1-3)O(1-5)
(f)	yttrium barium copper oxides with variable O content (>3)	MOFO	YBa2Cu3O(4-99)
(g)	any dodecamolybdates	MOFO	Mo12O40*

Alloy Search Field (ALLOY)

Description:

The alphanumerical search field Alloy Search Field allows the search of alloys, glasses and ceramic materials specified by percentages. The content of each constituent, an element or compound, can be specified by a percentage value or range. Additionally the form of the percentage information must be specified as

?	A	atom or mol percent
?	V	volume percent
?	W	weight percent
?	X	indefinite percent.

Note:

Compounds have to be entered using "Hill order".

Constituents in traces are specified as 0 %.

Tips and Hints:

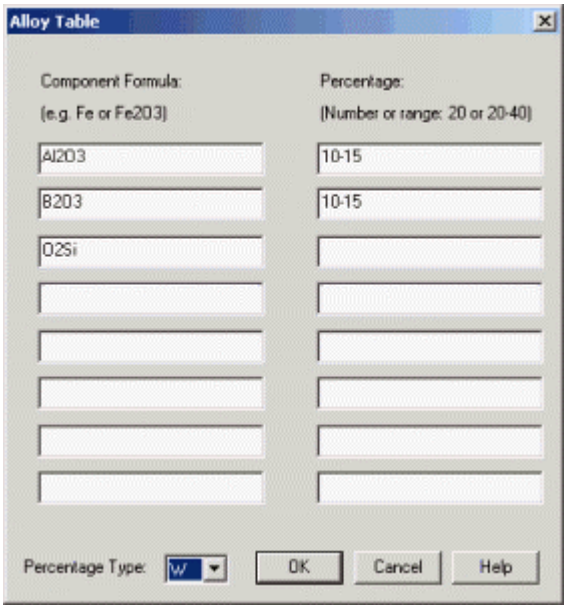
Use the alloy table (button F2) for search input.

Type of Indexing:

string (phrase)

Example:

Search for a silicium dioxide glass with 10-15 weight% Al2O3 and 10-15 weight% B2O3.



being equivalent to

query: alloy="Al2O3(10-15),B2O3(10-15),O2Si (W)"

Linearized Structure Formula (LSF)

Description:

The alphanumerical search field Linearized Structure Formula contains a linear representation of the structure of a compound. The formula may contain isotopes.

Compounds are divided into fragments, if discrete polyatomic ions, molecules, or ligands with unknown coordination exist. For multi-fragment compounds the molecular formulas of individual fragments are separated from one another by asterisks (*).

For systems, the formulas of individual compounds are separated from one another by a hush mark (#). Each compound can consist of several fragments.

For doped compounds, the formulas of the dopants are separated from the basis compound by the designation ‘#dot’.

Note:

If a compound includes an adduct, which has undefined prefix-factor, this adduct is formulated with the prefix-factor 99.

Tips and Hints:

Searches for compounds with isotopes or multi-fragment compounds with their reported stoichiometric multipliers as well as for doped materials and systems can be carried out using this field.

Type of Indexing:

string (phrase)

Examples:

	Search for	Field Name	Field Value
(a)	sodium carbonate	LSF	2Na(1+)*CO3(2-)=Na2CO3
(b)	hydrated nickel acetate	LSF	Ni(2+)*2CH3COO(1-)*99H2O= Ni(CH3COO)2*99H2O
(c)	boron doped silicium	LSF	Si#dotB
(d)	aqueous solution of sodium chloride	LSF	NaCl#H2O
(e)	system of zinc oxide and titanium dioxide	LSF	ZnO#TiO2

Molecular Formula (MF)

Description:

The alphanumerical search field Molecular Formula contains the molecular formula of a substance. Within multi-component compounds, each component is searchable separately.

Note:

The Molecular Formula has to be entered using "Hill order".

The formulas are arranged as follows:

- Carbon containing compounds are ordered
- number of carbon atoms
- number of hydrogen atoms
- alphabetic order of elements
- Non carbon containing compounds follow
- alphabetic order of elements

Hint:

Searching a specific compound in the MF field excludes all isotope labeled compounds. Searching an isotope molecular formula exactly hits the isotopic labeled compounds specified in the query.

Type of Indexing:

string (phrase)

Examples:

	Search for	Field Name	Field Value
(a)	sodium acetate	MF	C2H3NaO2
(b)	sodium chloride	MF	ClNa
(c)	sodium sulfate	MF	Na2O4S
(d)	Hafnium	MF	Hf
(e)	hydrofluoric acid	MF	FH

Fragment Molecular Formula (FRAGMF)

Description:

The search field fragment molecular formula contains the molecular formula of a fragment. It can be used to retrieve all compounds containing a given fragment (and the fragments themselves).

Note:

The fragment molecular formula has to be entered using "Hill order".

Tips and Hints:

The fragment molecular formula is combined with the order of the corresponding component. Therefore, a common search should be done by combination of the fragment molecular formula with an asterisk (*).

Type of Indexing:

string (phrase)

Examples:

	Search for	Field Name	Field Value
(a)	substances containing acetate fragments	FRAGMF	C2H3O2(1-)*
(b)	substances containing acetate fragments (in single-component compound)	FRAGMF	C2H3O2(1-):1
(c)	substances containing acetate fragments (in two-component compound)	FRAGMF	C2H3O2(1-):2
(d)	substances containing cyclotetraphosphate fragments	FRAGMF	O12P4(4-)*
(e)	substances containing hexacyanoferrate(III) fragments	FRAGMF	C6FeN6(3-)*

Fragment GMELIN Registry Number (FRAGRN)

Description:

The numerical search field, Fragment GMELIN Registry Number, contains the accession number which is assigned at the registration of a fragment. This number is an unambiguous identifier for the different fragments present in a multi-fragment compound.

Type of Indexing:

numerical

Example:

Search for	Field Name	Field Value
substances with the Fragment Gmelin Registry Number 2120	FRAGRN	2120

Ligand Molecular Formula (LIGMF) Description:

The alphanumerical search field Ligand Molecular Formula contains the abstract formula of the coordination centers and all ligand codes of a compound. The ordering of the formula is as follows:

1. all metal centers (ordered alphabetically)
2. the ligand codes (see LIGFO) are ordered in the following manner:
3. A, CN, CNO, CNR, CNS, CO, CS, D, L, Q, X
4. within the same ligand types, they are ordered on ascending denticity and the frequency is not taken into consideration

Note:

Charges are not taken into account.

Tips and Hints:

Searches for compounds using the GMELIN Ligand Search System are very powerful to look for a class of complexes with special connectivity.

Type of Indexing:

string (phrase)

Related Information:

LIG.LIGMF

Examples:

	Search for	Field Name	Field Value
(a)	hexa carbonyl chromium	LIGMF	Cr{CO}6
(b)	tetra halogeno palladium compounds	LIGMF	Pd{X}4
(c)	copper complexes with two halogenides and two ligands connecting by chalcogen atoms	LIGMF	Cu{Q}2{X}2
(d)	Platinum complex with two substituted isocyanide, one ligand connecting by pnictide atom and one ligand connecting by carbon	LIGMF	Pt{CNR}2{D}{L}
(e)	cobalt complexes with three chelate ligands connecting by chalcogen atoms	LIGMF	Co{(2)Q}3
(f)	nickel complex with two tridentate ligands connecting by one pnictide and two chalcogenide atoms	LIGMF	Ni{D(2)Q}2
(g)	ferrocene and substituted ferrocene compounds	LIGMF	Fe{(5)L}2
(h)	bridged ferrocenyl compounds	LIGMF	Fe{(10)L}

(i)	divanadium nonahalogenides	LIGMF	V2{X}9
(k)	molybdenum(6) halogenide(14) cluster	LIGMF	Mo6{X}14
(l)	molybdenum(4) tungsten(2) halogenide(14) cluster	LIGMF	Mo4W2{X}14

Ligand Formulas (LIGFO)

Description:

The search field, Ligand Formula, contains the ligand codes according to the Gmelin Ligand Search System, which describes the elements (in groups) and the number of the atoms that are connected to the central metal atom(s). A ligand formula is given for all structured compounds or fragments which contain at least one metal atom and at least one coordinating ligand atom of the classes "L, A, D, Q, X" or a special ligand.

The codes include the following elements:

Code	atom					
L:	C					
A:	B,	Si,	Ge			
D:	N,	P,	As,	Sb		
Q:	O,	S,	Se,	Te		
X:	H,	F,	Cl,	Br,	I,	At

There are the following "special" ligands:

Code:	CO,	CS,	CN,	CNS,	CNO,	CNR *)

*) The substituent R has no further bond to metal atoms.

The denticity of a ligand is put in parentheses in front of the ligand code.

If a ligand is described by a combination of the codes, they are ordered alphabetically and the denticity of the code is put in parentheses in front of the code.

Note:

The ligand formula describes only the denticity of the ligand not the connectivity to the metal center(s).

Type of Indexing:

string (phrase)

Related Information:

LIG.LIGFO

Examples:

	Search for	Field Name	Field Value
(a)	halogenid or hydride ligand μ-halogenide or μ-hydride ligand	LIGFO	X
(b)	ligand connecting by five C atoms to one or more metal centers e.g. η^5-cyclopentadienyl	LIGFO	(5)L
(c)	ligand connecting by two chalcogenides e.g. η^2- or μ-acides (like acetic acid), oxalate (bidentate), di-oles (like ethylene glycol), salicylates, acetylacetonates, dithiols, μ- bisulfido	LIGFO	(2)Q
(d)	ligand connecting by four chalcogenides e.g. silicate, phosphate, 12-crown-4, tetra-thiocyclohexadecane, oxalate (tetradentate)	LIGFO	(4)Q

(e)	ligand connecting by one pnictide und two chalcogenide atoms e.g. diole-amines, imino-diacetates	LIGFO	D(2)Q
(f)	ligand connecting by two pnictide und four chalcogenide atoms e.g. ethylenediaminetetraacetate	LIGFO	(2)D(4)Q

Further examples are available in chapter Ligand Search System ().

Ligand Formula Count (LIGFC)

Description:

In the field Ligand Formula Count, the frequency of a certain ligand within a compound is indexed.

For ligand codes see LIGFO.

Tips and Hints:

Different ligand formula counts can be combined with the "and" operator.

To restrict the search to one complex or complex anion – to one structure – the number of fragments (nfrag) should be set to 1 additionally. Because of this restriction no multifragment compounds are found. However you can find these compounds by the Fragment GMELIN Registry Number.

Type of Indexing:

string (phrase)

Related Information:

LIG.LIGFC

Examples:

	Search for	Field Name	Field Value
(a)	complex containing one halogenid or hydride, µ-halogenide or µ-hydride ligand	LIGFC	X:1
(b)	complex with six carbonyl ligands	LIGFC	CO:6
(c)	complex with three ligands connecting by two pnictides e.g. ethylenediamine, bipyridyl	LIGFC	(2)D:3

Example:

Search for complexes containing one ?^{5}-C ligand, one ligand connecting by two pnictide atoms and three halogenide (or hydride) ligands

Operator	Field Name	Field Value
	LIGFC	(5)L:1
and	LIGFC	(2)D:1
and	LIGFC	X:3
and	NFRAG	1

The hit set contains mono- as well as poly-nuclear complexes.

Number of Components (NC)

Description:

The search field Number of Components contains the total number of components of a compound.

A number of components of 1 (nc=1) means a one-component compound. These are substances like the elements, molecules, salts, complexes, adducts, mixed crystals (in simple formula description), alloys, glasses and ceramic materials (in formula description).

e.g. Au, H2O, NaCl, Fe(C5H5)2, Na2SO4*10H2O, Nb0.8Ta0.2C, Fe0.55Pd0.45, SiO2, YBa2Cu3O(7-x)

A number of components greater than 1 (nc>1) means a multi-component compound. These are heterogeneous compounds like systems or solutions of two or more compounds. Additionally, some homogeneous compounds, like doped compounds, mixed crystals (in complex formula description), alloys, glasses and ceramic materials (in tabular description) belong (not exclusive) to this category.

Example multi-component compounds	potential (linearized) formula	component 1	component 2
system iron – carbon	Fe#C	Fe	C
solution of sodium chloride in water	NaCl#H2O	NaCl	H2O
tin doped In2O3	In2O3#dotSn	In2O3	Sn
mixed crystal of zirconia and titanium oxide	(Zr,Ti)O2 ZrO2#TiO2	ZrO2	TiO2
brass with 30% zinc	Cu(b),Zn(30)(X%)	Cu – 70%	Zn – 30%
ceramics of 8 wt% yttrium oxide and zirconia	ZrO2(b),Y2O3(8)(W%)	ZrO2 – 92 wt%	Y2O3 – 8 wt%

Multi-component compounds have the fact "composition" showing information to each component.

Tips and Hints:

You can restrict the hit sets to one-component compounds, if nc=1 is combined with your query.

Type of Indexing:

numerical

Number of Fragments (NFRAG)

Description:

The search field Number of Fragments contains the total number of fragments of a compound.

A number of fragments of 1 (nfrag=1) means a component without fragmentation. These are substances like the elements, neutral molecules, neutral complexes (with known structure) and compounds without molecular units (e.g. solid-state compounds).

e.g. Au, H2O, Fe(C5H5)2, NaCl

For these compounds the number of components is 1.

A number of fragments greater than 1 (nfrag>1) means a multi-fragment compound. Compounds with more than one fragment are separated in the linearized formula by an asterisk. A one-component compound can consist of several fragments, e.g. as adducts, salts (of at least one ion with molecular unit).

Example multi-fragment compounds	number of fragments	number of components
FeCl3*6NH3	nfrag=2	nc=1
2Na(1+)*SO4(2-)=Na2SO4	nfrag=2	nc=1
Cu(2+)*SO4(2-)*5H2O= CuSO4*5H2O	nfrag=3	nc=1

All multi-component compounds are multi-fragment compounds, too. The number of fragments of multi-component compounds is the sum of the number of fragments of the single components.

Notes:

Rules to determine whether a compound is fragmented or not are as follows.

Solid state structures, ionic compounds:

- Substances are divided into formal fragments, if the compounds contain at least one discrete polyatomic ion or molecule in the crystal, the gas phase, the liquid phase, or in solution. The structures of these discrete ions or molecules are available.
  e.g. 2Na(1+)*SO4(2-)=Na2SO4 (nfrag=2, nc=1)
- Substances are not divided into fragments, if the compounds consist exclusively of one-atomic ions (including OH(1-), SH(1-), SeH(1-), and TeH(1-)) or have no discrete polyatomic ion or molecule.
  e.g. NaCl, KOH, CaTiO3 (nfrag=1, nc=1)

Organometallic and coordination compounds:

- Organometallic compounds and coordination compounds with known manner of ligand coordination are stored with the complete formula and structure.
  e.g. Fe(C5H5)2, [Co(NH3)3Cl3] (nfrag=1, nc=1)
- Organometallic salts and ionic coordination compounds with known manner of ligand coordination are divided into cations and anions. The complete structures of the ions are available.
  e.g. [Pd(CH3CN)4](2+)*2BF4(1-)=[Pd(CH3CN)4](BF4)2 (nfrag=2, nc=1)
- Organometallic compounds and coordination compounds with unknown manner of ligand coordination are divided into fragments by separating all ligands from the metal center.
  e.g. If there is an unknown coordination of thiocyanate to Co(3+) in [Co(NH3)5(SCN)]Cl2 (coordination by N or S atom possible), the formula is given as Co(3+)*5NH3*SCN(1-)*2Cl(1-)=[Co(NH3)5(SCN)]Cl2; (nfrag=4, nc=1).

The number of fragments can be determined only for compounds in formula description. Compounds given in percentage composition get nfrag=0.

Tips and Hints:

You can restrict the hit sets to one fragment, if nfrag=1 is combined with your query.

Type of Indexing:

numerical

Number of Structures (NSTRUC)

Description:

The search field Number of Structures contains the total number of structures of a compound.

Example	number of structures	
elements, simple salts like NaCl, solid state compounds like CaTiO3, alloys, glasses, ceramic materials	nstruc=0	no structure available
molecules like H2O, C60, neutral complexes Fe(C5H5)2	nstruc=1	
molecules, complexes, ionic compounds with two fragments like 2Na(1+)*SO4(2-), [Ru(py)2Cl2]*H2O, Fe(C5H5)2*C60	nstruc=2	
molecules, complexes, ionic compounds with three fragments like Cu(2+)*SO4(2-)*5H2O, Zn(2+)*TiF6(2-)*6H2O	nstruc=3	

The number of structures of compounds is the sum of the number of structures of the single fragments.

The number of structures of multi-component compounds is the sum of the number of structures of the single components.

Notes:

You should be aware that only molecular structures are available in the database.

Type of Indexing:

numerical

Molecular Weight (MW)

Description:

The search field Molecular Weight contains the molecular weight of a substance. The molecular weight is defined as the sum of the relative atomic masses of all atoms in a compound. It is related to single compounds.

Notes:

The molecular weight of compounds with more than one component, and compounds with undefined indices in the molecular formula, is indexed as zero.

Tips and Hints:

Searches with exact values requires the input of the digits behind the point, e.g. 19.9994 (D2O). A molecular weight of exact 19 are compounds with isotopes only, e.g. (19)F, (11)B(2)H4(1-), (7)Li(6)Li2, (4)He4(3)He.

Type of Indexing:

numerical

Examples:

	Search for	Field Name	Field Value
(a)	compounds with molecular weight between 186.01 – 186.15	MW	186.05-186.15
(b)	compounds with molecular weight lower 100	MW	<100
(c)	complex with molecular weight greater 5000	MW	>5000

CAS Registry Number (RN)

Description:

The search field Registry Number contains the CAS accession number in the Registry file.

CAS Registry Numbers have to be searched with a fixed format: 6 digits, hyphen, 2 digits, hyphen, 1 digit, (#######-##-#). Smaller registration numbers are filled with left-hand {leading} zeros.

Notes:

The CAS Registry Number present in the Gmelin database has been mainly extracted from the Gmelin handbook. There are only few CAS Registry Number available in primary literature that are available.

Type of Indexing:

string (phrase) with fixed format

Examples:

	Search for	Field Name	Field Value
(a)	substance with CAS Registry Number 102-54-5	RN	000102-54-5
(b)	substance with CAS Registry Number 77321-08-5	RN	077321-08-5
(c)	substance with CAS Registry Number 126543-78-0	RN	126543-78-0

Chemical Name (CN)

Description:

The search field Chemical Name contains the chemical names of the substances from the original literature.

Compounds can have multiple entries for chemical names such as systematic, trivial, and trade names. Additionally incomplete names are available describing only a part of the compound (e.g. the ligand) or steric information.

Notes:

In the GMELIN database not all compounds have a name. The names given do not necessarily conform to the IUPAC nomenclature.

Tips and Hints:

Name searches are not recommended to identify compounds, because names are ambiguous or non-systematic and are not available in many cases. In some cases name fragments might be useful to search for substance classes or complex compounds with same ligand. However there are more powerful methods available such as structure, substructure searches, or formula searches.

Type of Indexing:

string (phrase)

Related Information:

CNS

Examples:

	Search for	Field Name	Field Value
(a)	ferrocene	CN	Ferrocene
(b)	Alum	CN	Alum
(c)	adduct of (r)-binaphthol with tin tetrachloride	CN	(r)-binaphthol*tin tetrachloride

Chemical Name Segment (CNS)

Description:

The search field Chemical Name Segment uses the same source as the field Chemical Name. However, it is indexed differently allowing fast searching for segments of chemical names without entering truncation symbols.

In some cases name fragments might be useful to search for substance classes or complex compounds with the same ligands.

Type of Indexing:

string (wordwise)

Related Information:

CN

Examples:

	Search for	Field Name	Field Value
(a)	compounds containing the name term ferrocene	CNS	ferrocene
(b)	compounds containing the name term hexacyanoferrate	CNS	hexacyanoferrate
(c)	compounds containing the name term binaphthol	CNS	binaphthol

Example:

Search for compounds containing the name terms trans, chloro and iron

Operator	Field Name	Field Value
	CNS	trans
and	CNS	chloro
and	CNS	iron

Type of Substance (TYPE)

Description:

The search field Type of Substance contains the chemical classification of the substances.

Following classes are searchable:

- ALLOY
- COORDINATION COMPOUND
- DOPANT
- GLASS OR CERAMIC MATERIAL
- ISOMORPHOUS OR DIADOCHOUS COMPOUND, SOLID SOLUTION
- ISOTOPE OR ISOTOPE CONTAINING COMPOUND
- MINERAL (assigned to natural minerals only)
- POLYMER

Type of Indexing:

string (phrase)

Modification (MODTXT)

Description:

The search field Modification contains the modification of a substance. In many cases (e.g. minerals) the modification is identical to the chemical name.

Modifications can be:

Mineral name	e.g. calcite
Color	e.g. yellow
Crystal system	e.g. orthorhombic
Bravais type	e.g. face centered cubic
Space group (Hermann-Mauguin symbol)	e.g. p21/c
Crystal structure type	e.g. rutile
Numbers and Greek letters	e.g. .alpha.
Qualitative temperature and pressure references	e.g. high temperature
ortho / para	
singlet / triplet	

Notes:

A modification can consist of several designations, which are separated by a comma.

In multi-component systems the modification is assigned to the single component.

Tips and Hints:

The description of modifications is ambiguous or non-systematic in literature. Therefore it is possible that the same modification is recorded by several designations or combinations.

Type of Indexing:

string (phrase)

Entry Date (ED)

Description:

The search field Entry Date contains the date (year/month/day) when this compound was first entered into the database.

Dates have to be searched with a fixed format: yyyy/mm/dd.

Type of Indexing:

string (phrase)

Update Date (UPD)

Description:

The search field Update Date contains the date (year/month/day) when the last update of this compound was entered into the database.
Dates have to be searched with a fixed format: yyyy/mm/dd.

Type of Indexing:

string (phrase)

Ligands around Metals (LIG)

Search Fields:

LIG.LIGMF	Ligand Molecular Formula of one Center
LIG.LIGFO	Ligand Formulas of one Center
LIG.LIGFC	Ligand Formula Count of one Center

See also:

IDE	Identification of Substance
FOR	Formula Search Data
CMPS	Composition

Ligand Formulas of one Center (LIG.LIGFO)

Description:

The search field Ligand Formula of one Center contains the ligand codes according to the Gmelin Ligand Search System, which describes the elements (in groups) and the number of the atoms that are connected to one central metal atom. A ligand formula is given for all structured compounds or fragments which contain at least one metal atom and at least one coordinating ligand atom of the classes "L, A, D, Q, X" or a special ligand.

The codes include the following elements:

Code	atom					
L:	C					
A:	B,	Si,	Ge			
D:	N,	P,	As,	Sb		
Q:	O,	S,	Se,	Te		
X:	H,	F,	Cl,	Br,	I,	At

There are the following "special" ligands:

Code:	CO,	CS,	CN,	CNS,	CNO,	CNR *)

*) The substituent R has no further bond to metal atoms.

If a ligand is described by a combination of the codes, they are ordered alphabetically and the denticity of the code is put in parentheses in front of the code.

Note:

The ligand formula describes only the denticity of the ligand not the connectivity to the metal center.

In contrast to the search field Ligand Formula only one center is described here, even if the whole compound contains several metal centers. For a mononuclear complex both ligand formulas are identical.

Type of Indexing:

string (phrase)

Related Information:

LIGFO

Examples:

	Search for	Field Name	Field Value
(a)	halogenid or hydride ligand μ-halogenide or μ-hydride ligand	LIGFO	X
(b)	ligand connecting by two halogenide or hydride atoms e.g. η^2-hydrogen, η^2-BH4	LIGFO	(2)X
(c)	(monodentate) carbonyl	LIGFO	CO
(d)	ligand connecting by C and chalcogen e.g. μ-η^2-carbonyl (by C and O)	LIGFO	LQ
(e)	Ligand connecting by four pnictide atoms e.g. porphyrins, phthalocyanines, tetra-aza-cyclam	LIGFO	(4)D
(f)	ligand connecting by five C atoms to one or more metal centers e.g. η^5-cyclopentadienyl	LIGFO	(5)L
(e)	ligand connecting to metal(s) by C e.g. μ-carbonyl (only by C), bridged alkyl-, η^2 alken-, η^2-alkin ligands	LIGFO	(2)L

The hit set contains mono- as well as poly-nuclear complexes.

Ligand Molecular Formula of one Center (LIG.LIGMF)

Description:

The alphanumerical search field Ligand Molecular Formula of one Center contains the abstract formula of the single coordination centers and the corresponding ligand codes of a compound. The ordering of the formula is as follows:

1. metal center
2. the ligand codes (see LIG.LIGFO) are ordered in the following manner:
3. A, CN, CNO, CNR, CNS, CO, CS, D, L, Q, X
4. within the same ligand types, they are ordered on ascending denticity and the frequency is not taken into consideration

The details to each different metal center are displayed separately in field Ligands around Metals, respectively.

Note:

Charges are not taken into account.

In contrast to the search field Ligand Molecular Formula only one center is described here even if the whole compound contains several metal centers. For a mononuclear complex both ligand molecular formulas are identical.

Tips and Hints:

Searches for compounds using the GMELIN Ligand Search System are very powerful when looking for a class of complexes with special connectivity.

Type of Indexing:

string (phrase)

Related Information:

LIGMF

Examples:

	Search for	Field Name	Field Value
(a)	hexa carbonyl chromium	LIG.LIGMF	Cr{CO} 6
(b)	tetra halogeno palladium compounds	LIG.LIGMF	Pd{X}4
(c)	nickel complex with two tridentate ligands connecting by one pnictide and two chalcogenide atoms	LIG.LIGMF	Ni{D(2)Q}2

The hit set contains mono- as well as poly-nuclear complexes.

Ligand Formula Count of one Center (LIG.LIGFC)

Description:

In the field Ligand Formula Count of one Center the frequency of a certain ligand, relating to one metal center within a compound, is indexed.

For ligand codes see LIG.LIGFO.

Note:

In contrast to the search field Ligand Formula Count only one center is described here, even if the whole compound contain several metal centers. For a mononuclear complex both ligand formula counts are identical.

Tips and Hints:

Different ligand formula counts can be combined with the "proximity" operator.

This is a very powerful search code to tailor coordination compounds.

Type of Indexing:

string (phrase)

Related Information:

LIGFC

Example:

Search for complexes containing one ?^{5}-C ligand, one ligand connecting by two pnictide atoms and three halogenide (or hydride) ligands

Operator	Field Name	Field Value
	LIG.LIGFC	(5)L:1
proximity	LIG.LIGFC	(2)D:1
proximity	LIG.LIGFC	X:3

The hit set contains mono- as well as poly-nuclear complexes.

Formula Search Data Formula Search Data (FOR)

Search Fields:

NA	Number of Atoms
NE	Number of Elements
ELS	Element Symbol
ELC	Element Count

See also:

IDE	Identification of Substance
LIG	Ligands around Metals
CMPS	Composition

Number of Atoms (NA)

Description:

The numerical search field Number of Atoms contains the total number of atoms in a molecular formula MF. Thus NA will be multiple for multi-component compounds.

Note:

NA is a numerical value that can be searched for with exact values or open and close ranges.

Compounds with a negative number of atoms (NA = -1) have components with undefined stoichiometric indexes, like YBa2Cu3O(7-x), or adducts with an undefined prefix factor, like CuBr2*99H2O.

Tips and Hints:

The Number of Atoms must not be confused with the Number of Elements (NE) or the Element Count (ELC).

This search field is useful especially in combination with other search fields of this topic, especially for searching simple inorganic or solid-state compounds.

Type of Indexing:

numerical

Example:

Search for	Field Name	Field Value
compounds with 190 to 200 atoms	NA	190-200

Number of Elements (NE)

Description:

The numerical search field Number of Elements contains the number of different elements present in a molecular formula MF. Thus NA will be multiple for multi-component compounds.

Isotopes, including deuterium and tritium, are not treated as different elements.

Note:

NE is a numerical value that can be searched for with exact values or open and close ranges.

Tips and Hints:

The Number of Elements must not be confused with the Element Count (ELC) or the Number of Atoms (NA).

This search field is useful especially in combination with other search fields of this topic, especially for searching simple inorganic or solid-state compounds.

Type of Indexing:

numerical

Example:

Search for	Field Name	Field Value
compounds more than ten elements	NE	>10

Element Symbol (ELS)

Description:

The search field Element Symbol contains the symbol of each distinct element in the molecular formula.

Isotopes, including deuterium and tritium, are not treated as different elements.

Note:

Elements with atomic number greater 103 are available by the element symbols recommended by IUPAC (e.g. element #104 as Unq).

The term Qx represents positive charged compounds, the term Qy represents negative charged compounds.

Tips and Hints:

The Element Symbol must not be confused with the Element Count (ELC), the Number of Elements (NE) or the Number of Atoms (NA).

This search field is useful especially in combination with other search fields of this topic, especially for searching simple inorganic or solid-state compounds.

Type of Indexing:

string (phrase)

Examples:

Search for	Field Name	Field Value
zirconium and zirconium compounds	ELS	Zr

Search for phosphorus nitride compounds (of any stoichiometry)

Operator	Field Name	Field Value
	ELS	P
and	ELS	N
and	NE	2
and	NC	1

The hit set contains phosphorus nitride compounds without further elements.

Search for barium copper oxides with three up to four atoms

Operator	Field Name	Field Value
	ELS	Ba
and	ELS	Cu
and	ELS	O
and	NA	3-4
and	NC	1

The hit set contains barium copper oxides with various oxygen content and barium copper oxides with one further element as well as mixed crystals with further elements.

Element Count (ELC)

Description:
The numerical search field Element Count contains the respective counts of the distinct elements in a component molecular formula MF.

Isotopes, including deuterium and tritium, are not treated as different elements.

Note:

An element count is defined as the element symbol and the number of its occurrences per molecule.

Odd-numbered values result from compounds like mixed crystals, alloys and glasses or ceramic materials.

Negative element counts indicate compounds with the respective element in undefined stoichiometry.
The element count is fixed to two decimal places, even if the compound has more.

Tips and Hints:

The Element Symbol must not be confused with the Element Symbol (ELS), the Number of Elements (NE) or the Number of Atoms (NA).

Element counts can be used to restrict searches on the basis of number of elements. It is possible to exclude elements by ELC search combinations using the Boolean Operator NOT.

This search field is useful especially in combination with other search fields of this topic as well as with structure fragments to search for complexes being fragmented.

Type of Indexing:

string (phrase)

Examples:

Search for	Field Name	Field Value
compounds containing three ruthenium atoms	ELC	Ru3.00

Search for barium copper oxides with two Ba and three copper atoms per formula

Operator	Field Name	Field Value
	ELC	Ba2.00
and	ELC	Cu3.00
and	ELS	O
and	NC	1

The hit set contains compounds like ABa2Cu3(O,X), where A and/or X can be further element(s) or not available.

Search for a ruthenium complex containing four sulfur atoms but no phosphorus with maximal five different elements

Operator	Field Name	Field Value
	ELC	Ru1.00
and	ELC	S4.00
not	ELS	P
and	NE	5
and	NC	1

The hit set contains a number of mononuclear ruthenium complexes, as well as, some polynuclear complexes. There are also fragmented complexes with unknown ligand coordination.

Composition (CMPS)

Search Fields:

PERC	Percentage
PERT	Percentage Type

See also:

IDE	Identification of Substance
LIG	Ligands around Metals
FOR	Formula Search Data

Percentage (PERC)

Description:

The search field percentage contains the percentage values of alloys, glasses or ceramic materials. PERC is a numerical value that can be searched for with exact values or open and close ranges.

Note:

Constituents can be combined by search field MF using the proximity operator.

Tips and Hints:

Searches using the percentage field can be tailored individually because of the numerical percentage values and the separation from the percentage type.

Type of Indexing:

numerical

Related Information:

ALLOY

Example:

Search for alloys with more than 70 weight% palladium and 2-10 weight% rhodium

Operator	Field Name	Field Value
	MF	Pd
proximity	PERC	>70
and	MF	Rh
proximity	PERC	2-10
and	PERT	weight%

The hit set is not restricted to the number of constituents.

Percentage Type (PERT)

Description:

The search field percentage type contains the form of the percentage information of alloys, glasses or ceramic materials. The following types are available:

%	indefinite percent
atom%	atom or mol percent
volume%	volume percent
weight%	weight percent

Tips and Hints:

This search field is useful in combination with the percentage search field.

Type of Indexing:

string (phrase)

General Information (GEN)

Search Fields:

OCN	Occurrence in Nature

PUR	Purification
USE	Use of the Substance
HLDG	Handling
HEP	Health Protection
ECOL	Ecological Data
PHYB	Physiological Behavior
HIST	History
ECON	Economic Data

Occurence in Nature (OCN)

Description:

This field identifier is a group code indicating the Occurrence in Nature of a compound, like the occurrence in plants, animals, in the atmosphere, hydrosphere, lithosphere or in the universe.

Type of Indexing:

Group Code

Purification (PUR)

Description:

This field identifier is a group code indicating the Purification of a compound. Here the isolation or enrichment of a compound from a mixture, as well as, general purification methods are considered. However, the "working up" of a reaction mixture is indexed in the Reaction Details Purification / Isolation (RX.ISOL).

Type of Indexing:

Group Code

Use of the Substance (USE)

Description:

This field identifier is a group code indicating the Use of the Substance. Here the application of the compound in laboratory as well as in (chemical) industry is considered.

Note:

The use of a substance as catalyst is not indexed here, but under the group code Chemical Behavior in Behavior as Catalyst (BCAT).

Type of Indexing:

Group Code

Handling (HDLG)
Description:

This field identifier is a group code indicating the Handling, storage or disposal of a compound. Here, aspects like handling during transport, special storage conditions or removal, or waste disposal, are considered.

Type of Indexing:

Group Code

Health Protection (HEP)
Description:

This field identifier is a group code indicating the protection of persons from the effects of a compound or the degree of toxicity of a compound. Here information about MAC values, lethal doses, prophylaxis or therapeutic procedures can be searched.

Type of Indexing:

Group Code

Ecological Data (ECOL)
Description:

This field identifier is a group code indicating the effects of a compound on the environment.

Type of Indexing:

Group Code

Physiological Behavior (PHYB)

Description:

This field identifier is a group code indicating the Physiological Behavior of a compound including effects on men, animals, plants, microorganisms, or metabolism of a compound.

Type of Indexing:

Group Code

History (HIST)

Description:

This field identifier is a group code indicating the History of a compound.

Type of Indexing:

Group Code

Economic Data (ECON)

Description:

This field identifier is a group code indicating the Economic or commercial data of a compound.

Type of Indexing:

Group Code

Physical Properties (PHY)

Description:

The topic Physical Properties contains data for single-component systems.

This field identifier is a group code for Field Availability searches in the hierarchical system of the CrossFire database.

Type of Indexing:

Group Code

Acceptance Criteria

Data determined by experimental measurements in the abstracted article are indexed as values or corresponding keywords.

Values which have been calculated by classical (not quantum mechanical) methods or which come from experimentally measured data have also been accepted, e.g. rotational constants, enthalpy of vaporization, thermal expansion coefficient etc.

Note:

Data to multi-component systems are recorded in the topic Properties of / in Systems (MCS).

Values, which have been calculated by quantum mechanical methods, are indicated in the topic Quantum Chemical Calculations (QCC).

The topics on physical data follow the hierarchy described below:

Search Fields:

MOL	Molecular Properties
PHT	Information on Phase Transitions
CRY	Information on Condensed Phases
MEC	Mechanical Properties
THD	Thermal Properties
TRA	Transport Phenomena
TDD	Thermodynamic Data
ELE	Electric Properties
MAG	Magnetic Properties
OPT	Optical Properties
SPE	Spectroscopic Information

Information on Condensed Phase (CRY)

Search Fields:

COHA	Color / Habit
CGRO	Crystal Growth
CBND	Crystal Bonding
CDEF	Crystal Defects
SLAT	Superlattice
CEN	Crystal Energy
CRT	Crystal Structure

Color / Habit (COHA)

Description:

The search field contains general information on color and habit of a substance in the condensed phase. Information in the field COHA.NOTAT refers to the color of the substance in the corresponding solvent.

The following habits can be searched in the field COHA.HABIT:

- bipyramids
- blocks
- bricks
- columns
- cubes
- dodecahedrons
- fibres
- flakes
- leaves
- needles
- octahedrons
- parallelepipeds
- parallelograms
- pinacoids
- plates
- prisms
- pyramids
- rhombododecahedrons
- rhombohedrons
- rods
- skalenohedrons
- slabs
- tetrahedrons

The crystal habit may be strongly dependent upon the conditions of crystallization.

Fields:

Field Code	Full Name	Type of Indexing
COHA.COLOR	Color	string (phrase)
COHA.NOTAT	in Solvent	string (phrase)
COHA.HABIT	Habit	string (phrase)

Crystal Growth (CGRO)

Description:

Indication of crystallization mechanisms or preparation of single crystals, e.g. by the application of various methods, is given in the field CGRO.CRYS. Information on the growth of crystals, e.g. twin formation, or epitaxy is indicated in the field CGRO.FORM.

Note:

Searching for the special field codes requires the field value "described" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
CGRO.CRYS	Crystallization / Prepn. of Single Crystals	string (phrase)
CGRO.FORM	Growth Forms / Epitaxy	string (phrase)

Crystal Bonding (CBND)

Description:

The field Crystal Bonding gives indications on bond states, bond types or crystal structure of crystalline compounds, e.g. layer structures.

Type of Indexing:

Group Code

Crystal Defects (CDEF)

Description:

Indication on crystal defects; e.g. color centers, line defects, displacements, disorders, twinning, vacancies or surface defects, is given in this field.

Type of Indexing:

Group Code

Superlattice (SLAT)

Description:

The search field Superlattice indicates a solid system in which there exists a regular array of atoms of one species interspersed among the lattice structure of another species related by their crystal symmetry.

Type of Indexing:

Group Code

Crystal Energy (CEN)

Description:

The lattice energy is the energy associated with the construction of a crystal lattice relative to the energy of all constituent atoms separated by infinite distances. A characteristic term of the lattice energy is the Madelung constant determined solely by the geometry of an ionic crystal.

The field Crystal Energy gives indications on lattice energy as well as Madelung constants.

Type of Indexing:

Group Code

Crystal Structure (CRT)

Description:

The Crystal Structure type of a solid is the name of an isostructural prototype.The crystal type search field CRT.TYP contains terms describing the crystal structure types for the substances in the literature. The following terms are valid:

Antifluorite, Aragonite (CaCO3), Calcite (CaCO3), CdCl2,CdI2 (PbI2), Cooperite (PtS),

Corundum (Al2O3), CsCl, Cuprite (Cu2O), Cu, Diamond, Fluorite (CaF2), Graphite,

Ilmenite (FeTiO3), Inverted Spinel (FeIII)(MgFe(III)O4), Mg, NaCl, NiAs, PbO,

Perowskite (CaTiO3), Pyrite (FeS2), Rutile (TiO2), Silicates, Skutterudite (CoAs3),

Sphalerite, Spinel (MgAl2O4), Wurtzite (ZnS), W, Zinc blende (ZnS)

According to the translational lattice, crystals may be divided into seven crystal systems and 14 Bravais types. The crystal system search field CRT.SYST contains the crystal system names for the substances in the literature. The following names are given:

- cubic
- hexagonal
- trigonal (rhombohedral)
- tetragonal
- rhombic (=orthorhombic)
- monoclinic
- and triclinic.

The following Bravais types are given in the Bravais type search field CRT.BRAV:

- all-faces-centered orthorhombic
- body-centered cubic
- body-centered monoclinic
- body-centered orthorhombic
- body-centered tetragonal
- face-centered cubic
- one-face-centered orthorhombic
- simple cubic
- simple hexagonal
- simple monoclinic
- simple orthorhombic
- simple rhombohedral
- simple tetragonal
- simple triclinic

The unit cell of a crystal lattice requires three vectors for its description. The set of the three axes for the lattice length (a, b, c) is given in CRT.LENA(B,C) and the three lattice angles (alpha, beta, gamma) are given in CRT.ANGA(B;C).

The measuring temperature is given in CRYST.T and the molecules per unit cell in CRT.ZVAL.

The following methods can be searched in method of determination with the search field code CRT.MET:

- electron diffraction
- neutron diffraction
- powder X-ray diffraction
- single crystal X-ray diffraction
- X-ray diffraction

The symmetry group of a three-dimensional crystal pattern is called its space group. There are 230 crystallographic space groups. They are classified in 7 crystal systems (see CRT.SYST) and 32 crystallographic point groups. The crystal space group search field CRT.SGROUP contains the space group for a given substance in the literature.

Note:

Avoid confusion of the crystallographic space group with the point group of a molecule recorded in the search field PGR.

Indication on atomic coordinates, distances, angles or interplanar spacings is given in the field CRT.ATPOS.

Note:

Searching for the field CRT.ATPOS require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing	Unit
CRT.TYP	Crystal Type	string (phrase)	
CRT.SYST	Crystal System	string (phrase)	
CRT.BRAV	Bravais Type	string (phrase)	
CRT.LENA	Lattice Length A	numerical	Angstroem
CRT.LENB	Lattice Length B	numerical	Angstroem

CRT.LENC	Lattice Length C	numerical	Angstroem
CRT.ANGA	Lattice Angle .Alpha.	numerical	
CRT.ANGB	Lattice Angle .Beta.	numerical	
CRT.ANGC	Lattice Angle .Gamma.	numerical	
CRT.T	Temperature	numerical	°C
CRT.MET	Method of Determination	string (phrase)	
CRT.ZVAL	Molecules per Unit Cell	numerical	dimensionless
CRT.DEN	X-Ray Density	numerical	g/ml
CRT.MVOLO	Molar Volume	numerical	ml/mol
CRT.MVOLA	Specific Volume	numerical	l/kg
CRT.SGROUP	Space Group(s)	numerical	
CRT.ATPOS	Atomic Positions	string (phrase)	

Electric Properties (ELE)

Search Fields:

ELSR	Electronic Band Structure
ELCO	Electric Conductivity
SPCO	Superconductivity
PHCO	Photoconductivity
THEL	Thermoelectric Effects
DIC	Dielectric Constant
PIEZ	Piezoelectric Effects
PYRO	Pyroelectric Effects
FREL	Ferroelectricity
AFREL	Antiferroelectricity

Electronic Band Structure (ELSR)

Description:

The field Electronic Band Structure indicates discussion or calculation of (electron) band models, like band theory, valence band, conduction band, and Brillouin zone.

Type of Indexing:

Group Code

Electric Conductivity (ELCO)

Description:

The Electric Conductivity of a substance is its time rate of electricity flowing across a unit area per unit potential gradient. The electric conductivity search field is a numerical range searchable field and is linked to the associated temperature ELCO.T.

Information about pretreatment of samples is given in the field remarks ELCO.MR. Further information about the electric conductivity is given as a diagram or equation using the parameter field codes ELCO.DGM respectively ELCO.EQN. Indication of the electric charge mobility or the conduction mechanism is given in the parameter field ELCO.MOB. The search field is linked to the forms of state of the substance by parameter field code ELCO.S.

Note:

Searching for electric conductivity diagrams or equation field codes require the field value "available", the parameter field ELCO.MOB the field value "described" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing	Unit
ELCO	Electric Conductivity	numerical	S/cm
ELCO.T	Temperature	numerical	°C
ELCO.MR	Remarks	string (phrase)	
ELCO.DGM	Diagram	string (phrase)	
ELCO.EQN	Equation	string (phrase)	
ELCO.MOB	Conduction Mechanism	string (phrase)	
ELCO.S	Forms of State	string (phrase)	

Superconductivity (SPCO)

Description:

The superconductivity is the abrupt increase of electric conductivity of some materials at low temperatures. Indication on the general description of Superconductivity is given in the field SPCO.FLG.

Each substance has a transition temperature (onset-, midpoint-, zero-resistance temperature) Tc above which it is a normal conductor. The superconductivity SPCO.T field contains this critical temperature for a given substance in the literature.

Note:

Searching for superconductivity field codes require the field "described" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing	Unit
SPCO.FLG	superconductivity	string (phrase)	
SPCO.T	critical temperature	numerical	°C

Photoconductivity (PHCO)

Description:

The photoconductivity is the increase in electrical conductivity of nonmetallic substances when exposed to light. The production of voltage in semiconductor materials by light or other electromagnetic radiation is called photovoltaic effect.

The field Photoconductivity indicates information on photoconductivity or photovoltaic effects of a substance.

Type of Indexing:

Group Code

Thermoelectric Effects (THEL)

Description:

The thermoelectric effect is the production of current or voltage (thermal electromotive force) at a junction between two dissimilar metals or at a temperature gradient along a metal rod. The value depends on the metal, as well as, the temperature or temperature gradient, respectively.

The field Thermoelectric Effects indicates thermoelectric phenoma, e.g. Benedicks effect, Thomson effect, or Bridgman effect.

Type of Indexing:

Group Code

Dielectric Constant (DIC)

Description:

The Dielectric Constant is the ratio of the capacity of a condenser with the given substance as dielectric to the capacity of the same condenser with a vacuum as dielectric. The dielectric constant search field is a numerical range searchable field and is linked to the associated fields temperature DIC.T, frequency DIC.F and pressure DIC.P. Information about pretreatment of samples is given in the field remarks DIC.MR. The search field is linked to the forms of state, of the substance, by the parameter field code DIC.S.

Fields:

Field Code	Full Name	Type of Indexing	Unit
DIC	Electric Conductivity	numerical	
DIC.T	Temperature	numerical	°C
DIC.F	Frequency	numerical	Hz
DIC.P	Pressure	numerical	Torr
DIC.MR	Remarks	string (phrase)	
DIC.S	Forms of State	string (phrase)	

Piezoelectric Effects (PIEZ)

Description:

The piezoelectric effect is the electrical response of a substance induced by mechanical forces, and the mechanical response to an electrical force. The occurrence of piezoelectricity depends on the crystal structure. The crystal must belong to one of the non-centrosymmetric point groups.

The field Piezoelectric Effects indicates piezoelectric substances.

Type of Indexing:

Group Code

Pyroelectric Effects (PYRO)

Description:

The pyroelectric effect is the development of a spontaneous electrical polarization and is temperature dependent. This is mainly because the thermal expansion that occurs on heating changes the sizes (i.e. lengths) of the dipoles. The occurrence of pyroelectricity depends on the crystal structure. The crystal must belong to one of the non-centrosymmetric point groups.

The field Pyroelectric Effects indicates pyroelectric substances.

Type of Indexing:

Group Code

Ferroelectricity (FREL)

Description:

Ferroelectricity is due to parallel ordering of electric dipole moments in a substance in the absence of an applied electrical field. In ferroelectrics, domain structures are formed because adjacent dipoles tend to align themselves parallel to each other. Above a critical temperature ferroelectricity often disappears and a paraelectric state is generated.

The field Ferroelectricity indicates ferroelectric substances.

Type of Indexing:

Group Code

Antiferroelectricity (AFREL)

Description:

Antiferroelectricity is due to antiparallel ordering of electric dipole moments in a substance in the absence of an applied electrical field. The substance is built from two sublattices having equal and opposite electric polarization. Above a critical temperature antiferroelectricity disappears and a paraelectric state is generated.

The field Antiferroelectricity indicates the antiferroelectric substances.

Type of Indexing:

Group Code

Magnetic Properties (MAG)

Search Fields:

MAGS	Magnetostriction
GALV	Galvanomagnetic Effects
THMG	Thermomagnetic Effects
MSUS	Magnetic Susceptibility
CUWE	Curie Weiss Temperature
NEEL	Neel Temperature
CURI	Curie Temperature
MM	Magnetic Moment
MPRO	Magnetic Property

Magnetostriction (MAGS)

Description:

The field Magnetostriction indicates information on the volume change of substances under the influence of an external magnetic field.

Type of Indexing:

Group Code

Galvanomagnetic Effects (GALV)

Description:

The galvanomagnetic effect is any thermal or electric effect occurring in an electronic conductor or semiconductor in the presence of a magnetic field.

The field Galvanomagnetic Effects indicates information on

- Hall effect (formation of a transversal potential gradient)
- Ettingshausen effect (formation of a transversal temperature gradient)
- Galvanomagnetic Thomson effect (change of transversal resistivity)
- Nernst effect (formation of a longitudinal temperature gradient)

Type of Indexing:

Group Code

Thermomagnetic Effects (THMG)

Description:

Indication of Thermomagnetic Effects including all effects caused by a heat flow in electronic conductors or semiconductors in the presence of a magnetic field, e.g.:

- Righi-Leduc effect (formation of a transversal temperature gradient)
- Maggi-Righi-Leduc effect (change of thermal conductivity)
- Ettingshausen-Nernst effect (formation of a potential gradient)

is available.

Type of Indexing:

Group Code

Magnetic Susceptibility (MSUS)

Description:

The volumetric magnetic susceptibility is the difference in the magnetic permeability of a substance and of a vacuum, divided by the permeability of the vacuum. The specific (or mass) magnetic susceptibility of a substance is the quotient of its volumetric susceptibility and its density. The molar magnetic susceptibility of a substance is the product of its volumetric susceptibility and its molar volume. The Magnetic Susceptibility (specific: MSUS.VALA, molar: MSUS.VALO) field contains the values for a given substance in the literature**.**

The search field is a numerical range searchable field and is linked to the associated temperature MSUS.T. Further information about the magnetic susceptibility is given as a diagram or equation using the parameter field codes MSUS.DGM, and MSUS.EQN respectively. Information about pretreatment of samples or concentration of solutions is given in the field remarks MSUS.MR.

Note:

Searching for magnetic susceptibility diagram or equation field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing	Unit
MSUS.VALO	Molar Magnetic Susceptibility	numerical	ml/mol
MSUS.VALA	Specific Magnetic Susceptibility	numerical	l/kg
MSUS.T	Temperature	numerical	°C
MSUS.DGM	Diagram	string (phrase)	
MSUS.EQN	Equation	string (phrase)	
MSUS.MR	Remarks	string (phrase)	

Curie Weiss Temperature (CUWE)

Description:

The Curie-Weiss temperature is the temperature at which a plot of the reciprocal molar magnetic susceptibility against the absolute temperature T intersects the T-axis. The Curie-Weiss temperature can adopt positive, as well as, negative values.

The Curie-Weiss Temperature CUWE.T search field contains the values for a given substance in the literature and is a numerical range searchable field. Information about pretreatment of samples is given in the field remarks CUWE.MR.

Fields:

Field Code	Full Name	Type of Indexing	Unit
CUWE.T	Curie Weiss Temperature	numerical	K
CUWE.MR	Remarks	string (phrase)	

Neel Temperature (NEEL)

Description:

The Neel temperature is the temperature at which a substance experiences a phase transition from the antiferromagnetic to the paramagnetic state. The Neel temperature is also known as antiferromagnetic Curie point.

The Neel Temperature search field contains the values for a given substance in the literature and is a numerical range searchable field. Information about pretreatment of samples is given in the field remarks NEEL.MR.

Fields:

Field Code	Full Name	Type of Indexing	Unit
NEEL.T	Neel Temperature	numerical	K
NEEL.MR	Remarks	string (phrase)	

Curie Temperature (CURI)

Description:

The Curie temperature is the temperature above which a substance experiences a phase transition from the ferromagnetic to the paramagnetic state.

The Curie Temperature search field contains the values for a given substance in the literature and is a numerical range searchable field. Information about pretreatment of samples is given in the field remarks CURI.MR.

Fields:

Field Code	Full Name	Type of Indexing	Unit
CURI.T	Curie Temperature	numerical	K
CURI.MR	Remarks	string (phrase)	

Magnetic Moment (MM)

Description:

The magnetic dipole moment of a molecule is the moment due to the spin of electrons and nuclei. The Magnetic Dipole Moment is a numerical range searchable field.

Fields:

Field Code	Full Name	Type of Indexing	Unit
MM.VAL	magnetic moment	numerical	A*cm**2

Magnetic Property (MPRO)

Description:

The search field to Magnetic Property indicates if information about magnetic effects is available for a given substance in the literature.

Indication on the following magnetic phenomena is given in the field MPRO.PHEN:

- antiferromagnetic
- diamagnetic
- ferrimagnetic
- ferrimagnetic domains
- ferromagnetic
- ferromagnetic domains
- paramagnetic

Indication of the anisotropy of the magnetic susceptibility is given in the field MPRO.MAN.

Indication of the dependence of the spatial arrangement and orientation of the atomic magnetic moments in a crystal or indication of magnetic space groups (also designated as Schubnikow groups) is given in the field MPRO.MST.

Indication of the magnetization (magnetic dipole moment per unit volume) is given in the field MPRO.MAG.

Indication of the relationship between the magnetization or magnetic induction and the effective field strength given as a diagram is given in the field MPRO.MMD.

Indication of the relationship between the magnetization M, the magnetic field H, or the magnetic induction B and the temperature given as a diagram is available in the field MPRO.MPD.

Note:

Searching for magnetic anisotropy field codes require the field value "described", the field codes magnetic structure / space group, magnetization, magnetization diagram, and magnetic phase diagram require "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
MPRO.PHEN	Magnetic Phenomena	string (phrase)
MPRO.MAN	Magnetic Anisotropy	string (phrase)
MPRO.MST	Magnetic Structure / Space Group	string (phrase)
MPRO.MAG	Magnetization	string (phrase)
MPRO.MMD	Magnetization Diagram	string (phrase)
MPRO.MPD	Magnetic Phase Diagram	string (phrase)

Mechanical Properties (MEC)

Search Fields:

MVOL	Mole Volume
ELAS	Elastic Behavior
COM	Compressibility
PLAS	Plastic Behavior
STRE	Strength
HARD	Hardness
DEN	Density

Mole Volume (MVOL)

Description:

Indication of molar volume, molecular volume, atomic volume or ionic volume is given in the field Mole Volume.

This field is linked to the forms of state of the substance by parameter field code MVOL.S.

Fields:

Field Code	Full Name	Type of Indexing
MVOL.S	Forms of State	string (phrase)

Elastic Behavior (ELAS)

Description:

The elasticity of a substance is the response to stress, indicating the degree to which strain disappears from the substance when the stress has been removed.

The field Elastic Behavior indicates information on elastic behavior of a substance, e.g. elasticity coefficients, elastic modulus, torsional rigidity or shearing force.

Type of Indexing:

Group Code

Compressibility (COM)

Description:

The compressibility of a substance is the extent to which a material reduces its volume when it is subjected to compressive stresses.

The field Compressibility indicates information on compressible behavior of a substance.

This field is linked to the forms of state of the substance by parameter field code COM.S.

Fields:

Field Code	Full Name	Type of Indexing
COM.S	Forms of State	string (phrase)

Plastic Behavior (PLAS)

Description:

The plasticity of a substance is the property of a substance by which it undergoes plastic deformation when the applied stress exceeds a certain value, known as the yield value.

The field Plastic Behavior indicates information on the plastic behavior of a substance, e.g. plastic limit, superplasticity, or creep behavior.

Type of Indexing:

Group Code

Strength (STRE)

Description:

The strength of a substance is its resistance to a force producing or tending to produce permanent deformation, especially as described by its stress level at which it fractures or fails.

The Strength search field is a numeric range searchable field and is linked to the associated temperature STRE.T and to the kind of strength STRE.TYP.

Following strength types are valid:

- BEND STRENGTH
- COMPRESSION STRENGTH
- CREEP STRENGTH
- FATIGUE STRENGTH
- FRACTURE STRENGTH
- IMPACT STRENGTH
- NOTCH IMPACT STRENGTH
- SHEAR STRENGTH
- TENSILE STRENGTH
- TORSION STRENGTH
- IMPACT BENDING
- YIELD POINT

Fields:

Field Code	Full Name	Type of Indexing	Unit
STRE	Value of Strength	numerical	N/mm**2
STRE.TYP	Kind of Strength	string (phrase)	
STRE.T	Temperature	numerical	°C
STRE.MR	Remarks	string (phrase)	

Hardness (HARD)

Description:

The Hardness of a solid substance is its resistance to indentation, scratching, abrasion, or cutting. There are several scales of hardness numbers based on different methods of measurement:

- Identation hardness: Brinell, Knoop, Vickers, micro, Rockwell hardness
- Scratch hardness: Mohs hardness
- Scleroscope hardness

Following hardness types are valid: BRINELL HARDNESS, KNOOP HARDNESS, MICRO HARDNESS, MOHS HARDNESS, ROCKWELL HARDNESS, SCLEROSCOPE HARDNESS, VICKERS HARDNESS

Information about pretreatment of samples is given in the field remarks HARD.MR.

Note:

The displayed unit [e.g. N/mm**2] is not valid for Mohs, Rockwell and Scleroscope hardness, because they have no dimension in the GMELIN database.

Fields:

Field Code	Full Name	Type of Indexing	Unit
HARD	Value of Hardness	numerical	N/mm**2
HARD.VALU	Hardness without Unit		
HARD.TYP	Kind of Hardness	string (phrase)	
HARD.T	Temperature	numerical	°C
HARD.MR	Remarks	string (phrase)	

Density (DEN)

Description:

The density of a substance is the mass per unit volume at defined temperature and pressure.

The Density search field is a numeric range searchable field and is linked to the associated temperature DEN.T, the reference temperature DEN.RT, and to the pressure DEN.P. Information about pretreatment of samples is given in the field remarks DEN.MR. Further information about the density is given as a diagram or equation using the parameter field codes DEN.DGM respectively DEN.EQN. The field is linked to the forms of state of the substance by parameter field code DEN.S.

Note:

Searching for density diagram or equation field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing	Unit
DEN	Densitiy	numerical	g/ml
DEN.T	Temperature	numerical	°C
DEN.RT	Reference Temperature	numerical	°C
DEN.P	Pressure	numerical	Torr
DEN.MR	Remarks	string (phrase)	
DEN.DGM	Diagram	string (phrase)	
DEN.EQN	Equation	string (phrase)	
DEN.S	Forms of State	string (phrase)	

Molecular Properties (MOL)

Search Fields:

CONF	Conformation and Bonding Models
PGR	Symmetry / Point Group
IDA	Intramolecular Distances and Angles
VIB	Molecular Vibration
MCR	Molecular Rotation
EST	Electronic States
EDIS	Bond Dissociation Energy
ELP	Polarizability
DM	Dipole Moment
IP	Ionization Potential
PEF	Potential Energy Function

Conformation and Bonding Models (CONF)

Description:

The field Conformation and Bonding Models gives indications of conformation and bonding models or descriptions of molecular structure. The information indicated is more detailed than the structure shown in the database.

Type of Indexing:

Group Code

Symmetry / Point Group (PGR)

Description:

The field Symmetry / Point Group contains the Schoenflies symbol of the point group, which the molecule exhibits.

Note:

Avoid confusion of the symmetry point group of a molecule with its crystal space group recorded in the search field CRYST.SGROUP**.**

Type of Indexing:

String (phrase)

Intramolecular Distances and Angles (IDA)

Description:

The group code Intramolecular Distances and Angles gives indications of intramolecular distances, bond angles and dihedral angles of structure.

You can search for the determination method using the associated field code IDA.MET. Following methods can be searched:

- Electron Diffraction
- Empirical Calcn. (Phys. Properties)
- ESR Spectroscopy
- EXAFS Spectroscopy
- Fluorescence Spectroscopy
- Infrared Spectroscopy
- Microwave Spectroscopy
- Neutron Diffraction

- NMR Spectroscopy
- Powder X-Ray Diffraction
- Raman Spectroscopy
- Single Crystal X-Ray Diffraction
- Ultraviolet Spectroscopy
- X-Ray Diffraction
- X-Ray Spectroscopy

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
IDA.MET	Method of Determination	string (phrase)	

Molecular Vibration (VIB)

Description:

Indication of fundamental vibrations, force constants, anharmonicity constants and vibration-rotation-interaction constants is given in the fields VIB.FUND, VIB.FORCE, VIB.ANHRM and VIB.ROTA.

Note:

Searching for the special field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
VIB.FORCE	Force Constants	string (phrase)
VIB.FUND	Fundamental Vibrations	string (phrase)
VIB.ANHRM	Anharmonicity Constants	string (phrase)
VIB.ROTA	Vibration-Rotation-Interaction Constants	string (phrase)

Molecular Rotation (MRC)

Description:

The Molecular Rotation constant is inversely proportional to the moment of inertia of a molecule rotating about a particular axis. The search field contains the rotation constants for the vibrational ground state in the electronic ground state (Ao, Bo, Co).

Indication of centrifugal distortion or Coriolis coupling is given in the search field MRC.CENT.

Note:

Searching for centrifugal distortion require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing	Unit
MRC.CONA	Rotational Constant A(0)	numerical	Hz
MRC.CONB	Rotational Constant B(0)	numerical	Hz
MRC.CONC	Rotational Constant C(0)	numerical	Hz
MRC.CENT	Centrifugal Distortion	string (phrase)	

Electronic States (EST)

Description:

The field Electronic States gives indications of properties of electronic energy levels e.g. term values, lifetimes, fine or hyperfine structure.

Note:

Assignments of UV bands to transitions between electronic states are indicated in the UV.ASSIG search field.

Type of Indexing:

Group Code

Bond Dissociation Energy (EDIS)

Description:

The field Bond Dissociation Energy is the amount of energy needed to break a single bond of one type in a molecule.

The field Bond Dissociation Energy gives indications of bond energy in the electronic ground state.

Type of Indexing:

Group Code

Polarizability (ELP)

Description:

The electric Polarizability of a molecule is the induced electric dipole moment per unit field strength.

If the polarizability of an ion is determined the whole compound containing the ion is stated by formula or chemical name. You can search for this associated information using the parameter field code ELP.COFO.

Type of Indexing:

Numerical (range)

Unit:

The default unit in the CrossFire database for this fact is ml.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
ELP.COFO	Complete Formula	string (phrase)

Dipole Moment (DM)

Description:

The dipole moment is the electric moment of the charge density in an asymmetrical molecule.

You can search for the determination method using the associated field code DM.MET. Following methods can be searched:

- Electric Constant, Permittivity
- Dielectric Relaxation
- IR Spectroscopy
- Microwave Spectroscopy
- Molecular Beam Electric Resonance

e.g the method dielectric constant means that the dipole moment value is calculated from the dielectric constant.

Type of Indexing:

Numerical (range)

Unit:

The default unit in the Gmelin database for this fact is D.

Note:

D = Debye = 3.33 10-30 C m

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
DM.MET	Method of Determination	string (phrase)

Ionization Potential (IP)

Description:

The Ionization Potential is the energy required to remove an electron from the neutral molecule bond infinity.

Valid determination methods in the field IP.MET are as follows:

- Electron Impact
- Mass Spectroscopy
- Photoelectron Spectroscopy
- Photoemission Yield Spctr.
- Photoionization

Possible types of the ionization process in the field IP.TYP are:

- Adiabatic
- Vertical
- Not Given

Generally, only the first ionization potential is recorded numerically. Further ionization potentials are indicated in the field IP.POT.

Indication of additional information on ion formation (like ionization cross section, electron affinity) is given in the field IP.IONFORM.

Type of Indexing:

Numerical (range)

Unit:

The default unit in the CrossFire database for this fact is eV.

Note:

eV = 1.6021 10-19 Joule

Note:

Searching for higher ionization potentials require the field value "available", formation of ions the field value "described", or more general "*".

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
IP.MET	Method of Determination	string (phrase)
IP.TYP	Kind of Ionization	string (phrase)
IP.POT	Higher Ionization Potentials	string (phrase)
IP.IONFORM	Formation of Ions	string (phrase)

Potential Energy Function (PEF)

Description:

Indication of Potential Energy Function is given in this field.

You can search for information given as diagram or equation using the associated parameter fields PEF.DGM respectively PEF.EQN.

Note:

Searching for potential energy diagrams or equations, requires the field value "available" or more general "*".

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
PEF.DGM	Diagram	string (phrase)
PEF.EQN	Equation	string (phrase)

Optical Properties (OPT)

Search Fields:

RI	Refractive Index
CDIC	Circular Dichroism
OA	Optical Anisotropy

OR	Optical Rotation
MAGO	Magnetooptical Effects
ELOP	Electrooptical Effects

Refractive Index (RI)

Description:

The refractive index is the ratio of the velocity of light in a vacuum to the velocity of light in the substance. The Refractive Index is a numerical range searchable field and is linked to the associated temperature RI.T and wave length RI.W. Indication of birefringence is given in the field code RI.BR. Information about pretreatment of samples is given in the field remarks RI.MR. The refractive index is linked to the forms of state of the substance by parameter field code RI.S.

Note:

Searching for birefringence field code requires the field value "yes" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing	Unit
RI	refractive index	numerical	
RI.T	temperature	numerical	°C
RI.W	wave length	numerical	nm
RI.MR	remarks	string (phrase)	
RI.BR	birefringence	string (phrase)	
RI.S	forms of state	string (phrase)	

Circular Dichroism (CDIC)

Description:

Circular dischroism is due to the phenomen that planar polarization converts to elliptic polarization when linearly polarized incident light passes through an active medium, e.g. an optically active substance. Optically active substances absorb left and right polarized light unequally.

The field Circular Dichroism indicates information on circular dichroism or optical rotary dispersion of a substance.

Type of Indexing:

Group Code

Optical Anisotropy (OA)

Description:

The behavior of a substance whose effect on electromagnetic radiation varies with the direction of the propagation is designated as optical anisotropy.

The field Optical Anisotropy indicates information on optical anisotropic behavior of substances.

Type of Indexing:

Group Code

Optical Rotation (OR)

Description:

The optical rotation is the rotation of the plane of polarization in a beam of light as it passes through an optically active substance.

The field Optical Rotation indicates the optical rotary power of an optical active substance.

Type of Indexing:

Group Code

Magnetooptical Effects (MAGO)

Description:

Magnetooptic effects relate to the effect of magnetism on the propagation of light.

The field Magnetooptical Effects indicates information on magnetooptical effects of substances, e.g. Faraday effect, magneto-optic Kerr effect, magneto-optical-rotational-dispersion (MORD) or Zeeman effect.

Type of Indexing:

Group Code

Electrooptical Effects (ELOP)

Description:

Electrooptic effects are the alteration of the optical behavior, e.g. refractive properties, by an applied electric field.

The field Electrooptical Effects indicates information on electrooptical effects of substances, e.g. Kerr effect, Stark effect, or Pockels effect.

Type of Indexing:

Group Code

Information on Phase Transition (PHT)

Search Fields:

STAT	State Diagram
TP	Triple Point
CRP	Critical Point
TSS	Transition Point Solid / Solid
HTSS	Transition Enthalpy Solid / Solid
STSS	Transition Entropy Solid / Solid
GTSS	Transition Gibbs Energy Solid / Solid
MP	Melting Point
HFUS	Melting Enthalpy
SFUS	Melting Entropy
GFUS	Melting Gibbs Energy
MPFI	Melting Point (Further Information)
SP	Sublimation Point
HSUB	Sublimation Enthalpy
SSUB	Sublimation Entropy
GSUB	Sublimation Gibbs Energy
SPFI	Sublimation Point (Further Information)
BP	Boiling Point
HVAP	Boiling Enthalpy
SVAP	Boiling Entropy
GVAP	Boiling Gibbs Energy
VP	Vapor Pressure
VPFI	Vapor Pressure (Further Information)

State Diagram (STAT)

Description:

The field State Diagram indicates a phase (state) diagram as a plot of pressure versus temperature for a certain substance (one component).

Type of Indexing:

Group Code

Note:

Phase diagrams of multi-component systems are indicated in the search field META.

Triple Point (TP)

Description:

The Triple Point is the thermodynamic state at which three phases of a substance exist in equilibrium recorded in the fields temperature TP and pressure TP.P.

The search field phases contains the description of the three phases existing at the triple point. You can search for this associated information using the parameter field code TP.PHAS.

Fields:

Field Code	Full Name	Type of Indexing	Unit
TP.PHAS	Phases	string (phrase)	
TP.P	Pressure	numerical	Torr
TP	Temperature	numerical	°C

Critical Point (CRP)

Description:

The Critical Point CRP is the temperature above which a gas cannot be liquified, regardless of the pressure. The critical pressure CRP.P of a substance is the minimum pressure required for liquefaction at the critical temperature. The critical density CRP.DEN is the density exhibited by a substance at critical temperature and critical pressure.

The critical volume CRP.MVOLO(MVOLA) of a substance is the molar (specific) volume at critical pressure and critical temperature.

Fields:

Field Code	Full Name	Type of Indexing	Unit
CRP.P	Pressure	numerical	Torr
CRP	Temperature	numerical	°C
CRP.DEN	Density	numerical	g/ml
CRP.MVOLO	Molar Volume	numerical	ml/mol
CRP.MVOLA	Specific Volume	numerical	l/kg

Transition Point Solid / Solid (TSS)

Description:

The (crystal) Transition Point Solid / Solid is the thermodynamic state at which two crystalline modifications are in equilibrium. The TSS field contains the temperature at which a phase transition between two specified crystalline phases occurs. It is linked to the associated pressure by parameter field codes TSS.P. The crystalline modifications are displayed in the field TSS.PHAS1 and TSS.PHAS2.

Fields:

Field Code	Full Name	Type of Indexing	Unit
TSS.PHAS1	Solid Phase 1	string (phrase)	
TSS.PHAS2	Solid Phase 2	string (phrase)	
TSS.P	Pressure	numerical	Torr
TSS	Temperature	numerical	°C

Transition Enthalpy Solid / Solid (HTSS)

Description:

The (specific) enthapy of phase transition is the change in enthalpy for conversion of one mole (gram) of a substance from one solid phase 1 into phase 2 without change in temperature.

The transition enthalpy is linked to the associated temperature and pressure by parameter field codes HTSS.T resp. HTSS.P. The crystalline modifications are displayed in the field HTSS.PHAS1 and HTSS.PHAS2.

Fields:

Field Code	Full Name	Type of Indexing	Unit
HTSS.PHAS1	Solid Phase 1	string (phrase)	
HTSS.PHAS2	Solid Phase 2	string (phrase)	
HTSS.T	Temperature	numerical	°C
HTSS.P	Pressure	numerical	Torr
HTSS.ENTHO	Molar Transition Enthalpy	numerical	J/mol
HTSS.ENTHA	Specific Transition Enthalpy	numerical	J/g

Transition Entropy Solid / Solid (STSS)

Description:

The (specific) entropy of phase transition is the change in entropy for conversion of one mole (gram) of a solid phase 1 into a different phase 2 without change in temperature.

The transition entropy is linked to the associated temperature and pressure by parameter field codes STSS.T resp. STSS.P. The crystalline modifications are displayed in the field STSS.PHAS1 and STSS.PHAS2.

Fields:

Field Code	Full Name	Type of Indexing	Unit
STSS.PHAS1	Solid Phase 1	string (phrase)	
STSS.PHAS2	Solid Phase 2	string (phrase)	
STSS.P	Pressure	numerical	Torr
STSS.T	Temperature	numerical	°C
STSS.ENTRO	Molar Transition Entropy	numerical	J/(mol*K)
STSS.ENTRA	Specific Transition Entropy	numerical	J/(g*K)

Transition Gibbs Energy Solid / Solid (GTSS)

Description:

The (specific) Gibbs energy of phase transition is the change in Gibbs energy for conversion of one mole (gram) of a solid phase 1 into a different phase 2 without change in temperature.

The transition Gibbs enthalpy is linked to the associated temperature and pressure by parameter field codes GTSS.T resp. GTSS.P. The crystalline modifications are displayed in the field GTSS.PHAS1 and GTSS.PHAS2.

Fields:

Field Code	Full Name	Type of Indexing	Unit
GTSS.PHAS1	Solid Phase 1	string (phrase)	
GTSS.PHAS2	Solid Phase 2	string (phrase)	
GTSS.P	Pressure	numerical	Torr
GTSS.T	Temperature	numerical	°C
GTSS.FRENO	Molar Gibbs Energy of Transition	numerical	J/mol
GTSS.FRENA	Specific Gibbs Energy of Transition	numerical	J/g

Melting Point (MP)

Description:

The Melting Point or freezing point of a substance is the temperature at which the solid and liquid phases are in thermodynamic equilibrium.

The MP search field is linked to the associated pressure by parameter field code MP.P and to the solvent, from which the substance was crystallized, by parameter field code MP.SOL. Decomposition of the substance during melting is indicated in associated parameter field MP.DEC.

Fields:

Field Code	Full Name	Type of Indexing	Unit
MP	Temperature	numerical	°C
MP.P	Pressure	numerical	Torr
MP.DEC	Decomposition	string (phrase)	
MP.SOL	Solvent	string (phrase)	

Melting Enthalpy (HFUS)

Description:

The (specific) enthalpy of fusion is the change in enthalpy when one mole (gram) of a solid substance is converted into liquid without a change in temperature.

The Melting Enthalpy is linked to the associated temperature and pressure by parameter field codes HFUS.T resp. HFUS.P and to the solvent from which the substance was crystallized by parameter field code HFUS.SOL.

Fields:

Field Code	Full Name	Type of Indexing	Unit
HFUS.T	Temperature	numerical	°C
HFUS.P	Pressure	numerical	Torr
HFUS.SOL	Solvent	string (phrase)	
HFUS.ENTHO	Molar Enthalpy Of Melting	numerical	J/mol
HFUS.ENTHA	Specific Enthalpy Of Melting	numerical	J/g

Melting Entropy (SFUS)

Description:

The (specific) entropy of fusion is the change in entropy for the transition of one mole (gram) of solid substance into liquid at constant temperature.

The Melting Entropy is linked to the associated temperature and pressure by parameter field codes SFUS.T resp. SFUS.P and to the solvent from which the substance was crystallized by parameter field code SFUS.SOL.

Fields:

Field Code	Full Name	Type of Indexing	Unit
SFUS.T	Temperature	numerical	°C
SFUS.P	Pressure	numerical	Torr
SFUS.SOL	Solvent	string (phrase)	
SFUS.ENTRO	Molar Entropy Of Melting	numerical	J/(mol*K)
SFUS.ENTRA	Specific Entropy Of Melting	numerical	J/(g*K)

Melting Gibbs Energy (GFUS)

Description:

The (specific) Gibbs energy of fusion is the change in Gibbs energy when one mole (gram) of a solid substance is converted into liquid without change in temperature.

The Melting Gibbs Energy is linked to the associated temperature and pressure by parameter field codes GFUS.T resp. GFUS.P and to the solvent from which the substance was crystallized by parameter field code GFUS.SOL.

Fields:

Field Code	Full Name	Type of Indexing	Unit
GFUS.T	Temperature	numerical	°C
GFUS.P	Pressure	numerical	Torr
GFUS.SOL	Solvent	string (phrase)	
GFUS.FRENO	Molar Gibbs Energy Of Melting	numerical	J/mol
GFUS.FRENA	Specific Gibbs Energy Of Melting	numerical	J/g

Melting Point (Further Information) (MPFI)

Description:

The search field Melting Point (Further Information) indicates if further information about the melting point is given as diagram, table, or equation.

Note:

Searching for the special field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
MPFI.DGM	Diagram	string (phrase)
MPFI.TAB	Table	string (phrase)
MPFI.EQN	Equation	string (phrase)

Point of Sublimation (SP)

Description:

The Point of Sublimation is the temperature at which the vapor pressure of a solid substance is equal to the external pressure.

The SP search field is linked to the associated pressure by parameter field code SP.P and to the solvent from which the substance was crystallized by parameter field code SP.SOL.

Fields:

Field Code	Full Name	Type of Indexing	Unit
SP	Temperature	numerical	°C
SP.P	Pressure	numerical	Torr
SP.SOL	Solvent	string (phrase)	

Sublimation Enthalpy (HSUB)

Description:

The (specific) enthalpy of sublimation is the change in enthalpy for conversion of one mole (gram) of a solid substance into vapor without change in temperature.

The Sublimation Enthalpy is linked to the associated temperature and pressure by parameter field codes HSUB.T resp. HSUB.P and to the solvent from which the substance was crystallized by parameter field code HSUB.SOL.

Fields:

Field Code	Full Name	Type of Indexing	Unit
HSUB.T	Temperature	numerical	°C
HSUB.P	Pressure	numerical	Torr
HSUB.SOL	Solvent	string (phrase)	
HSUB.ENTHO	Molar Sublimation Enthalpy	numerical	J/mol
HSUB.ENTHA	Specific Sublimation Enthalpy	numerical	J/g

Sublimation Gibbs Energy (GSUB)

Description:

The (specific) Gibbs energy of sublimation is the change in Gibbs energy for conversion of one mole (gram) of a solid substance into vapor without change in temperature.

The Sublimation Gibbs Energy is linked to the associated temperature and pressure by parameter field codes GSUB.T resp. GSUB.P and to the solvent from which the substance was crystallized by parameter field code GSUB.SOL.

Fields:

Field Code	Full Name	Type of Indexing	Unit
GSUB.T	Temperature	numerical	°C
GSUB.P	Pressure	numerical	Torr
GSUB.SOL	Solvent	string (phrase)	
GSUB.FRENO	Molar Gibbs Energy Of Sublimation	numerical	J/mol
GSUB.FRENA	Specific Gibbs Energy Sublimation	numerical	J/g

Sublimation Entropy (SSUB)

Description:

The (specific) entropy of sublimation is the change of entropy for the transition of one mole (gram) of a solid substance to saturated vapor at constant temperature and under equilibrium conditions.

The Sublimation Entropy is linked to the associated temperature and pressure by parameter field codes SSUB.T resp. SSUB.P and to the solvent from which the substance was crystallized by parameter field code SSUB.SOL.

Fields:

Field Code	Full Name	Type of Indexing	Unit
SSUB.T	Temperature	numerical	°C
SSUB.P	Pressure	numerical	Torr
SSUB.SOL	Solvent	string (phrase)	
SSUB.ENTRO	Molar Sublimation Entropy	numerical	J/(mol*K)
SSUB.ENTRA	Specific Sublimation Entropy	numerical	J/(g*K)

Sublimation Point (Further Information) (SPFI)

Description:

The search field Sublimation Point (Further Information) indicates if further information about the melting point is given as diagram, table, or equation.

Note:

Searching for the special field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
SPFI.DGM	Diagram	string (phrase)
SPFI.TAB	Table	string (phrase)
SPFI.EQN	Equation	string (phrase)

Boiling Point (BP)

Description:

The Boiling Point is the temperature at which the vapor pressure of a liquid equals the external pressure. The normal boiling point is the temperature at which the vapor pressure equals the normal atmospheric pressure.

The BP search field is linked to the associated pressure by parameter field code BP.P. Decomposition of the substance during boiling is indicated in associated parameter field BP.DEC.

Fields:

Field Code	Full Name	Type of Indexing	Unit
BP	Temperature	numerical	°C
BP.P	Pressure	numerical	Torr
BP.DEC	Decomposition	string (phrase)	

Boiling Enthalpy (HVAP)

Description:

The (specific) enthalpy of vaporization is the enthalpy change required to convert one mole (gram) of liquid substance into saturated vapor at constant temperature.

The Boiling Enthalpy is linked to the associated temperature and pressure by parameter field codes HVAP.T resp. HVAP.P.

Fields:

Field Code	Full Name	Type of Indexing	Unit
HVAP.T	Temperature	numerical	°C
HVAP.P	Pressure	numerical	Torr
HVAP.ENTHO	Molar Vaporization Enthalpy	numerical	J/mol
HVAP.ENTHA	Specific Vaporization Enthalpy	numerical	J/g

Boiling Entropy (SVAP)

Description:

The (specific) entropy of vaporization is the change in entropy for the transition of one mole (gram) of liquid substance into vapor at constant temperature and under equilibrium conditions.

The Boiling Entropy is linked to the associated temperature and pressure by parameter field codes SVAP.T resp. SVAP.P.

Fields:

Field Code	Full Name	Type of Indexing	Unit
SVAP.T	Temperature	numerical	°C
SVAP.P	Pressure	numerical	Torr
SVAP.ENTRO	Molar Vaporization Entropy	numerical	J/(mol*K)
SVAP.ENTRA	Specific Vaporization Entropy	numerical	J/(g*K)

Boiling Gibbs Energy (GVAP)

Description:

The (specific) Gibbs energy of vaporization is the change in Gibbs energy when one mole (gram) of a liquid substance is converted into vapor.

The Boiling Gibbs Energy is linked to the associated temperature and pressure by parameter field codes SVAP.T resp. SVAP.P.

Fields:

Field Code	Full Name	Type of Indexing	Unit
GVAP.T	temperature	numerical	°C
GVAP.P	pressure	numerical	Torr
GVAP.FRENO	molar Gibbs energy of vaporization	numerical	J/mol
GVAP.FRENA	specific Gibbs energy vaporization	numerical	J/g

Vapor Pressure (VP)

Description:

The Vapor Pressure of a pure solid or liquid substance is the pressure exerted by its vapor under equilibrium conditions.

You can search for the associated temperature using the parameter field code VP.T. The vapor pressure is linked to the forms of state of the substance by parameter field code VP.S.

Fields:

Field Code	Full Name	Type of Indexing	Unit
VP	Pressure	numerical	Torr
VP.T	Temperature	numerical	°C
VP.S	Forms of State	string (phrase)	

Vapor Pressure (Further Information) (VPFI)

Description:

The search fields Vapor Pressure (Further Information) indicates if information about vapor pressure is given as a diagram, table or equation.

This field is linked to the forms of state of the substance by parameter field code VPFI.S.

Note:

Searching for the special field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
VPFI.DGM	Diagram	string (phrase)
VPFI.EQN	Table	string (phrase)
VPFI.TAB	Equation	string (phrase)
VPFI.S	Forms of State	string (phrase)

Spectroscopic Information (SPE)

Search Fields:

NMR	NMR Spectroscopy
IR	IR Spectroscopy
NQR	NQR Spectroscopy
ESR	ESR Spectroscopy
MS	Mass Spectroscopy
UV	UV/VIS Spectroscopy
MOE	Moessbauer Spectroscopy
ROT	Rotational Spectroscopy
RAS	Raman Spectroscopy
UPS	UV Photoelectron Spectroscopy
XPS	X-Ray Photoelectron Spectroscopy
XSPE	X-Ray Spectroscopy
AUG	Auger Spectroscopy
FLS	Fluorescence Spectroscopy
PHS	Phosphorescence Spectroscopy
LUS	Luminescence Spectroscopy
EEL	Electron Energy Loss Spectroscopy

NMR Spectroscopy (NMR)

Description:

NMR spectroscopy is based on resonance of nuclei (nuclear spin I>0) with a magnetic field and an electromagnetic field. Usually the frequency of the electromagnetic field is swept. The NMR Spectroscopy search field is linked to the associated search fields solvent NMR.SOL and temperature parameters NMR.T. The corresponding spin-spin coupling atoms are searchable in NMR.NUI. Indications about a shown spectrum is given in the parameter field code NMR.DGM, as well as, further information about signals and intensities (NMR.SIGNAL), linewidths or dynamic effects (NMR.LINDYN), and description of spectra (NMR.DESCR).

Note:

Searching for spectrum diagram, signals / intensities, linewidths, or spectrum description field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing	Unit
NMR.NUC	Nucleus	string (phrase)	
NMR.DGM	Spectrum Diagram	string (phrase)	
NMR.NUI	Spin-Spin Coupling to Nuclei	string (phrase)	
NMR.SOL	Solvent	string (phrase)	
NMR.T	Temperature	numerical	°C
NMR.SIGNAL	Signal / Intensities	string (phrase)	
NMR.LINDYN	Linewidths	string (phrase)	
NMR.DESCR	Description	string (phrase)	

IR Spectroscopy (IR)

Description:

The IR absorption spectrum of a substance is produced by its interaction with electromagnetic radiation (usually in the range 10-10000 cm^{-1}) due to vibrational transitions. The IR Spectroscopy search fields are linked to the associated search fields solvent IR.SOL and temperature parameters IR.T. The wavelength range is searchable with IR.SPEC. Indications about a shown spectrum is given in the parameter field code IR.DGM as well as further information about bands and intensities (IR.BANDS), and description of spectra (IR.DESCR).

Note:

Searching for spectrum diagram, bands / intensities, or spectrum description field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing	Unit
IR.DGM	Spectrum Diagram	string (phrase)	
IR.SOL	Solvent	string (phrase)	
IR.SPEC	Spectral Range	numerical	cm**-1
IR.T	Temperature	numerical	°C
IR.BANDS	Bands / Intensities	string (phrase)	
IR.DESCR	Description	string (phrase)	

NQR Spectroscopy (NQR)

Description:

The NQR-Spectrum is based on resonance between the nuclear quadrupole moment and a variable electric field gradient. The nuclei are searchable with the parameter field NQR.NUC. Indications about a shown spectrum is given in the parameter field code NQR.DGM as well as further information about quadrupole splitting (NQR.SPLIT), and description of spectra (NQR.DESCR).

Note:

Searching for spectrum diagram, quadrupole splitting, or spectrum description field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing

NQR.NUC	Nucleus	string (phrase)
NQR.DGM	Spectrum Diagram	Y
NQR.SPLIT	Quadrupole Splitting	Y
NQR.DESCR	Description	Y

ESR Spectroscopy (ESR)

Description:

ESR spectroscopy is determined by measuring the paramagnetic properties of atoms or molecules in a magnetic field. Resonance absorption occurs on irradiation with electromagnetic waves of appropriate frequency. Hyperfine coupling is due to interaction of the unpaired electrons with nuclei possessing a magnetic moment. The ESR Spectroscopy search fields contain the coupling nuclei ESR.NUI, g-factors ESR.GFAC, and solvent ESR.SOL and temperature parameters ESR.T. Indications about a shown spectrum is given in the parameter field code ESR.DGM, as well as, description of spectra in ESR.DESCR.

Note:

Searching for spectrum diagram, g-factors, or spectrum description field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing	Unit
ESR.DGM	Spectrum Diagram	string (phrase)	
ESR.GFAC	G-Factors	string (phrase)	
ESR.NUI	Hyperfine Coupling To Nuclei	string (phrase)	
ESR.SOL	Solvent	string (phrase)	
ESR.T	Temperature	numerical	°C
ESR.DESCR	Description	string (phrase)	

Mass Spectroscopy (MS)

Description:

Method based on sending an ionized beam of molecules or molecule fragments through an inhomogeneous magnetic field to achieve a separation depending on the mass/charge ratio of the particles. Indications about a shown spectrum is given in the parameter field code MS.DGM, as well as, further information of a given molecular peak (MS.PEAK), the fragmentation (MS.FRAG), and description of spectra (MS.DESCR).

Note:

Searching for the special field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
MS.DGM	Spectrum Diagram	string (phrase)
MS.PEAK	Molecular Peak	string (phrase)
MS.FRAG	Fragmentation Pattern	string (phrase)
MS.DESCR	Description	string (phrase)

UV / VIS Spectroscopy (UV)

Description:

The UV and VIS absorption spectrum of a substance is produced by its interaction with electromagnetic radiation (usually in the range 200-800 nm) due to electronic transitions. The UV / VIS Spectroscopy search field contains solvent (UV.SOL) and spectral range parameters (UV.SPEC) for ultraviolet and visible spectra. Indications about a shown spectrum is given in the parameter field code UV.DGM as well as further information of assignments (UV.ASSIG), and description of spectra (MS.DESCR).

Note:

Searching for spectrum diagrams, assignment, or spectrum description field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing	Unit
UV.DGM	Spectrum Diagram	string (phrase)	
UV.SOL	Solvent	string (phrase)	
UV.SPEC	Spectral Range	numerical	nm
UV.ASSIG	Assignment	string (phrase)	
UV.DESCR	Description	string (phrase)	

Moessbauer Spectroscopy (MOE)

Description:

Gamma-ray nuclear resonance absorption spectroscopy, with frozen Moessbauer nuclides, is searchable in the parameter field MOENUC. Indications about a shown spectrum are given in the parameter field code MOEM, as well as, further information of chemical shifts (MOE.SHIFTS), quadrupole splitting (MOE.SPLIT), and description of spectra (MOE.DESCR).

Note:

Searching for spectrum diagrams, chemical shifts, quadrupole splitting, or spectrum description field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
MOE.NUC	Nucleus	string (phrase)
MOE.DGM	Spectrum Diagram	string (phrase)
MOE.SHIFTS	Chemical Shifts	string (phrase)
MOE.SPLIT	Quadrupole Splitting	string (phrase)
MOE.DESCR	Description	string (phrase)

Rotational Spectroscopy (ROT)

Description:

The field Rotational Spectroscopy indicates a molecular spectrum produced by rotational-level transition. It is produced in the far-infrared region between 50 and 200 µm and in the microwave region.

Type of Indexing:

Group Code

Raman Spectroscopy (RAS)

Description:

Raman spectroscopy is a method in which the sample is illuminated with monochromatic light, usually generated by a laser. The scattered light produced by the sample is first scatter with exactly the same energy and wavelength as the incident light and second Raman scatter, which is usually much less intense than the first one and emerges at either longer or shorter wavelength than the incident light.

The field Raman Spectroscopy indicates the application of, or information to, a vibrational (Raman) spectrum of a substance.

Type of Indexing:

Group Code

UV Photoelectron Spectroscopy (UPS)

Description:

UV photoelectron spectroscopy (UPS) is a method in which a surface is bombarded with photons in the ultraviolet energy range and the resulting electronic emission spectrum is analyzed for information about molecular orbital characteristics or occupied and unoccupied density of states of substances.

The field UV Photoelectron Spectroscopy indicates the application of, or information to, a UV photoelectron spectrum of a substance.

Type of Indexing:

Group Code

X-Ray Photoelectron Spectroscopy (XPS)

Description:

X-Ray photoelectron spectroscopy (XPS) is a method in which a substance is irradiated with X-rays and the energies of the photoelectrons emitted from the substance surface are determined.

The field X-Ray Photoelectron Spectroscopy indicates the application of, or information to, an X-ray photoelectron spectrum of a substance.

Type of Indexing:

Group Code

X-Ray Spectroscopy (XSPE)

Description:

X-ray spectroscopy measures the absorption of X-rays by samples, especially at energies in the region of absorption edges.

The field X-Ray Spectroscopy indicates the application of X-ray spectroscopy e.g. EXAFS, XANES or EDAX.

Type of Indexing:

Group Code

Auger Spectroscopy (AUG)

Description:

Auger Spectroscopy is a method to analyze the energy of secondary (Auger) electrons ejected from a solid surface upon irradiation with accelerated electrons or X-ray photons.

The field Auger Spectroscopy indicates the application of, or information to, an Auger spectrum of a substance.

Type of Indexing:

Group Code

Fluorescence Spectroscopy (FLS)

Description:

Fluorescence spectrum is produced by the emission of radiation following absorption of and excitation by radiant energy.

The field Fluorescence Spectroscopy indicates the application of, or information to, a fluorescence spectrum of a substance.

Type of Indexing:

Group Code

Phosphorescence Spectroscopy (PHS)

Description:

The phosphorescence spectroscopy is a method based on the emission of light to spin-forbidden decay of electrons from excited states to the ground state.

The field Phosphorescence Spectroscopy indicates the application of, or information to, a phosphorescence spectrum of a substance.

Type of Indexing:

Group Code

Luminescence Spectroscopy (LUS)

Description:

Luminescence spectroscopy is a method based on the emission of light from a non thermal excitation. Luminescence is obtained under a variety of excitation sources, e.g. electromagnetic radiation, particles (like electron beam), electric field.

The field Luminescence Spectroscopy indicates the application of or information to a luminescence spectrum of a substance.

Type of Indexing:

Group Code

Electron Energy Loss Spectroscopy (EEL)

Description:

An electron energy loss spectrum is a method in which a substance is bombarded with monochromatic electrons and the distribution of the energy loss by scattered electrons is determined.

The field Electron Energy Loss Spectroscopy indicates the application of or information to an electron energy loss spectrum of a substance.

Type of Indexing:

Group Code

Thermodynamic Data (TDD)

Search Fields:

CP	Specific Heat at Constant Pressure
CPFI	Cp (Further Information)
CV	Specific Heat at Constant Volume
CVFI	Cv (Further Information)
HFOR	Enthalpy of Formation
HFFI	Enthalpy of Formation (Further Information)
GFOR	Gibbs Energy of Formation
GFFI	Gibbs Energy of Formation (Further Information)
SFOR	Entropy of Formation
SFFI	Entropy of Formation (Further Information)
EQST	Equation of State
ACEN	Acentric Factor

Specific Heat at Constant Pressure (CP)

Description:

The Specific (Molar) Heat Capacity at Constant Pressure is the enthalpy necessary to raise the temperature of one mole (one mass unit) of substance one degree at constant pressure.

The coefficient field is a numerical, range searchable field and is linked to the associated temperature CP.T and pressure CP.P, as well as, to the forms of state of the substance by parameter field code CP.S.

Fields:

Field Code	Full Name	Type of Indexing	Unit
CP.VALO	Cp (molar)	Numerical	J/mol*K
CP.VALA	Cp (specific)	Numerical	J/g*K
CP.T	Temperature	Numerical	°C
CP.P	Pressure	Numerical	Torr
CP.MR	Remarks	string (phrase)	
CP.S	Forms of State	string (phrase)	

Cp (Further Information) (CPFI)

Description:

The search field CP (Further Information) indicates if further information about the specific heat at constant pressure is given as a diagram, table, or equation in the fields CPFI.DGM, CPFI.TAB and CPFI.EQN.

The search field is linked to the forms of state of the substance by parameter field code CPFI.S.

Note:

Searching for the special field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
CPFI.DGM	Cp as Diagram	string (phrase)
CPFI.TAB	Cp as Table	string (phrase)
CPFI.EQN	Cp as Equation	string (phrase)
CPFI.S	Forms of State	string (phrase)

Specific Heat at Constant Volume (CV)

Description:

The Specific (Molar) Heat Capacity at Constant Volume is the internal energy required to raise the temperature of one mole (one gram) of substance one degree at constant volume.

The coefficient field is a numerical, range searchable field and is linked to the associated temperature CV.T and pressure CV.P as well as to the forms of state of the substance by parameter field code CV.S.

Fields:

Field Code	Full Name	Type of Indexing	Unit
CV.VALO	Cv (molar)	numerical	J/mol*K
CV.VALA	Cv (specific)	numerical	J/g*K
CV.T	Temperature	numerical	°C
CV.P	Pressure	numerical	Torr
CV.REM	Remarks	string (phrase)	
CV.STATE	Forms of State	string (phrase)	

Cv (Further Information) (CVFI)

The search field CV (Further Information) indicates if further information about the specific heat at constant volume is given as a diagram, table, or equation in the fields CVFI.DGM, CVFI.TAB and CVFI.EQN.

The search field is linked to the forms of state of the substance by parameter field code CVFI.S.

Note:

Searching for the special field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
CVFI.DGM	Cv as Diagram	string (phrase)
CVFI.TAB	Cv as Table	string (phrase)
CVFI.EQN	Cv as Equation	string (phrase)
CVFI.S	Forms of State	string (phrase)

Enthalpy of Formation (HFOR)

Description:

The (specific) Enthalpy of Formation is the change in enthalpy associated with the formation of one mole (one gram) of a substance from its elements in their standard states at specified temperature and pressure.

The coefficient field is a numerical, range searchable field and is linked to the associated temperature HFOR.T and pressure HFOR.P as well as to the forms of state of the substance by parameter field code HFOR.S.

Fields:

Field Code	Full Name	Type of Indexing	Unit
HFOR.VALO	Molar Enthalpy of Formation	numerical	J/mol
HFOR.VALA	Specific Enthalpy of Formation	numerical	J/g
HFOR.T	Temperature	numerical	°C
HFOR.P	Pressure	numerical	Torr
HFOR.S	Forms of State	string (phrase)	

Entropy of Formation (Further Information) (SFFI)

Description:

The search field Entropy of Formation (Further Information) indicates if further information about the Gibbs energy of formation is given as a diagram, table, or equation in the fields SFFI.DGM, SFFI.TAB and SFFI.EQN.

The search field is linked to the forms of state of the substance by parameter field code SFFI.S.

Note:

Searching for the special field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
SFFI.DGM	Diagram	string (phrase)
SFFI.TAB	Table	string (phrase)
SFFI.EQN	Equation	string (phrase)
SFFI.S	Forms of State	string (phrase)

Enthalpy of Formation (Further Information) (HFFI)

Description:

The search field Enthalpy of Formation (Further Information) indicates if further information about the enthalpy of formation is given as a diagram, table, or equation in the fields HFFI.DGM, HFFI.TAB and HFFI.EQN.

The search field is linked to the forms of state of the substance by parameter field code HFFI.S.

Note:

Searching for the special field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
HFFI.DGM	Diagram	string (phrase)
HFFI.TAB	Table	string (phrase)
HFFI.EQN	Equation	string (phrase)
HFFI.S	Forms of State	string (phrase)

Gibbs Energy of Formation (GFOR)

Description:

The (specific) Gibbs Energy of Formation is the change in Gibbs energy associated with the isothermal formation of one mole (one gram) of the substance from the elements in their standard states at specified temperature and pressure.

The coefficient field is a numerical, range searchable field and is linked to the associated temperature GFOR.T and pressure GFOR.P as well as to the forms of state of the substance by parameter field code GFOR.S.

Fields:

Field Code	Full Name	Type of Indexing	Unit
GFOR.VALO	Molar Gibbs Energy of Formation	numerical	J/mol
GFOR.VALA	Specific Gibbs Energy of Formation	numerical	J/g
GFOR.T	Temperature	numerical	°C
GFOR.P	Pressure	numerical	Torr
GFOR.S	Forms of State	string (phrase)	

Gibbs Energy of Formation (Further Information) (GFFI)

Description:

The search field Gibbs Energy of Formation (Further Information) indicates if further information about the Gibbs energy of formation is given as a diagram, table, or equation in the fields GFFI.DGM, GFFI.TAB and GFFI.EQN.

The search field is linked to the forms of state of the substance by parameter field code GFFI.S.

Note:

Searching for the special field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
GFFI.DGM	Diagram	string (phrase)
GFFI.TAB	Table	string (phrase)
GFFI.EQN	Equation	string (phrase)
GFFI.S	Forms of State	string (phrase)

Entropy of Formation (SFOR)

Description:

The (specific) Entropy of Formation is the change in entropy associated with the formation of one mole of a substance from its elements in their standard states at specified temperature and pressure.

The entropy of formation (specific: SFOR:VALA, molar: SFOR.VALO) search field is a numerical, range searchable field and is linked to the associated temperature SFOR.T and pressure SFOR.P, as well as, to the forms of state of the substance by parameter field code SFOR.S.

Fields:

Field Code	Full Name	Type of Indexing	Unit
SFOR.VALO	Molar Entropy of Formation	numerical	J/mol*K
SFOR.VALA	Specific Entropy of Formation	numerical	J/g*K
SFOR.T	Temperature	numerical	°C
SFOR.P	Pressure	numerical	Torr
SFOR.S	Forms of State	string (phrase)	

Equation of State (EQST)

Description:

The equation of state describes the state of a substance in terms of the relationship of the basic physical quantities of volume, pressure, and temperature.

The field Equation of State indicates a thermodynamic equation of state.

Type of Indexing:

Group Code

Acentric Factor (ACEN)

Description:

The Pitzer Acentric Factor is a measure of nonsphericity or acentricity of a molecule's potential force field.

Fields:

Field Code	Full Name	Type of Indexing
ACEN.VAL	Acentric Factor	numerical

Search Fields:

TEC	Thermal Expansion
TCND	Thermal Conductivity

Thermal Expansion (TEC)

Description:

The Thermal Expansion coefficient is the ratio of the change in length per unit length or change in volume per unit volume to the change of temperature.

The coefficient field is linked to the associated temperature TEC.T and to the kind of expansion TEC.LIN or TEC.CUB, as well as, to the forms of state of the substance by parameter field code TEC.S.

Note:

Searching for density diagram or equation field codes requires the field value "yes" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing	Unit
TEC	expansion coefficient	numerical	K**-1
TEC.LIN	linear expansion	string (phrase)	
TEC.CUB	cubic expansion	string (phrase)	
TEC.T	temperature	numerical	°C
TEC.MR	remarks	string (phrase)	
TEC.S	forms of state	string (phrase)	

Thermal Conductivity (TCND)

Description:

The Thermal Conductivity of a substance is the time rate of heat transfer by conduction, across unit area, through unit thickness of substance, for unit difference of temperature.

The coefficient field is linked to the associated temperature TCND.T and to the forms of state of the substance by parameter field code TCND.S.

Fields:

Field Code	Full Name	Type of Indexing	Unit
TCND	thermal conductivity	numerical	cal/(m*s*K)
TCND.T	temperature	numerical	°C
TCND.MR	remarks	string (phrase)	
TCND.S	forms of state	string (phrase)	

Transport Phenomena (TRA)

Search Fields:

DYVI	Dynamic Viscosity
KIVI	Kinematic Viscosity
NONT	Non-Newtonian Behavior

Dynamic Viscosity (DYVI)

Description:

The Dynamic Viscosity is the ratio of the shearing stress to the shear of the motion of a fluid, melt, or suspension. It is independent of the velocity distribution and the dimensions of the system. For a gas it is independent of pressure except at very low pressures.

The dynamic viscosity field contains the values for the dynamic viscosity of substances given at specified temperatures. You can search for this associated information using the parameter field code DYVI.T.

The search field remarks contain concentration details of solutions, as well as, information to further specialize conditions relating to the dynamic viscosity values. You can search for this associated information using the parameter field code DYVI.MR.

The forms of state of the substance can be restricted by the associated parameter field code DYVI.S

Type of Indexing:

Numerical (range)

Unit:

The default unit in the CrossFire database for this fact is P.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
DYVI.T	Temperature	numerical	°C
DYVI.MR	Remarks	string (phrase)	
DYVI.S	Forms of State	string (phrase)	

Kinematic Viscosity (KIVI)

Description:

The Kinematic Viscosity of a substance is the ratio of the dynamic viscosity to its density.

The values are given at specific temperatures. These temperatures can be searched using the associated parameter field code KIVI.T.

The search field remarks contain concentration details of solutions, as well as, information to further specialize conditions relating to the dynamic viscosity values. You can search for this associated information using the parameter field code KIVI.MR.

The forms of state of the substance can be restricted by the associated parameter field code KIVI.S

Type of Indexing:

Numerical (range)

Unit:

The default unit in the CrossFire database for this fact is St.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
KIVI.T	Temperature	numerical	°C
KIVI.MR	Remarks	string (phrase)	
KIVI.S	Forms of State	string (phrase)	

Non-Newtonian Behavior (NONT)

Description:

Compounds show Non-Newtonian Behavior if their viscosity at a given temperature is not a constant, but depends on the shear velocity or the shear stress.

Type of Indexing:

Group Code

Properties of / in Systems Properties of / in Systems (MCS)

Search Fields:

SOR	Sorption
DIF	Diffusion
AZE	Formation of Azeotrope
DIST	Distribution
MULT	System Components
META	Multicomponent System Data
ETEC	Eutectic Temperature
PTEC	Peritectic Temperature
MULS	Solubility In Systems
VPR	Vapor Pressure of Solution
SLB	Solubility
SLBP	PL-Value
ST	Surface Tension

Sorption (SOR)

Description:

The Sorption search field contains the availability of references about adsorption, absorption, desorption and chemisorption. It is divided into the sorption of a substance, or a title compound.

Search Fields:

SPTO	Sorption to Title Compound
SPOF	Sorption of Title Compound

Sorption to Title Compound (SPTO)

Description:

The Sorption to Title Compound search field contains the availability of references about adsorption, absorption, desorption and chemisorption to a substance, a title compound. The title compound is the adsorbent. The other component, the adsorbate, is searchable in the associated field SPTO.PA.

Further information about the sorption is given as a diagram, table or equation using the parameter field codes SPTO.DGM, SPTO.TAB respectively SPTO.EQN. Further data are given in the field SPOF.

Note:

Searching for a diagram, table or equation field require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
SPTO.PA	Other Component	string (phrase)
SPTO.DGM	Diagram	string (phrase)
SPTO.TAB	Table	string (phrase)
SPTO.EQN	Equation	string (phrase)

Sorption of Title Compound (SPOF)

Description:

The Sorption of Title Compound search field contains the availability of references about adsorption, absorption, desorption and chemisorption of a substance, a title compound. The title compound is the adsorbate. The other component, the adsorbent, is searchable in the associated field SPOF.PA.

Further information about the sorption is given as a diagram, table or equation using the parameter field codes SPOF.DGM, SPOF.TAB respectively SPOF.EQN. Further data are given in the field SPTO.

Note:

Searching for a diagram, table or equation field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
SPOF.PA	Other Component	string (phrase)
SPOF.DGM	Diagram	string (phrase)
SPOF.TAB	Table	string (phrase)
SPOF.EQN	Equation	string (phrase)

Diffusion (DIF)

Description:

The Diffusion search field contains the availability of references about diffusion of a substance into a second one without the influence of external forces. It is divided into the diffusion of a substance, or a title compound.

Search Fields:

DIFOF	Diffusion of Title Compound
DIFIN	Diffusion into Title Compound

Diffusion of Title Compound (DIFOF)

Description:

The diffusion coefficient is the ratio of the mass flux to the concentration gradient in a system, which is free of external force fields and is homogeneous with respect to temperature and pressure. The Diffusion of Title Compound search field contains references to the diffusion of a title compound into a second compound and eventually the diffusion coefficient of a given substance (gas, liquid, but also solid) in the literature through the second one.

The field is linked to the associated temperature DIFOF.T and to the compound (other phase) DIFOF.PA through which the given substance diffuses.

Fields:

Field Code	Full Name	Type of Indexing	Unit
DIFOF.PA	Other Component	string (phrase)	
DIFOF	Diffusion Coefficient	numerical	cm**2/s
DIFOF.T	Temperature	numerical	°C

Diffusion into Title Compound (DIFIN)

Description:

The diffusion into title compound is the diffusion of a substance into the title compound without influence of external forces. The Diffusion into Title Compound search field contains references to the diffusion of a substance into the title compound for a given substance in the literature.

The field is linked to the compound (other phase) DIFOF.PA which diffuses through the given substance.

Fields:

Field Code	Full Name	Type of Indexing
DIFIN.COMP	Other Component	string (phrase)

Azeotropes (AZE)

Description:

An azeotrope is a solution with an extremum boiling point at which composition of liquid and vapor phases are equal; therefore, there is no change in composition on boiling. The azeotrope field contains the azeotropy of the title compound with another substance in the literature. Both are recorded as GRN.

Fields:

Field Code	Full Name	Type of Indexing
AZE.PG	Azeotropes (GRN)	string (phrase)
AZE.PA	Azeptropes	string (phrase)

Distribution (DIST)

Description:

A substance distributes itself between two immiscible solvents so that the ratio of its concentrations in the two solvents is approximately a constant. The distribution coefficient gives the ratio of the concentrations in the two phases at a specified temperature at the equilibrium state. The two phases can be specified in the search fields DIST.PHAS1 and DIST.PHAS2. The Distribution search field contains references to the distribution of a given substance in the literature between two phases and eventually the distribution coefficient. The distribution coefficient search field DISTR is a numerical search field and is linked to the associated temperature DIST.T.

Fields:

Field Code	Full Name	Type of Indexing	Unit
DIST.PHAS1	Phase 1	string (phrase)	
DIST.PHAS2	Phase 2	string (phrase)	
DIST.COEFF	Distribution Coefficient	numerical	
DIST.T	Temperature	numerical	°C

System Components (MULT)

Description:

In the GMELIN file a heterogeneous multicomponent system is defined as a compound consisting of pure "corner components" e.g. RbBr#ScBr3. Phases that are formed in such systems (System Components) can be retrieved in the field MULT by GRN or chemical name.

Fields:

Field Code	Full Name	Type of Indexing
MULT.GRN	component registry number	string (phrase)
MULT.PA	component name(s)	string (phrase)

Multicomponent System Data (META)

Description:

Indication of phase, solubility or melting diagrams of heterogeneous multicomponent systems is given in the field META.DGM.

Indication on metastable phases of heterogeneous multicomponent systems is given in the field META.PHAS.

Note:

Searching for a diagram field code requires the field value "available", for metastabile phases the field value "described" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
META.DGM	Phase / Solubility / Melting Diagram	string (phrase)
META.PHAS	Metastable Phases	string (phrase)

Eutectic Temperature (ETEC)

Description:

The Eutectic Temperature is the temperature on which co-crystallization of two phases occurs. It is the lowest possible liquid temperature in a system containing two stable phases. The liquid curve forms a singularity at this temperature in the melting diagram of a heterogeneous multicomponent system. The eutectic temperature field ETEC.T contains the values for a given substance in the literature. The concentration of the phases at the eutectic point is given in the remark field ETEC.MR.

Fields:

Field Code	Full Name	Type of Indexing	Unit
ETEC.T	Eutectic Temperature	numerical	°C
ETEC.MR	Remarks	string (phrase)	

Peritectic Temperature (PTEC)

Description:

The Peritectic Temperature is the temperature at which the melt of a heterogeneous multicomponent system begins to react with the solid phase to form a new compound. Normally this temperature is identical with the incongruent melting point of this compound. The peritectic temperature field contains the values for the hetereogeneous multicomponent system in the literature. The

concentration of the phases at the peritectic point is given in the remark field PTEC.MR.

Fields:

Field Code	Full Name	Type of Indexing	Unit
PTEC.T	Peritectic Temperature	numerical	°C
PTEC.MR	Remarks	string (phrase)	

Solubility in Systems (MULS)

Description:

The search field Solubility in Systems indicates information on solubility or miscibility in heterogeneous multicomponent systems.

Type of Indexing:

Group Code

Vapor Pressure of Solution (VPR)

Description:

Indication of the vapor pressure of a heterogeneous multicomponent system as a diagram, table or equation is given in the fields VPR.DGM, VPR.TAB or VPR.EQN.

Note:

Searching for special field codes require the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
VPR.DGM	Diagram	string (phrase)
VPR.TAB	Table	string (phrase)
VPR.EQN	Equation	string (phrase)

Solubility (SLB)

Description:

The Solubility of a substance is the maximum concentration of a compound in a binary mixture at a given temperature forming a homogeneous solution. Entries with the solubility unit mol/l can be found in the field SLB.VAL. Entries with other solubility units other than mol/l can be found in the field SLB.VALU. The solvent is given in the associated search field SLB.SOL. The solubility is linked to the associated temperature by the parameter field code SLB.T.

A qualitative description of the solubility of a compound can be retrieved in the field SLB.TXT.

Fields:

Field Code	Full Name	Type of Indexing	Unit
SLB.TXT	Description of Solubility	string (phrase)	

SLB.VAL	Solubility (molar)	numerical	mol/l
SLB.VALA	Solubility (weight)	numerical	
SLB.VALU	Solubility (other)	numerical	
SLB.T	Temperature	numerical	°C
SLB.SOL	Solvent	string (phrase)	
SLB.UNIT	Solubility Unit	string (phrase)	

PL-Value (SLBP)

Description:

The solubility product is the product of the concentrations of the ions of a substance in a saturated solution. It is contained in the search field SLBP.SOLPRO. The corresponding PL- Value is given in the search field SLBP.VAL. The field SLBP.TXT additionally displays a qualitative description on solubility. The temperature at which the solubility product was measured is searchable in the parameter field SLBP.T

Fields:

Field Code	Full Name	Type of Indexing	Unit
SLBP.TXT	Description of Solubility	string (phrase)	
SLBP.VAL	PL-Value	numerical	
SLBP.SOLPRO	Solubility Product	numerical	mol/l
SLBP.T	Temperature	numerical	°C
SLBP.SOL	Solvent	string (phrase)	

Surface Tension (ST)

Description:

The surfaces tend to contract to a minimum area, the surface tension is caused by cohesive forces between the molecules. It is measured as a force per unit length along the surface or the work, which must be done to extend the surface by a unit area. The Surface Tension search field contains the values for a given substance in the literature and is linked to the associated temperature ST.T. Further information about the samples is given in the field remarks ST.MR. The surface tension is linked to the forms of state of the substance by the parameter field code ST.S.

Fields:

Field Code	Full Name	Type of Indexing	Unit
ST	Surface Tension	numerical	erg/cm**2
ST.T	Temperature	numerical	°C
ST.MR	Remarks	string (phrase)	
ST.S	Forms of State	string (phrase)	

Electrochemistry (EC)

Search Fields:

ELYS	Electrolysis
TRAN	Transference Number
ION	Ionic Mobility
ELTR	Behavior As Electrode
CELL	Electrochemical Cell
POT	Electrochemical Reaction
ELTC	Electrolytic Conductivity

Electrolysis (ELYS)

Description:

Indication on a detailed description of Electrolysis, with general conditions and phenomena arising from the flow of current, is given in the field ELYS .FLG. Further data are given in the numerical search field decomposition potential ELYS.POT.

Note:

Searching for the electrolysis field code requires the field value "described" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing	Unit
ELYS.FLG	Electrolysis	string (phrase)	
ELYS.POT	Decomposition Potential	numerical	V

Transference Number (TRAN)

Description:

The transference number is the fraction of the electrical current carried by a single ion in an electrolytic solution.

The field Transference Number indicates information on transference number of compounds or ions.

Type of Indexing:

Group Code

Ion Mobility (ION)

Description:

The ionic mobility is the migration velocity of ions in an electric field of homogenous field strength. The Ion Mobility search field is a numeric range searchable field and is linked to the associated temperature ION.T. Further information about the samples is given in the field remarks ION.MR.

Fields:

Field Code	Full Name	Type of Indexing	Unit
ION	Ionic Mobility	numerical	m**2/(V*s)
ION.T	Temperature	numerical	°C
ION.MR	Remarks	string (phrase)	

Behavior as Electrode (ELTR)

Description:

The field Behavior as Electrode indicates detailed information on compounds as electrodes or parts of an electrode. This includes all processes, which change the electrode mechanically, optically, chemically, or physically, as well as, a description of the use and stability of the electrode, information to material composition or quality, polarization or adsorption phenomena, and overvoltage.

Type of Indexing:

Group Code

Electrochemical Cell (CELL)

Description:

The Electrochemical Cell potential field CELL.POT contains the values for cells using substances of the file as electrode material, as electrolyte, or as a compound of the electrolyte. The electrochemical cell potential field is a numeric range searchable field and is linked to the associated temperature CELL.T. A pair of electrodes dipping into an ionic medium called electrolyte (solid, liquid or gas) and connected by an external electric conductor constitutes an electrochemical cell. The description of cell field CELL.DESCR contains the description of cells using substances of the file as electrode material, as a compound of the electrolyte.

Fields:

Field Code	Full Name	Type of Indexing	Unit
CELL.DESCR	description of cell	string (phrase)	
CELL.POT	cell potential	numerical	V
CELL.T	temperature	numerical	°C

Electrochemical Reaction (POT)

Description:

An electrochemical reaction is a reaction where electrons between the reaction partners and external sources are exchanged. You can search for the reaction partners by GRN or chemical name and the associated potential value and kind of potential (POT.PTYP). The field is linked to the associated parameters temperature (POT.T), solvent (POT.SOL), method of determination (POT.MET), the reference electrode (POT.REL), and the supporting electrolyte (POT.ELYT). Further information is indicated in the search field potential diagram (POT.DGM).

Note:

Searching for a potential diagram field code requires the field value "available" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing	Unit
POT.EGRN	Coreactant(s) (Registry Number)	string (phrase)	
POT.EDN	Coreactant(s) (Name)	string (phrase)	
POT.PGRN	Product(s) (Registry Number)	string (phrase)	
POT.PRO	Product(s) (Name)	string (phrase)	
POT	Potential Value	numerical	V
POT.PTYP	Kind of Potential	string (phrase)	
POT.T	Temperature	numerical	°C
POT.SOL	Solvent	string (phrase)	
POT.MET	Method of Determination	string (phrase)	
POT.REL	Reference Electrode	string (phrase)	
POT.DGM	Potential Diagram	string (phrase)	
POT.ELYT	Supporting Electrolyte	string (phrase)	

Electrolytic Conductivity (ELTC)

Description:

The molar (specific) electrolytic conductivity is the reciprocal of the resistivity, per mole (gram) per unit volume of solution.

The equivalent electrolytic conductivity is the molar electrolytic conductivity per number of equivalents.

The field is linked to the associated parameters temperature (ELTC.T), solvent (ELTC.SOL), and kind of conductivity (ELTC.KIND). Further information about the samples is given in the field remarks ELTC.MR.

Note:

$S\ cm^{2}\ mol^{-1} = 10^{-3}\ S\ cm^{-1}\ l\ mol^{-1}$

Fields:

Field Code	Full Name	Type of Indexing	Unit
ELTC.VALO	Molar Electrolytic Conductivity	numerical	S*l/(cm*mol)
ELTC.VALA	Specific Electrolytic Conductivity	numerical	S*l/(cm*g)
ELTC.AEVAL	Equivalent Conductivity	numerical	cm**2/(? *val)
ELTC.T	Temperature	numerical	°C
ELTC.SOL	Solvent	string (phrase)	
ELTC.KIND	Kind Of Conductivity	string (phrase)	
ELTC.MR	Remarks	string (phrase)	

Chemical Properties (CHE)

Description:

The group Chemical Data contains information about:

Search Fields:

CHB	Chemical Behavior
RCLA	Reaction with Substance Classes
SURF	Surface Reaction
RX	Reaction
RX	Reaction Details

Tips and Hints:

The Reactions are stored in the facts Reaction Identification Data and Reaction Details. These reactions have been registered and hence assigned a Reaction Identification Number.

Surface Reaction (SURF)

Description:

The field Surface Reaction indicates chemical changes (reactions) of the surface of a substance. The formation of surface compounds is described.

The focus is on the substance where the surface reaction takes place.

Type of Indexing:

Group Code

Reaction (RX)

Description:

All chemical syntheses and reactions of inorganic or organometallic compounds can be retrieved in the RX fields.

The Reaction Identification Data are stored in six fields. These contain the keys to the reactants and products, which can be searched for by GRN, name, or by structure (if available). The parameter data to any reaction, such as solvent, catalyst, and further conditions, is stored in the corresponding fact Reaction Details.

Note:

Phase transformations are stored in Transition Point Solid / Solid.

Reaction Identification Fields:

Field Code	Full Name	Type of Indexing
RX:ID	Reaction ID	numerical
RX.RGRN	Reactant(s) (GRN)	numerical
RX.RCT	Reactant(s) (Name)	string (phrase)
RX.PGRN	Product(s) (GRN)	numerical
RX.PRO	Product(s) (Name)	string (phrase)
RX.NVAR	Number of Reaction Details	numerical

Reaction ID (RX.ID)

Description:

The Reaction ID is assigned when a chemical reaction is registered in the Gmelin Information System. The Reaction ID is an unambiguous identifier of a reaction. The Reaction ID is the accession number of the reaction record in CrossFire. It is an integer, which does not contain further information.

Type of Indexing:

numerical

Reactant(s) (GRN) (RX.RGRN)

Description:

Reactants (starting materials) are defined as compounds that form the product(s). Inorganic starting materials are registered compounds and are therefore present as title compounds with data. Organic starting materials have usually no further data in the Gmelin database; they will be present and have minimal "identification" data in addition to the structure.

Starting materials are searchable either by GRN (in the RX.RGRN field) or by names (in the RX.RCT field).

Tips and Hints:

Searching for reactions by GRN is useful for compounds having no molecular or no completely defined molecular structure. So you can tailor all reactions of a title compound into preparations and reactions.

You can perform reaction searching for compounds with full structures directly in the structure editor using the reaction editmode. Here you can search with full structures or substructures.

Type of Indexing:

numerical

Example:

Searching for substances that have been prepared from copper(II) sulfide (GRN unknown).

Step 1:
Searching for GRN of copper(II) sulfide in substance context:

Operator	Field Name	Field Value
	MOFO	CuS
And	NC	1

Display of Identification Data including the GRN. The first hit describes the usual CuS compound; GRN = 13690.

Step 2:
Searching for reactions with copper(II) sulfide as a starting material in reaction context:

Operator	Field Name	Field Value
	RX.RGRN	13690

Reactant(s) (Name) (RX.RCT)

Description:

Reactants (starting materials) are defined as compounds that form the product(s). Inorganic starting materials are registered compounds and are therefore present as title compounds with data. Organic starting materials have usually no further data in the Gmelin database, they will be still present and have minimal "identification" data in addition to the structure.

Starting materials are searchable either by GRN (in the RX.RGRN field) or by names (in the RX.RCT field).

Note:

The search field contains formulas and, if present, chemical names.

Tips and Hints:

Name searches are not recommended to identify compounds, because names are ambiguous or non-systematic and complete chemical names are not available in many cases. In some cases, name fragments might be useful to search for substance classes. However there are more powerful methods available such as structure or substructure searches, or GRN search.

Type of Indexing:

string (phrase)

Product(s) (GRN) (RX.PGRN)

Description:

Reaction products are registered compounds and are therefore present as title compounds with data. The main focus of the Gmelin database is the formation of inorganic and organometallic compounds.

Reaction products are searchable either by GRN (in the RX.PGRN field) or by names (in the RX.PRO field).

Tips and Hints:

Searching for reactions by GRN is useful for compounds having a partially defined or undefined molecular structure. You can tailor all reactions of a title compound into preparations and reactions.

You can perform reaction searching for compounds with full structures directly in the structure editor using the reaction editmode. Here you can search with full structures or substructures.

Type of Indexing:

numerical

Example:

Searching for preparations of Bi2Sr2CaCu2O8 (GRN unknown).

Step 1:
Searching for GRN of calcium titanate in substance context:

Operator	Field Name	Field Value
	MOFO	Bi2Sr2CaCu2O8
And	NC	1

Display of Identification Data including the GRN. The first hit is Bi2Sr2CaCu2O8 without further specification; the GRN is 24127.

Step 2:
Searching for reactions with copper(II) sulfide as a starting material in reaction context:

Operator	Field Name	Field Value
	RX.PGRN	24127

Product(s) (Name) (RX.PRO)

Description:

Reaction products are registered compounds and are therefore present as title compounds with data. The main focus of the Gmelin database are the formation of inorganic and organometallic compounds.

Reaction products are searchable either by GRN (in the RX.PGRN field) or by names (in the RX.PRO field).

Note:

The search field contains formulas and, if present, chemical names additionally.

Tips and Hints:

Name searches are not recommended to identify compounds, because names are ambiguous or non-systematic and complete chemical names are not available in many cases. In some cases, name fragments might be useful to search for substance classes. However there are more powerful methods available such as structure or substructure searches, or GRN search.

Type of Indexing:

string (phrase)

Number of Details (RX.NVAR)

Description:

This field gives the number of reaction details.

Note:

At the moment the RX.NVAR field is always 1, because the reaction details are linked to one registered reaction.

Type of Indexing:

numerical

Reaction Details

Reaction Detail Fields:

Field Code	Full Name	Type of Indexing
RX.NYD	Yield (Numeric)	numerical
RX.YD	Yield	string (phrase)
RX.RGT	Reagent	string (phrase)
RX.IGRN	Intermediate(s) (GRN)	numerical
RX.INT	Intermediate(s) (Name)	string (phrase)
RX.BPRO	Byproduct	string (phrase)
RX.SOL	Solvent	string (phrase)
RX.CGRN	Catalyst(s) (GRN)	numerical
RX.CAT	Catalyst(s) (Name)	string (phrase)
RX.IND	Industrial Synthesis	string (phrase)
RX.SCON	Special Conditions	string (phrase)
RX.GCON	General Conditions	string (phrase)
RX.ISOL	Purification / Isolation	string (phrase)
RX.KIN	Kinetics	string (phrase)
RX.UPD	Update Date	string (phrase)

Yield (Numeric) (RX.NYD)

Description:

The yields of products are stored in this field. Only the absolute yield for the pure product quoted by the author is accepted.

In this field the yield is indexed as a numerical value. You can search with single values or ranges, as well as, greater than / less than a certain value.

Note:

The yield 0 % means that the desired product was not formed. If only a trace of a product is formed the yield is stored as <1 %. Quantitative yields are expressed as >99 % yield.

Type of Indexing:

numerical

Related Information:

RX.YD

Example:

	Search for	Field Name	Field Value
(a)	reactions with product yields greater than 98%	RX.NYD	>98
(b)	reactions with product yields between 84 and 85 %	RX.NYD	84-85
(c)	reactions with product yields less than 5 %	RX.NYD	<5

Yield (RX.YD)

Description:

The yields of products are stored in this field. Only the absolute yield for the pure product quoted by the author is accepted.

In this field the yield is indexed as a string. This means the reaction yield has to match exactly with the entered string for a hit.

Note:

The yield 0 % means that the desired product was not formed. If only traces of a product is formed the yield is stored as <1 %. Quantitative yields are expressed as >99 % yield.
If mathematic signs are added for a search, the input has to be set in quotation marks.

Type of Indexing:

string (phrase)

Related Information:

RX.NYD

Examples:

	Search for	Field Name	Field Value
(a)	reactions with product yields greater than 98%	RX.YD	">98"
(b)	reactions with product yields between 84 and 85 %	RX.YD	84-85
(c)	reactions with product yields less than 5 %	RX.YD	"<5"

Reagent (RX.RGT)

Description:

Reagents are compounds, which take part in the reaction but do not make a contribution to the product, e.g. compounds for pH adjustment, reducing agents, or oxidizing agents. Further undefined compounds, which cannot be expressed by formula but only by name, are also available in this field, like air, charcoal, or Rh-catalyst supported on SiO2 (Rh/SiO2).
Reagents have no GRN.

Note:

Alternative agents are linked by "or".

Type of Indexing:

string (phrase)

Intermediate(s) (GRN) (RX.IGRN)

Description:

Intermediates are stored as non-isolated compounds formed in a one-pot reaction, or compounds of intermediate steps for which measured data are available.

Intermediates are searchable either by GRN (in the RX.IGRN field) or by names (in the RX.INT field).

Type of Indexing:

numerical

Intermediate(s) (Name) (RX.INT)

Description:

Intermediates are stored as non-isolated compounds formed in a one-pot reaction, or compounds of intermediate steps for which measured data are available.

Intermediates are searchable either by GRN (in the RX.IGRN field) or by names (in the RX.INT field).

Tips and Hints:

Name searches are not recommended to identify compounds, because names are ambiguous or non-systematic and complete chemical names are not available in many cases. In some cases name fragments might be useful to search for substance classes.

Type of Indexing:

string (phrase)

Byproduct (RX.BPRO)

Description:

By-products are compounds, which are produced during the reaction but have no focus or are not characterized. By-products can be precipitated salts like AgCl, formed gases like CO2, or organic compounds.

Type of Indexing:

string (phrase)

Solvent (RX.SOL)

Description:

This field contains information on the solvent, or the solvent mixture, used in the reaction. If solvents are also reaction partners, they are stored as reactants.

There are some special solvent descriptions available:

for reactions in melt:	melt
for reactions without solvent: e.g. at higher temperatures	neat (no solvent)
Solid-state reactions:	neat (no solvent, solid phase)
gas-phase reactions:	neat (no solvent, gas phase)

Type of Indexing:

string (phrase)

Catalyst(s) (GRN) (RX.CGRN)

Description:

Catalysts are compounds that do not appear in the stoichiometric equation of the reaction. They only influence the rate of the reaction. In the Gmelin database catalysts are inorganic or organometallic compounds and neither identical with a starting material nor an acid-base catalyst.

Catalysts are searchable either by GRN (in the RX.CGRN field) or by names (in the RX.CAT field).

Type of Indexing:

numerical

Catalyst(s) (Name) (RX.CAT)

Description:

Catalysts are compounds that do not appear in the stoichiometric equation of the reaction. They only influence the rate of the reaction. In the Gmelin database catalysts are inorganic or organometallic compounds and neither identical with a starting material nor an acid-base catalyst.

Catalysts are searchable either by GRN (in the RX.CGRN field) or by names (in the RX.CAT field).

Tips and Hints:

Name searches are not recommended to identify compounds, because names are ambiguous or non-systematic and complete chemical names are not available in many cases. In some cases name fragments might be useful e.g. to search for substance classes.

Type of Indexing:

string (phrase)

Industrial Synthesis (RX.IND)

Description:

The field Industrial Synthesis indicates the corresponding reaction as an industrial reaction.

Note:

Searching for industrial synthesis field code requires the field value "yes" or more general "*".

Type of Indexing:

string (phrase)

Special Conditions (RX.SCON)

Description:

This field contains information on special reaction conditions related to a list of controlled terms.

Following special conditions are valid:

- electric arc
- electrochem. process
- electrolysis
- high pressure
- irradiation (uv/vis)
- other radiation
- sonication

Type of Indexing:

string (phrase)

General Conditions (RX.GCON)

Description:

The field General Conditions contains a short description of the performance of the reaction. Details like protective gas, reaction time, temperature, pressure, or special performance of a reaction are described.

Type of Indexing:

string (phrase)

Purification / Isolation (RX.ISOL)

Description:

The field General Conditions contains a short description of the purification/isolation of the reaction products. Details to methods of separation and purification are described. Further elemental analysis or purity details of the products are indicated. Methods of identification are noted especially for compounds, which are not isolated.

Type of Indexing:

string (phrase)

Kinetics (RX.KIN)

Description:

The field Kinetics indicates descriptions of kinetics of the reaction, e.g. rate constants, reaction order or activation energies.

Note:

Searching for industrial synthesis field code requires the field value "available" or more general "*".

Type of Indexing:

string (phrase)

Update Date (RX.UPD)

Description:

The search field Update Date contains the date (year/month/day) when the last update of this reaction was entered into the database.

Dates have to be searched with a fixed format: yyyy/mm/dd.

Type of Indexing:

string (phrase)

Chemical Behavior Chemical Behavior (CHB)

Search Fields:

DP	Decomposition
STAB	Information on Stability
FLAP	Flash Point
BCAT	Behavior as Catalyst
BINH	Behavior as Inhibitor
ACBS	Behavior as Acid / Base
COLL	Colloid Chemical Behavior
POLY	Polymerisation
ASS	Association
SOHY	Solvation / Hydration

Decomposition (DP)

Description:

The decomposition point is the temperature at which a substance decomposes thermally. The Decomposition Point search field is a numeric range searchable field. Decomposition in solutions is linked to the associated solvent by the DP.SOL search field.

Fields:

Field Code	Full Name	Type of Indexing	Unit
DP	Temperature	numerical	°C
DP.SOL	Solvent	string (phrase)	

Information on Stability (STAB)

Description:

The search field Information on Stability displays a description of the stability, as well as, the behavior of a substance influenced by light, moisture or air.

Fields:

Field Code	Full Name	Type of Indexing
STAB	Description of Stability	string (phrase)

Flash Point (FLAP)

Description:

The Flash Point is the lowest temperature at which a liquid gives off sufficient vapor to form an ignitable mixture with air near the surface of the liquid or within the vessel used.

Fields:

Field Code	Full Name	Type of Indexing	Unit
FLAP.T	Flash Point	numerical	°C

Behavior as Catalyst (BCAT)

Description:

The field Behavior as Catalyst indicates information and references of a compound catalysing organic or inorganic reactions.

Note:

You can search for the corresponding inorganic reaction, which is catalysed, using the field RX.CGRN or RX.CAT.

Type of Indexing:

Group Code

Behavior as Inhibitor (BINH)

Description:

The field Behavior as Inhibitor indicates the behavior of a compound as an inhibitor. They can be designated as reaction inhibitors, negative catalysts, or radical scavengers.

Type of Indexing:

Group Code

Behavior as Acid / Base (ACBS)

Description:

The field Behavior as Acid / Base indicates the behavior of a compound as an acid or base. The acid-base behavior is the object of the article, or how the pH, pKS, or pKB values are determined.

Type of Indexing:

Group Code

Colloid Chemical Behavior (COLL)

Description:

The field Colloid Chemical Behavior indicates information on colloids, gels, sols, aerosols smoke or mist.

Type of Indexing:

Group Code

Polymerisation (POLY)

Description:

The field Polymerisation indicates information on the polymerisation or oligomerisation of a compound. Only the polymerisation of a substance with itself is recorded, no co-polymerisation.

Type of Indexing:

Group Code

Association (ASS)

Description:

The field Association indicates information on the association of the molecules of a compound.

Type of Indexing:

Group Code

Solvation / Hydration (SOHY)

Description:

The field Solvation / Hydration indicates information on the solvation or hydration of a compound. The focus is the substance without solvate molecules.

Type of Indexing:

Group Code

Reaction with Substance Classes (RCLA)

Description:

Indication on the chemical behavior, against classes of compounds, is given in the fields RCLA.REAC and RCLA.NOREAC. The classes of substances are specified in the field RCLA.CLASS. The product substance classes are specified in the field RCLA.PROD.

Note:

Searching for "does react" and "does not react" field codes requires the field value "yes" or more general "*".

Fields:

Field Code	Full Name	Type of Indexing
RCLA.REAC	does react	string (phrase)
RCLA.NOREAC	does not react	string (phrase)
RCLA.CLASS	reaction with	string (phrase)
RCLA.PROD	reaction product	string (phrase)

Quantum Chemical Calculations (QCC)

Description:

The topic Quantum Chemical Calculations contains data derived from quantum mechanical methods.

This field identifier is a group code for Field Availability searches in the hierarchical system of the CrossFire database.

Type of Indexing:

Group Code

Note:

Values which have been calculated by classical (not quantum mechanical) methods or which come from experimentally measured data are not recorded here, but under the corresponding property.

Search Fields:

QUAN	Quantum Chemical Calculations

Quantum Chemical Calculations (QUAN)

Description:

The Quantum Chemical Calculations QCC.PROP search field refers to quantum chemical calculations performed for a substance. The calculated properties are available in this field together with a classification of the corresponding quantum chemical method of calculation QCC.MET.

Following calculation methods are valid:

- ab initio calculation
- electron correlation and CI calculation
- empirical method
- further quantum calculation
- other semiempirical calculations
- relativist. calculation
- semiempirical NDO calculation
- statist. model calculation
- valence bond calculation

Fields:

Field Code	Full Name	Type of Indexing
QCC.PROP	calculated properties	string (phrase)
QCC.MET	method of calculation	string (phrase)

Bibliographic Information Bibliographic Information (BIB)

Search Fields:

CNR	Citation Number
CIT	Citation
AB	Abstract

Citation Number (CNR)

Description:

Every reference in the Gmelin Database has been assigned a citation number, which can be used to access a certain citation directly.

Fields:

Field Code	Full Name	Type of Indexing
CNR	Citation Number	Numerical

Abstract

Description:

The content of the abstract field is taken from the original literature from 1995 to the present. However, there are also sometimes abstracts available from journals before 1995.

Tips and Hints:

The Boolean Operators AND, OR, NOT can be used to find occurrences of the indicated terms anywhere in the abstract. In the case of PROXIMITY the entire abstract is considered as information unit. Therefore, the PROXIMITY operator works like AND.

You can link words using the Operators NEAR or NEXT.

Search Fields:

TI	Title
AB	Abstract
ALA	Abstract Language
AB.KW	Keywords

Title (TI)

Description:

The content of the Title field is taken from the original literature from 1995 to the present. However, there are also titles available from journals before 1995.

Tips and Hints:

The Boolean Operators AND, OR, NOT can be used to find occurrences of the indicated terms anywhere in the abstract. In the case of PROXIMITY the entire abstract is considered as information unit. Therefore, the PROXIMITY operator works like AND.

You can link words using the operators NEAR or NEXT.

Fields:

Field Code	Full Name	Type of Indexing
TI	Abstract Title	string (word)

Example:

Search for all documents where bioactive substances are determined:

Operator	Field Name	Field Value
	TI	Bioactive

Example:

Search for documents where a relationship between the structure of drugs has been published:

Operator	Field Name	Field Value
	TI	structur*
and	TI	drug*

Abstract (AB)

Description:

The content of the Abstract field is taken from the original literature from 1995 to the present. However, there are also abstracts available from journals before 1995.

Tips and Hints:

The Boolean Operators AND, OR, NOT can be used to find occurrences of the indicated terms anywhere in the abstract. In the case of PROXIMITY the entire abstract is considered as information unit. Therefore, the PROXIMITY operator works like AND.

You can link words using the operators NEAR or NEXT.

Fields:

Field Code	Full Name	Type of Indexing
AB	Abstract	string (word)

Example:

Search for all documents where anticancer or antimetastatic substances are described:

Operator	Field Name	Field Value
	AB	Anticancer
or	AB	antimetastat*

Example:

Search for documents with the phrase catalytic activity in the abstract:

Operator	Field Name	Field Value
	AB	catalyt*
And	AB	Activity

Example:

Search for documents concerning with p-type semiconductors:

Operator	Field Name	Field Value
	AB	P
next	AB	Type
and	AB	semiconductor*

Abstract Language (ALA)

Description:

The Abstract Language field contains the language of the literature abstract. In general, the abstract is available in English.

Fields:

Field Code	Full Name	Type of Indexing
ALA	Abstract Language	string (phrase)

Keywords (AB.KW)

Description:

This field contains keywords, index headings or similar items, which are present in an article.

Fields:

Field Code	Full Name	Type of Indexing
AB.KW	Abstract Keyword	string (phrase)

Example:

Search for all documents with keyword photochemistry or similar phrases:

Operator	Field Name	Field Value
	AB.KW	photochem*

Example:

Search for documents dealing with kinetics and catalysis (including variations):

Operator	Field Name	Field Value
	AB.KW	kinetic*
and	AB.KW	*catal*

Citation (CIT)

Search Fields:

AU	Author
PY	Publication Year
CO	CODEN
LA	Language
JT	Journal Title

Author (AU)

Description:

The Author field contains the surname of the author, the first name or abbreviations as they were written in the original publication. For publications with more than one author each author name will be separately indexed. Use LIST to look in the index and see exactly how a particular author has been cited. The surname is always separated by a comma and a space from first names or affixes e.g. "van der". Titles such as "Dr.", "Sir" or "Prof." are ignored. The five names mentioned in the article are given, further names are displayed as "et al.".

Authors can be indexed as follows:

- Adams, Richard D.
- Arduengo, Anthony J. III
- Baudler, Marianne
- Cotton, F. Albert
- Schnering, H. G. von
- Simon, A.

Tips and Hints:

To ensure that all references from a particular author are found it is recommended that the EXPAND function (<F2>, LIST) is used to check the way the author has been cited. Thus it is often useful to use truncation when author searches are carried out and restrict the search to surname only.

Fields:

Field Code	Full Name	Type of Indexing
AU	Author	string (phrase)

Related Information:

PY, CO, JT, LA

Examples:

	Search for	Field Name	Field Value
(a)	articles published by authors with surname Adams	AU	Adams, *
(b)	articles published by all authors beginning with Adam	AU	Adam*
(c)	articles published by Richard Adams	AU	Adams, Richard
(d)	articles published by Richard Adams including other first names	AU	Adams, Richard*
(e)	articles published by R. Adams – including Richard Adams – or other first names starting with R	AU	Adams, R*

Example:

Using the PROXIMITY operator will only retrieve those publications of F. Albert Cotton from Polyhedron (PLYHDE):

Operator	Field Name	Field Value
	AU	Cotton, F. Albert
proximity	CO	PLYHDE

Publication Year (PY)

Description:

The content of the Publication Year field is the publication year of the article cited. It should not be confused with the entry date.

Fields:

Field Code	Full Name	Type of Indexing
PY	Publication Year	Numerical

Related Information:

AU, CO, JT, LA

Example:

Search for all substances reported in 2000 in the journal J. Orgmet. Chem. (JORCAI):

Operator	Field Name	Field Value
	PY	2000
proximity	CO	JORCAI

CODEN (CO)

Description:

Journal titles may be searched for using the CASSI CODEN. A list of CODENs of the journals considered is contained in the Appendix. CASSI CODENs are unique, unambiguous, six-character codes assigned to journals and other serial and non-serial publications. They are used instead of the abbreviated journal titles to search for references from a particular publication.

Fields:

Field Code	Full Name	Type of Indexing
CO	CODEN	string (phrase)

Related Information:

AU, PY, JT, LA

Example:

Search for substances published in the journals Inorg. Chim. Acta and J. Mol. Catal. A Chem.:

Operator	Field Name	Field Value
	CO	ICHAA3
or	CO	JMCCF2

Journal Title (JT)

Description:

The title of the journal is present in this field if it could be assigned via the CODEN.

You can request a list of the journal titles if you use the LIST (<F2>) function in the citation query input mask.

Fields:

Field Code	Full Name	Type of Indexing
JT	Journal Title	string (phrase)

Language (LA)

Description:

The Language of the original publication is contained in this field.

You can see the valid languages by using the EXPAND function (<F2>, LIST).

Tips and Hints:

All data in the Gmelin database is in English. This field will tell you the language of the original article.

Fields:

Field Code	Full Name	Type of Indexing
LA	Language	string (phrase)

Related Information:

AU, PY, CO, JT

3

Gmelin Special Features

Gmelin Special Features

3D Structures

Stereochemical Information

Polyhedra

Gmelin Ligand Search System

3D Structures

The Gmelin database contains a large collection of inorganic and organometallic compounds. Most of them are available with structures. However, you should be aware that only compounds or compound parts, which are formed by discrete molecules or ions, have a structure; e.g. all molecules or coordination compounds. Compounds with a solid-state structure, alloys, glasses, or ceramic materials do not have a structure in the Gmelin database.

Many of the structures in the Gmelin database have been entered with three dimensional coordinates. This is necessary to describe stereochemistry in coordination compounds correctly. Because of the more complex stereocenters in inorganic chemistry, which cannot be expressed by normal up and down bonds, the stereochemical description in the Gmelin database is different from the Beilstein database.

The structures in Gmelin are displayed three-dimensionally. To get a real impression of a 3D structure you need to be able to rotate this structure along the three axis of the coordination system. This is possible with the structure editor. Copy a structure from Display Hits to the Commander and launch the structure editor. Select the menu item "3D Rotate" from Edit mode menu and you will be able to rotate the selected objects.

Stereochemical Information

The structures of fragments or compounds in the Gmelin file are defined by the connectivity of atoms, the total charge and by stereodescriptors which mark a certain polyhedron.

Two principal different stereochemical aspects can be searched for:

- Stereochemical information on bonds
- Stereochemical information on centers.

Stereochemical information on bonds

Specified double bond information (cis or trans) can be searched for if the bond attribute "Double Steric" is chosen in the structure editor, and the structure is drawn as desired.

Additionally, stereoinformation on single bonds (eclipsed and staggered-configuration) is stored in the database, e.g. for dipyridyl derivates. However, these descriptors are not searchable.

Stereochemical information on centers

Stereochemical information on centers can be searched for by adding stereo center search attributes on a chiral atom. These attributes are expressed by polyhedra (Polyhedra).

In the case of trigonal pyramidal, tetrahedral, or octahedral centers, a stereodescriptor is set if one, or more than one, possible configuration of a stereocenter can be assigned. In all other cases the mentioning of a polyhedral center within a compound in the original literature is sufficient for the designation of a polyhedral descriptor. The polyhedral descriptor fix also the ligand configuration. If the configuration is unknown, no descriptor is set.

All stereocenters are drawn three-dimensionally. Fragments with stereochemical information are assigned either an absolute or a racemic configuration.

Further, chiral isomers with at least a known sign of optical rotation, but unknown polyhedral geometry, are distinguished. However, these descriptors are not searchable. They are displayed as (+)- or (-)-enantiomers, respectively.

Stereochemical Search

In the structure editor, coordination polyhedras can be specified if the edit mode is set to "Inorganic".

A exact stereochemical search can only be done with structures built up by polyeders from the template "polyatom". These polyeders have a fixed numbering of the ligand positions.

In the "query options" menu structure related attributes can be set and stereo searching can be performed.

Polyhedra

Another feature of the structure editor and the CrossFire server, in combination with the Gmelin database, is the capability to enter stereo center search attributes for coordination compounds. These attributes are called "polyeder". They can be entered in the atom attribute dialog box of the structure editor, if the edit mode is set to "Inorganic".

The following descriptors are available to describe polyhedra in the Gmelin file:

a) Simple Polyhedra

Descriptor	Polyhedron
P-3	trigonal pyramid
T-4	tetrahedron
SP-4	square planar
SP-5	square pyramid
TB-5	trigonal bipyramid
OC-6	octahedron
TP-6	trigonal prism
PB-7	pentagonal bipyramid
CU-8	cube
SA-8	square antiprism
DD-8	dodecahedron

HB-8	hexagonal bipyramid
TPS-9	tricapped trigonal prism
HB-9	heptagonal bipyramid

These polyhedra can be used for a stereochemical search in combination with structures built up from the polyatom template.

b) Two polyhedra, linked by a chain of bonds

Descriptor	Polyhedron	
22E	two triangles	(eclipsed)
22S	two triangles	(staggered)
23E	triangle plus tetrahedron	(eclipsed)
23S	triangle plus tetrahedron	(staggered)
33E	two tetrahedra	(eclipsed)
33S	two tetrahedra	(staggered)
24E	triangle plus square pyramid	(eclipsed)
24S	triangle plus square pyramid	(staggered)
25E	triangle plus octahedron	(eclipsed)
25S	triangle plus octahedron	(staggered)
44E	two square pyramids	(eclipsed)
44S	two square pyramids	(staggered)
45E	square pyramid plus octahedron	(eclipsed)
45S	square pyramid plus octahedron	(staggered)
55E	two octahedra	(eclipsed)
55S	two octahedra	(staggered)

In contrast to the "simple polyhedra" these polyhedra are only displayable.

Gmelin Ligand Search System

The fact editor allows the formulation of queries, which gives you fast and easy access to classes or coordination compounds via ligand codes. This Gmelin Ligand Search System describes the elements (in groups) in combination to the number of the atoms that are connected to the central metal atom(s).

Complete ligand molecular formulas are available for all structured compounds or fragments which contain at least one metal atom and at least one coordinating ligand atom of the classes "L, A, D, Q, X" or a "special" ligand.

Single ligands are indexed for complete compounds (LIGFO) and also for single centers in multinuclear compounds (LIG.LIGMF).

The codes include the following elements:

Code	atom
L:	C
A:	B, Si, Ge
D:	N, P, As, Sb
Q:	O, S, Se, Te
X:	H, F, Cl, Br, I, At

There are the following "special" ligands:

Code:	CO,	CS,	CN,	CNS,	CNO,	CNR *)

*) The substituent R has no further bond to metal atoms.

If a ligand is described by a combination of the codes, they are ordered alphabetically and the denticity of the code is put in parentheses in front of the code.

Note:

The ligand formula describes only the denticity of the ligand not the connectivity to the metal center(s).

Examples:

	Search for	Field Name	Field Value
(a)	halogenid or hydride ligand μ-halogenide or μ-hydride ligand	LIGFO	X
(b)	ligand connecting by two halogenide or hydride atoms e.g. η²-hydrogen, η²-BH4	LIGFO	(2)X
(c)	(monodentate) carbonyl	LIGFO	CO
(d)	ligand connecting by C and chalcogen e.g. μ-η²-carbonyl (by C and O)	LIGFO	LQ
(e)	ligand connecting to metal(s) by C e.g. μ-carbonyl (only by C), bridged alkyl-, η² alken-, η²-alkin ligands	LIGFO	(2)L
(f)	ligand connecting by three C atoms e.g. η³-allyl, η^1-yl-η²-alkenyl	LIGFO	(3)L
(g)	ligand connecting by four C atoms e.g. η^4-butadiene, norbornadiene, cycloocta1,5-diene	LIGFO	(4)L
(h)	ligand connecting by five C atoms to one or more metal centers e.g. η^5-cyclopentadienyl	LIGFO	(5)L
(i)	ligand connecting by six C atoms e.g. η^6-cyclobenzene	LIGFO	(6)L
(k)	ligand connecting by ten C atoms to one or more metal centers e.g. two bridged η^5-cyclopentadienyl	LIGFO	(10)L
(l)	ligand connecting by twelve C atoms e.g. η^6,η^6-cyclophanes	LIGFO	(12)L
(m)	ligand connecting by two chalcogenides e.g. η²- or μ-acides (like acetic acid), oxalate (bidentate), di-oles (like ethylene glycol), salicylates,	LIGFO	(2)Q

	acetylacetonates, dithiols, µ- bisulfido		
(n)	ligand connecting by three chalcogenides e.g. tri-ole, µ-carbonato, bis(alkylthio)-sulfide, 2,6-diformyl-phenolate	LIGFO	(3)Q
(o)	ligand connecting by four chalcogenides e.g. silicate, phosphate, 12-crwon-4, tetra-thiocyclohexadecane, oxalate (tertadentate)	LIGFO	(4)Q
(p)	ligand connecting by six chalcogenide atoms e.g. 18-crown-6, bridged TeO6, SbO6, IO6	LIGFO	(6)Q
(q)	ligand connecting by two pnictide atoms e.g. ethylenediamine, η^2-nitrogen, bipyridine, di-substituated phosphinoalkans (like dppm, dppe), di-substituated arsine (like diars)	LIGFO	(2)D
(r)	ligand connecting by three pnictide atoms e.g. terpyridine, tri-aza-cyclononane, tris-pyrazolyl-borates, triphos	LIGFO	(3)D
(s)	ligand connecting by four pnictide atoms e.g. porphyrins, phthalocyanines, tetra-aza-cyclam	LIGFO	(4)D
(t)	ligand connecting by five pnictide atoms e.g. cobalamin	LIGFO	(5)D
(u)	ligand connecting by one pnictide und one C atom e.g. benzylamine, phenylpyridine	LIGFO	DL
(v)	ligand connecting by one pnictide und two chalcogenide atoms e.g. diole-amines, imino-diacetates	LIGFO	D(2)Q
(w)	ligand connecting by two pnictide und two chalcogenide atoms e.g. disalicylidene-diiminato ligands	LIGFO	(2)D(2)Q

	(like salen)		
(x)	ligand connecting by two pnictide und four chalcogenide atoms e.g. ethylenediaminetetraacetate	LIGFO	(2)D(4)Q
(y)	ligand connecting by two pnictide und four chalcogenide atoms e.g. cryptand (222)	LIGFO	(2)D(6)Q
(z)	ligand connecting by three group III and two C atoms e.g. carboranes (like close-C2B9H11)	LIGFO	(3)A(2)L

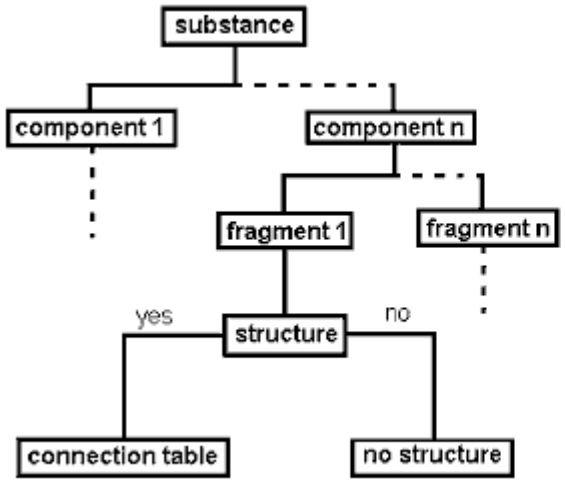
4

Guidelines for Searching

Guidelines for Searching

In order to get good retrieval results on searching for compounds in the GMELIN database with CrossFire, the user should have some knowledge of how these compounds are stored.

Substance Hierarchy in the GMELIN file



General Information on Searching for Compounds

In general compounds can be searched using compound formulas, formula data, or structures. Combined searches are also possible.

Searching for compound formulas

- by code MOFO. Here the formula can be entered in the usual chemical description, e.g. NaCl, K2SO4, FeCl3*6NH3, Fe(C5H5)2.
  Index ranges can also be used in formulas, e.g. BaCuO(1-3), PN(1-10).
  Asterisks at the end of a formula increase the formula search by further elements, e.g. Ba2Cu3O7*. Combinations are also possible, e.g. Y(0-1)Ba2Cu3O(6-8)*.
  It is not possible to display this field via the expand command.

- by code MF. Here the molecular formula has to be entered in the "Hill order", i.e. "carbon" first, "hydrogen" next, and then all further elements in alphabetic order, e.g. C10H10Fe for ferrocene.
  Formulas of compounds without "carbon" are always entered in alphabetic order, e.g. ClNa for sodium chloride, K2O4S for potassium sulfate.

Consequently, an input "hf" means the element "hafnium"; hydrofluoric acid must be entered as "fh".

- by code LSF. Compounds can consist of more than one fragment being separated in the linearized structure formula field by an asterisk (see Compound Formulas with more than one Fragment)

Note:

To tailor the search to a one component compound the formula search should additionally be restricted by the number of components (nc=1).

Searching for formula data

- by code ELS. The symbol of each distinct element of the molecular formula can be entered.

- by code ELC. The respective count of the distinct elements in a molecular formula can be fixed.

- by code NE. The total number of elements of the molecular formula can be restricted.

- by code NA. The total number of atoms of the molecular formula can be restricted.

Note:

To tailor the search to a one component compound the formula search should additionally be restricted by the number of components (nc=1).

Searching for full / sub structures

- Structures - even complex structures - are easily drawn using the structure editor.

- Predefined templates - on the menu bar or in menu "file" - are available.

- Atom attributes can be specified, like atom symbols, atom charge, atom mass.

- Free sites on atoms vary the bondings to this atom. If "free sites" remain zero, no further bondings are considered as drawn. If the number of "free sites" is changed, the coordination sphere of the atom is increased further by the respective count.

- If the edit mode is set to "Inorganic", coordination polyhedras can be specified.

- In the "query options" menu structure related attributes can be set and stereo searching can be performed.

Compound Formulas with more than one Component

These are heterogeneous multi-component compounds, like systems or solutions of two or more compounds. There are also homogeneous compounds, like alloys, glasses, ceramic materials, solid solutions, minerals, and doped compounds, that belong (not exclusive) to this category. All these compounds have the number of components greater than one (nc>1).

- First, compounds can be stored in a kind of tabular form containing the components of alloys, glasses and ceramics together with their atomic, volume, weight, or undefined percentages. On searching for these compounds the search fields ALLOY, PERC and PERT are recommended.

  Example:
  Pd(b),Rh(2-3) (W%), this means a palladium based alloy containing 2-3 weight % rhodium.
  Al2O3(10-15),B2O3(10-15),O2Si (W%), this means a silicium dioxide (Hill order) glass containing 10-15 weight % aluminium oxide and 10-15 weight % boron oxide.

- Second, and this is the normal case, compounds are stored with their line formula. These compounds can consist of one, or more, component, and each component can consist of one or more than one fragment, and each fragment may or may not have a structure.
  Each component can be searched by its molecular formula, e.g. by MOFO or MF. The single fomulas can be combined.

  Example:
  MF=BaO and MF=CuO and MF=O3Y2 and NC=3, this means a three-component substance of the compounds BaO, CuO and Y2O3.

  Compounds with more than one component can be given in the field LSF (linearized structure formula) in the following style:

  ABC#XYZ the single components ABC and XYZ are separated by a hash sign (#)
  (A,B)Z the single component parts are separated by a comma, giving the components AZ and BZ
  A(x)B(1-x)C x:0.9-0.95; gives the components A0.95B0.05C and A0.9B0.1C

- Formulas of type 2 and 3 often refer to solid solutions, minerals or diadochous compounds. Type 1 often refers to homogeneous or heterogeneous multicomponent compounds.

Compound Formulas with more than one Fragment

Compounds with more than one fragment are separated in the linearized structure formula field by an asterisk.

Example: 2Na(1+)*SO4(2-)=Na2SO4

Normally, the formula is repeated in the conventional manner after the '=' symbol as shown in the example above.

Rules whether a compound is fragmented or not are as follows:

Solid state structures and ion lattices:

- Substances, which contain in the crystal, the gas phase, the liquid phase, or in solution

  discrete polyatomic ions
  are divided into formal fragments if there is at least one structurable fragment, e.g. 2Na(1+)*SO4(2-)=Na2SO4.

- on lattices, which consist exclusively of one-atomic ions (including OH-, SH-, SeH-, and TeH-), or solid state structures without discrete ions or molecules, have no structure in the database; the formula is given without fragmentation, e.g. NaCl, KOH, CaTiO3.

Organometallics and Coordination Compounds:

- Organometallic compounds, and coordination compounds with known manner of ligand coordination, are stored with the complete formula and structure, e.g. Cr(CO)6,
  Fe(C5H5)2, (Co(NH3)3Cl3).

- Organometallic salts, and coordination compounds with known manner of ligand coordination, are divided into cations and anions. The complete structure of the ions are available, e.g. (Pd(CH3CN)4)(2+)*2BF4(1-)=(Pd(CH3CN)4)(BF4)2

- Organometallic compounds, and coordination compounds with unknown manner of ligand coordination, are divided into fragments by separating all ligands from the metal center. E.g., if there is an unknown coordination of the dianion of oxalic acid to Fe(2+) in [Fe(OOCCOO)2](2-) (mono- or bidentate), the formula is given as Fe(2+)*2OOCCOO(2-). E.g. if there is an unknown coordination of thiocyanate to Co(2+) in [Co(NH3)5(SCN)](2+) (coordination by N or S atom), the formula is given as Co(2+)*5NH3*SCN(1-). Additional the complete structure of the complex ion (Co(NH3)5(SCN))(2+) can be available (in this case twice with Co-SCN and Co-NCS coordination).

Note:

Clusters with unknown ligand coordination are not divided further; hydrogen atoms are not separated from the cluster units; the cluster cores get no structure; the structures of the ligands are given e.g. if the coordination of CO in the cluster H2Os3(CO)10 is unknown, the formula is given as H2Os3*10CO; the cluster core gets no structure.

General Information on Structures

Note:

You should be aware that only molecular structures are available, for instance all coordination compounds or molecules.

Single bonds, double bonds and triple bonds are available as bond types in the database, but note, the bond type is no criterion for registration. If one is not sure about the bond order, the bond type 'any bond' should be preferred in the search query. There are no tautomeric or aromatic bonds. In the case of keto/enol tautomerism, the ketonic form is always stored. Different tautomers are stored explicitly. All pi-interactions within organometallic pi-complexes are drawn as single bonds.

Structures of fragments are identical if the connectivity of the chosen atoms and the overall charge are the same. Only additional stereodescriptors can differentiate them further.

Main group organometallic compounds

In the gray area between covalent and ionic bonds, usually both formulations occur in the original literature for main group organometallic compounds. From the point of view of input conventions the following rules are generally favored by the Gmelin file, but one may find both alternatives, and it is recommended that you search for both structures to ensure completeness:

- Lithiumorganic compounds are stored with a covalent Li-C single bond
- Sodium- and potassiumorganic compounds are stored in ionic form (more than one fragment)
- Grignard compounds are stored in the covalent form
- Organometallic compounds with metals of the main groups III-VI are stored in the covalent form

Transition metal organometallic compounds

Transition metal organometallic compounds are input with the connectivity of atoms given in the original literature. If the connectivity is unknown, the compounds are separated formally into the central metal atoms and the surrounding ligands.

Stereochemistry

Stereochemistry is a further identification criterion of the structures in the Gmelin file. Two principal different stereochemical aspects can be searched for:

Stereochemical information on bonds and on centers.

Specified double bond information (cis or trans) can be searched for if the bond attribute "Double Steric" is chosen in the structure editor, and the structure is drawn as desired.

All stereocenters are drawn three-dimensionally. Fragments with stereochemical information are assigned either an absolute or a racemic configuration.

In the case of trigonal pyramidal, tetrahedral, or octahedral centers, a stereodescriptor is set if one, or more than one, possible configuration of a stereocenter can be assigned. This also applies to all pi-descriptors and all descriptors linking two polyhedra by a chain of bonds.
In all other cases the mentioning of a polyhedral center within a compound in the original literature is sufficient for the designation of a polyhedral descriptor. In the case of sterical isomers the polyhedral descriptor fix also the ligand configuration. If the configuration is unknown, no descriptor is set.

The polyhedron descriptors in the GMELIN file are as follows:

Descriptor	Polyhedron
P-3	trigonal pyramid
T-4	tetrahedron
SP-4	square planar
SP-5	square pyramid
TB-5	trigonal bipyramid
OC-6	octahedron
TP-6	trigonal prism
PB-7	pentagonal bipyramid
CU-8	cube
SA-8	square antiprism
DD-8	dodecahedron

HB-8	hexagonal bipyramid
TPS-9	tricapped trigonal prism
HB-9	heptagonal bipyramid

Note:

Additional to isomerism on double bonds stereoinformation on single bonds (eclipsed and staggered-configuration) is stored in the database. Further chiral isomers with at least known sign of optical rotation but unknown polyhedral geometry are distinguished. However, these descriptors are not searchable.

Identical Molecular Formula - New Compound?

Searching for a certain molecular formula may often give more than one hit.

The following criteria are responsible for a further registration of a compound with molecular formula identical to another:

- different charge
- isotope marked atoms in the formula
- the substance types

- glass or ceramic material
- Isomorphous, diadochous compounds, solid solutions
- Isotope or isotope containing compounds
- Minerals
- Polymer

- modifications of inorganic compounds
- different connectivity of atoms in the structure
- additional stereodescriptors

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