CrossFire™ Beilstein Data Fields Reference Guide

MDL Information Systems GmbH

Distributed by

Theodor-Heuss-Allee 108

D- 60486 Frankfurt

Germany

Phone: +49-69-5050 4242

Fax: +49-69-5050 4245

http://www.mdl.com

CrossFire Beilstein Reference Guide: Version 4.0., April 2004, for MDL CrossFire Commander Version 7 and CrossFire Server Version 7.

Customer Support

MDL Information Systems GmbH offers a Helpdesk service for our customers. The Helpdesk will give you help for the use of the system and will answer all questions you might have to Beilstein or its products.

The Helpdesk can be contacted via E-mail, phone or fax.

Europe Helpdesk

Phone:	+41 61 486-8880
Fax:	+41 61 486-8889
E-mail:	support@mdl.com

UK Helpdesk

Phone:	+44 1276 701-520
Fax:	+44 1276 701-501
E-mail:	support@mdl.com

US HelpDesk

Phone:	+1-800-326 3002 (toll free) +1-510-895 2213 (outside USA)
Fax:	+1-510-895 6092 (outside USA)
E-mail:	support@mdl.com

Japan Helpdesk

Phone:	+81-3-3230-2641
Fax:	+81-3-3230-2761
E-mail:	jsupp@mdl.com

Table of Contents

1. General

Introduction

Searching

The Database Contents

Acceptance Criteria for Substances

Acceptance Criteria for Attributes

Substance Types

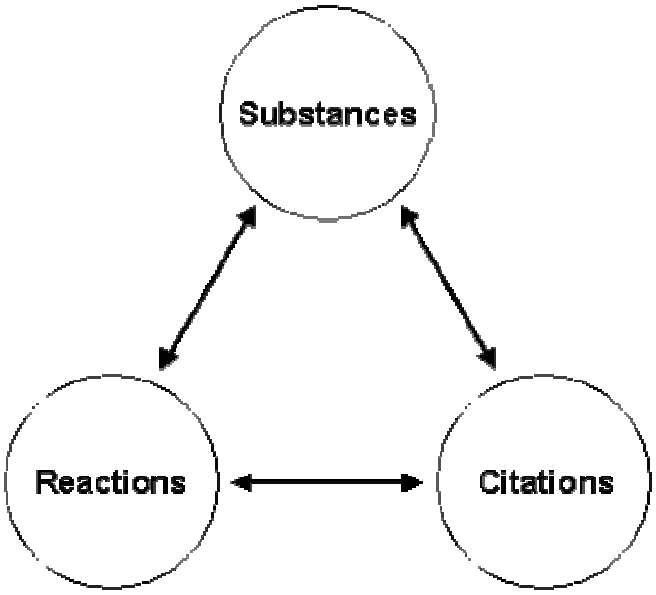
Searching for Facts

1.1. Introduction

The CrossFire system is a complete chemical information system comprising of the Beilstein Database, the CrossFire search and retrieval server software and the CrossFire Commander client. The CrossFire Commander runs under Microsoft Windows or on an Apple Macintosh and provides the user interface suite for MDL's products. Since the different products, for example CrossFire and AutoNom, have different interface requirements, the Commander configures itself accordingly.

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 unit. 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 organic 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 how you want, whether in terms of Substances (Structures and Properties), Reactions or Citations and provides hyperlinks between the different forms.



Substances:

The database contains over 30 million reports on properties of about 9 million organic compounds. You can access the structures and their associated chemical, physical, ecological, toxicological and pharmacological and bibliographic information. 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 9 million reactions which are searchable, with CrossFire as reaction substructures; you can define the role of a structure or substructure in the reaction, and search using reaction attributes such as reaction centers, bond fate and atom-atom mapping. Hyperlinks are provided to substances and to literature references.

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, if you are using CrossFire Abstracts or CrossFire EcoPharm. 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 mouse click on the hyperlink calls up the substance record for one of the reaction partners. Similarly when viewing some properties, simply click on 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 compounds, 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 organic chemistry problems but can lead to chance discoveries.

1.2. Searching

With CrossFire you can search for Structures, Reactions, Properties, Bibliographic and other factual information.

Structures:

Full structures, substructures, generic structures, stereoisomers and tautomers 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 only. Query atom types such as „X" any halogen can be set as can Atom lists (e.g. A1= C, N, O, S). Predefined generic groups, e.g. ALK (alkyl) and user defined generic groups (Markush structures) are easily input.

Reactions:

As for structures plus reaction role (reactant or product), reaction center, bond fate and atom-atom mapping.
Thus you can search for half reactions of the type:
? => A
"how do I make this type of compound"
A => ?
"what do these starting materials give"
or full reactions of the type:
A => B
"general or specific transformations".

Properties:

Search for Numeric values and ranges, strings and keywords. The CrossFire database contains more than 30 million reports on chemical, physical, physiological properties. You can search, for example, for chemical name, reaction conditions, pharmacological data. All of these are stored in discrete fields.

1.3. The Database Contents

There are three different data sources for the file:

1. The Beilstein Handbook from the Basic Series to Supplement IV covering the literature from 1779 to 1959. For more than 1.1 million compounds the complete Handbook information is available.

2. Primary literature data from 1960 to 1979: this data source contains ca. 3 million additional compounds. Specific data is available for melting point, boiling point, density, refractive index, optical rotatory power, isolation from natural products and chemical derivatives. All other physical and chemical properties are available as keywords together with corresponding references to the original literature. This data source provides the basis for the production of the Beilstein Handbook supplement V. This part of the file is being continuously updated to provide data for all data fields.

3. Primary literature data >1979: in contrast to source 2. detailed information for all physical and chemical properties have been abstracted from the literature. All data fields contain references as well as data. The category "Pharmacological and Ecological Data" is also included. The yearly growth is in the range of ca. 250.000 structures with 220.000 reactions and ca. 40.000 citations.

1.4. Acceptance Criteria for Substances

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

Substances are registered in the database if they contain, besides carbon, only the following elements out of the Periodic Table:

Group I: H, Li, Na, K, Rb, Cs

Group II: Mg, Ca, Sr, Ba

Group III: B

Group IV: C, Si

Group V: N, P, As

Group VI: O, S, Se, Te

Group VII: F, Cl, Br, I

These are designated as Beilstein substances. A further prerequisite is that an acceptable piece of data is given for the substance or that the substance is referred to in connection with another substance (components of mixtures or preparative methods).

Inorganic substances (Gmelin substances) are in general not registered (see exceptions below). These are:

- Substances which contain, besides carbon, the elements which are not mentioned in the list above
- Substances which do not contain carbon, and
- Elements

As an exception from the boundary Beilstein Gmelin areas the following substances are not treated as Beilstein substances:

- CO, CS, CO_2, CS_2, COS, C_3O_2, C_3S_2
- Carbonic acid and its thio analogs along with their salts with inorganic cations
- HCN, HOCN, HSCN and the corresponding iso-acids together with all metal salts and complexes of these acids
- Dicyanogene
- Phosgene
- Metal carbides

- Metal salts of formic acid, acetic acid, and oxalic acid
- Fullerenes, which consist only of carbon
- Carboranes

1.5. Acceptance Criteria for Attributes

Acceptable data for the Beilstein Database fall into the following categories:

1. Identification
2. Bibliographical Data
3. Chemical Data
4. Physical Properties
5. Ecological Data
6. Pharmacological and Ecological Data

General rules for accepted data will be discussed in the relevant chapters (PHY, CHE, ECO etc.). Subjects are sorted in a hierarchical order. To find information to a specific topic use the help index or the help find function.

1.6. Substance types

Beilstein has extended the concept of substances to enable the abstraction of environmental, pharmacological and toxicological data. It now allows the acceptance of substances whose identity is not necessarily given by means of a structure. Substances will continue to be "chemical substances" in their organic chemical sense.

Beilstein distinguishes between several types of substances:

1. Pure substances with a structural formula:

A Classical Beilstein compounds

2. Substances which may be described by means of names or information about the components:

B Biomolecules: (biopolymers [carbohydrates, nucleic acids, proteins], enzymes, hormones, etc.)

M Mixtures: (composed of components)

composition completely given

composition partially given

composition completely not given

P Polymers:

monomers given

monomers not given

1.6.1. Classical Beilstein compounds

Substances of this type may consist of one (e.g. benzene) or more fragments (e.g. salts, complexes, addition compounds, each with defined molar ratios).

Peptides with up to 12 amino acids and polysaccharides with up to 6 carbohydrate units are abstracted. Larger peptides and polysaccharides are registered by means of their names as biomolecules.

⇒ To prevent gaps due to the separation into Beilstein and Gmelin areas, the rules have been modified in the following cases:

- Compounds with more than one fragment:

If salts or adducts contain a Gmelin (inorganic) component as well as a Beilstein fragment, these multi-fragment compounds and their data are abstracted, as long as the Beilstein fragment is the one under investigation.

- Reference compounds:

If in the preparation or the chemical behavior references are made to starting materials or products which are defined as Gmelin compounds and which are necessary for the correct description of the reaction (e.g. lead tetraacetate in the oxidative acetoxylation of furan) the structure of the Gmelin compound, but not its data, are abstracted.

The same applies to the acceptance of the physical properties of multi-component systems or to azeotropes.

⇒ In addition to pure isolated compounds which fulfill the classical Beilstein compound definition the following may be abstracted under certain defined conditions:

- Stereoisomeric mixtures:

Stereoisomers (enantiomers, diastereoisomers) which are not isolated from product mixtures are accepted, if defined data can be assigned to individual isomers in the mixture by means of spectroscopic measurements (e.g. NMR, UV).

If individual stereoisomers in a mixture have been identified and assigned configurations (e.g. spectroscopically) they are recorded as pure stereoisomers but only with those data which can be assigned to them.

Enantiomeric mixtures are abstracted if the ratio of the enantiomers is at least 80:20 (enantiomeric excess 60 %). Mixtures with less enrichment are not accepted with the exception of racemates which are dealt with as if they were pure compounds. Enantiomers with an optical purity of 98 % (corresp. to ca. 96 % ee) are treated as pure compounds.

Diastereoisomeric mixtures are abstracted as such provided there are satisfactory data (e.g. bp, mp, etc.) available. Stereocenters in the mixture which remains unseparated are entered as unsteric.

- Short lived ions and radicals:

These are considered when satisfactory data are available which can be assigned to the ion or radical.

- Compounds containing isotopes:

If the position of the label in the compound is known the marked compound is abstracted provided that acceptable data are available. The degree of labeling is not an acceptance criterion since low degrees of labeling can be important in ecological, medical or pharmacological investigations. If the position of the labels is not known or the labeled substance is only used as tracer (e.g. for detection of metabolic products) together with the unlabelled substance, only the unmarked compound is abstracted provided that there are acceptable data available.

1.6.2. Biomolecules

Here are included all biomolecules such as carbohydrates, nucleic acids, proteins, enzymes, hormones, etc. for which a structure entry is not possible.

Peptides with up to 12 amino acids and polysaccharides with up to 6 carbohydrate units are, however, abstracted with a structure (see Classical Beilstein Compounds). The biomolecule is completely described by its name.

1.6.3. Mixtures

Mixtures are only abstracted when it is clear from the publication that the substance or its components belong to the area of organic chemistry. Frequently they are chemical products which are commercially available as pesticide or a cleaning material. The active components are then usually known but various additives in various concentrations are used by different manufacturers.

This substance type is divided into different substance types.

Mixtures (Composition completely given)

"Composition known" means that not only the components (names or structures) but also their concentrations in the mixture are known completely and exactly (author's values). The mixtures name would not need to be known.

Mixtures (Composition partially given)

"Composition partly known" means that the qualitative and/or quantitative composition (components, concentrations) are not completely known. Alternatively all data are available but for the concentrations only ranges are given. The mixture is described by means of its name.

Mixtures (Composition completely not given)

"Composition unknown" means that there are no data available for the components nor their concentrations. Only the name of the mixture is given (and the certainty that a mixture is being dealt with). The mixture is completely described by its name.

1.6.4. Polymers

Here are included the synthetic polymers. This substance type is divided into two substance types.

Polymers (Monomers given)

Polymers of this type are described by the name of the polymer and the structure of the monomers (structure entry for the components). The names of the polymers are entered with a strict syntax.

Polymers (Monomers not given)

This type of substance is completely described by its name only.

1.7. Searching for Facts

The database contains Numeric and textual data in more than 450 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 very straightforward. High flexibility is given by option to carry out Numeric, text, Field Availability and hierarchical searching. A successful search retrieves records, each of which contains 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

Numeric Fields

Text Fields

Keyword Fields

Truncation

Operators

Field Availability Search

Hierarchical Group Code Search

1.7.1. Substance Factual Search

This is a search for specific 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 graphical reactions and citations.

1.7.2. Reaction Factual Search

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

1.7.3. Citation Factual Search

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

1.7.4. Numeric Searching

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

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

Numeric values are also present in some String fields, where they are searchable as strings.

1.7.5. Text Searching

Searching for strings or partial strings can be carried out in the text fields. To search for a partial String use the truncation wild card symbols. It is highly recommendable to look in the index, use "List", 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 (Phrase) (plus)

The phrase is only split at certain symbols.

e.g. Author

The splitting occurs such that each author name is indexed as a phrase.

String (Wordwise)

The entry is split into words at the following symbols:

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

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

1.7.6. Keyword Searching

Many topics in the Beilstein database have fields of the type Description. These fields contain entries, which usually stem 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 LIST function of the CrossFire system before starting a search. The keywords can be copied out of the list into the edit mask for searching.

1.7.7. Truncation

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

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

Right, left and middle truncations 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. Pharmacological Data, to make sure that all occurrences of a term are found. Thus to retrieve the records with both antiinfluenza and antiinfluenzal the following should be input:

pharm.com=antiinfluenza*

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

1.7.8. Operators

In the operator column of the CrossFire Commander Fact Editor as well as in the fact query window of the Commander itself the Boolean operators, AND, NOT, OR and PROXIMITY can be input. For the Beilstein Abstracts databases the two additional operators NEAR and NEXT are also available.

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. cns = "furan" and nmr.nuc = "13C"

This will result in a list of compounds, where the compounds name contains the word "furan" and where the compounds also have 13C-NMR data available. 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. cns = "furan" or cns = "thiophene"

This will result in a list of compounds, where the chemical name of the compounds either contain the fragments "furan" or "thiophene".

When using this operator with hit lists, e.g. from structure searches, the resulting list will contain all records present in 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. ln = 26334 not (elc = n1 or elc = n2)

This example will retrieve all pyridine compounds that contain one carboxamide or amidine group and that do contain more than 2 nitrogen atoms.

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 ºC measured in the pressure range of 750 to 760 mm.

NEAR Operator

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

e.g. ab=fibrinogen* near ab=receptor*

e.g. pharm.com=neutrophil* near pharm.com=chemoattract*

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=capillar* next ab=electrophor*

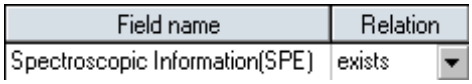
1.7.9. Field Availability Search

This is a search for the occurrence of a fact in the database. Thus you can search for all compounds, which were isolated from natural products by entering INP in the Field Name column and leaving the Value column empty.

1.7.10. Hierarchical Group Code Search

This is a search for the presence of data in any of a specified group of fields. Data fields are grouped together according to the hierarchy of the Beilstein Database. The group fields, e.g. Spectral Data (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.



2. Data Field Description

The Beilstein Database is organized hierarchically according to the following top level hierarchy:

Basic Indexes (BI)

Identification Data (IDE)

Bibliographic Information (BIB)

References (REFX)

Chemical Data (CHE)

Physical Data (PHY)

Pharmacological and Ecological Data (PED)

In the following all levels of the hierarchy down to the field level is described in detail.

2.1. Basic Indexes (BI)

Basic Indexes are collective indexes, which allow convenient searching without thinking about field codes. The Beilstein databases under the CrossFire system offer the following Basic Indexes:

- All BRN's (ABRN)
- All Chemical Names (ACN)
- All Chemical Names Segment (ACNS)
- Substance Basic Index (BISUB)
- Reaction Basic Index (BIREA)
- Citation Basic Index (BICIT)
- EcoPharm Basic Index (BIPHARM)

2.1.1. All BRN's (ABRN)

Description:

This is the basic index for BRN's. It contains all BRN's out of the field which have the extension **.**PB, **.**BRN or **.***BRN. It is useful in such a case where referenced compounds need to be found.

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

Type of Indexing:

Numeric

2.1.2. All Chemical Names (ACN)

Description:

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

This Basic Index contains the following fields:

Field Code	Field Name
CN	Chemical Name
AUN	Autoname
CCN	Composition: Comp.Name

CDER	Derivative
POT.PRO	Product
.CN, .PA	All fields with the extension

Type of Indexing:

String (phrase)

2.1.3. All Chemical Name Segments (ACNS)

Description:

This is the basic index for Chemical Names Segment. The Chemical Name Segment Index uses the same sources like the All Chemical Name Index. However, it is indexed differently allowing fast searching for segments of chemical names without entering truncation symbols.

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

This Basic Index contains the following fields:

Field Code	Field Name
CN	Chemical Name
AUN	Autoname
CCN	Composition: Comp.Name
CDER	Derivative
POT.PRO	Product
.CN, .PA	All fields with the extension

Type of Indexing:

String (wordwise)

2.1.4. 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 CrossFire Commander without specifying a field name and with staying in substance context the keywords will automatically be searched in this index.

The Substance Basic Index contains the following fields:

Field Code	Field Name
CN	Chemical Name
AUN	Autoname
CCN	Composition: Comp. Name
BRN	Beilstein Registry Number
RN	CAS Registry Number
INP	Isolation from Natural Product
RSTR	Related Structure
PUR	Purification
CNF.OBJ	Object of Investigation
EM.MET	Electrical Moment Method
IP.MET	Ionization Potential Method
CSYS	CSYS
NMR.NUC	NMR Nucleus
NMR.NUI	NMR Coupling Nuclei
ESR.NUI	ESR Coupling Nuclei
NQR.NUC	NQR Nucleus
DE.MET	Method
.SOL	All fields with the extension (except RX.SOL)
.KW / .COM	All fields with the extension
.CN / .PA	All fields with the extension

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

Type of Indexing:

String (wordwise)

2.1.5. 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 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
RX.PRO	Product
RX.RGT	Reagent
RX.CAT	Catalyst
RX.SOL	Solvent
RX.COND	Other Conditions
RX.SUB	Subject Studied
RX.TYP	Reaction Type
RX.PRT	Prototype Reaction
RX.COM	Comment

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

Type of Indexing:

String (wordwise)

2.1.6. 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 CrossFire Commander without specifying a field name and with staying in citation context the keywords will automatically be searched in this index.

The Citation Basic Index (BICIT) is only visible and searchable for the Abstracts databases.

The Citation Basic Index contains the following fields:

Field Code	Field Name
AU	Author

TI	Title
AB	Abstract
AB.KW	Abstract Keywords
JT	Journal Title
PA	Patent Assignee

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

Type of Indexing:

String (wordwise)

2.1.7. EcoPharm Basic Index (BIPHARM)

Description:

This is the basic index for Ecopharm data. A user has to enter the fieldname BIPHARM= and a keyword to perform searches in this basic index. It contains the following fields out of the EcoPharm area:

Pharmacological Data

Field Code	Field Name
PHARM.E	Effect
PHARM.EP	Endpoint of Effect
PHARM.SP	Species or Test-System
PHARM.RA	Route of Application
PHARM.KD	Kind of Dosing
PHARM.MR	Method
PHARM.FD	Further Details
PHARM.TY	Type
PHARM.RE	Results
PHARM.META	Metabolite
PHARM.COM	Comment

Ecological Data/Ecotoxicology

Field Code	Field Name
ECT.E	Effect
ECT.EP	Endpoint of Effect
ECT.SP	Species or Test-System

ECT.RA	Route of Application
ECT.KD	Kind of Dosing
ECT.MR	Method
ECT.FD	Further Details
ECT.TY	Type
ECT.RE	Results
ECT.META	Metabolite
ECT.COM	Comment

Ecological Data/Exposure/Exposure Assessment

Field Code	Field Name
ECA.HE	Exposure
ECA.SO	Sources
ECA.COM	Comment

Ecological Data/Exposure/Concentration in the Environment

Field Code	Field Name
ECC.SP	Species
ECC.ME	Media
ECC.LO	Location
ECC.MR	Method, Remarks
ECC.COM	Comment

Mobility/Transport and Distribution

Field Code	Field Name
ECTD.TY	Type
ECTD.ME	Media
ECTD.RE	Results
ECTD.MR	Method, Remarks
ECTD.COM	Comment

Mobility/Bioaccumulation, Biomagnification, Biomonitoring

Field Code	Field Name
BIO.SP	Species
BIO.ME	Media

MIO.MR	Method, Remarks
BIO.MAG	Biomagnification
BIO.MON	Biomonitoring
BIO.COM	Comment

Transformation and Degradation./Biodegradation

Field Code	Field Name
BIOD.TY	Type
BIOD.IN	Inoculum
BIOD.DP	Degradation Product
BIOD.MR	Method, Remarks
BIOD.COM	Comment

Transformation and Degradation/Abiotic Degradation, Hydrolysis

Field Code	Field Name
ECDH.TY	Type
ECDH.DP	Degradation Product
ECDH.MR	Method, Remarks
ECDH.COM	Comment

Transformation and Degradation/Abiotic Degradation, Photolysis

Field Code	Field Name
ECDP.TY	Type
ECDP.DP	Degradation Product
ECDP.MR	Method, Remarks
ECDP.COM	Comment

Transformation and Degradation/Stability in Soil

Field Code	Field Name
ECS.TY	Type
ECS.MR	Method, Remarks
ECS.COM	Comment

Transformation and Degradation/Oxygen Demand

Field Code	Field Name
EOD.TY	Type
EOD.MR	Method, Remarks
EOD.COM	Comment

USE

Field Code	Field Name
USE.LH	Laboratory Use and Handling
USE.PT	Use Pattern
USE.COM	Comment

The EcoPharm Basic Index belongs to the substance context and a search will result in a substance/structure hitset.

The EcoPharm Basic Index (BIPHARM) is only visible and searchable for the EcoPharm databases.

Type of Indexing:

String (wordwise)

2.2. Bibliographic Information (BIB)

The field area bibliographic information consists of the following topics and fields:

Citation Number (CNR)

Citation Number (CNR)

Citation (CIT)

Document Type (DT)

Authors (AU)

Patent Author (PA)

Patent Country Code (PCC)

Patent Number (PN)

Patent Year (PPY)

Coden (CO)

Journal Title (JT)

Journal/Review without Coden (JTW)

ISBN (ISB)

Country Code (CC)

Language Code (LA)

Editor (EDT)

Location of Publication (LO)

Volume (VL)

Article Number (NB)

Publication Year (PY)

Page (PAG)

Citation (Unresolved) (URES)

Abstracts (AB)

Title (TI)

Abstract (AB)

Language (ALA)

Keywords (AB.KW)

2.2.1. Bibliographic Information (BIB)

Description:
This field identifier is a group code in the hierarchy of the Beilstein database. The database contains citations from Journals, Patents and books or monographs. Titles of Journals with Coden will be found in the JT field, for Journals and other works without Coden the title is stored in the JTW field. Patents are stored in the patent fields. Citations that could not be classified into one of these groups are stored in the unresolved citation field. At next lower level in the BIB group, DT distinguishes between the different types of sources. Journals, Patents and books or reviews are contained in the database. Currently only journals are abstracted. The data fields contain bibliographic data, such as authors, Coden etc. BIB and the specific fields are searchable via Field Availability. Fields belonging to the data field level are also searchable as strings.

Example:
Search for substance records from the journal with the Coden: LACHDL in the Facts mask.

Field Name	Value
CO	LACHDL

Tips and Hints:
There are some compounds, which have no bibliographical data. These are compounds, which only occur as references in the data for other compounds, e.g. starting materials in reactions or preparations. Once you have carried out a search for bibliographic information it is possible to display the BIB fields of each citation (possibly more than one for a particular compound) by selecting HIT in the Display main menu. You have to be in the "full display mode".

Type of Indexing:
Group Code

Related Information:
AU, CO, LA, VL, NB, PY, PAG.

2.2.2. Citation Number (CNR)

Description:

Every reference in the Beilstein database has been assigned a citation number, which can be used to access a certain citation directly.

Type of Indexing:

Numeric

2.2.2.1. Citation Entry Date (CED)

Description:

The search field Citation Entry Date contains the date (year/month/day) when the citation was first entered into the database. Dates have to be searched with a fixed format: yyyy/mm/dd.

Type of Indexing:

String (phrase)

2.2.2.2. Citation Update Date (CUPD)

Description:

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

Type of Indexing:

String (phrase)

2.2.3. Citation

2.2.3.1. Document Type (DT)

Description:

DT contains information describing the type of source, e.g. journals, patents or other publications.

Tips and Hints:

Since there are no other types of sources at present you should not use the code DT for Field Availability searches.

Related Information:

AU, CO, PAG, LA, VL, NB, PY

Type of Indexing:

String (phrase)

2.2.3.2. Authors (AU)

Description:

The AU field contains the surname of the author and the given or further names (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. A comma and a space always separate the surname from first names or affixes e.g. "van der". Titles such as "Dr.", "Sir" or "Prof." are ignored. The first five names mentioned in the article are given, further names are displayed (not indexed) as "et al.".

For citation originating from the Handbook, only the surnames are present.

Example1:

Adams, *	published by authors with the surname Adams
Adam*	published by all authors beginning with Adam
Adam, Paul	published by Paul Adam.
Adam, Paul*	published by Paul Adam including other first names.
Adam, P*	published by P. Adam including Adam, Paul or other first names starting with P

Example2:

Operator	Field Name	Value
	AU	Schmidt, Richard R
PROXIMITY	CO	TETRAB

Using the PROXIMITY Operator will only retrieve those publications of Richard R. Schmidt from Tetrahedron (TETRAB).

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 surnames only.

Type of Indexing:

String (phrase)

Related Information:

CO, PAG, LA, VL, NB, PY.

2.2.3.3. Patent Author (PA)

Description:

The PA field contains the name of companies or a single inventor of a patent. The assignee names have not been standardized. Use LIST command to view the index.

Type of Indexing:

String (phrase)

2.2.3.4. Patent Country Code (PCC)

Description:

The country code of the country issuing the patent is stored in the CC field.

Type of Indexing:

String (phrase)

2.2.3.5. Patent Number (PN)

Description:

Every patent has a unique patent number, which can be searched, in this field. The PN field contains the two-letter country code and the patent number.

Type of Indexing:

String (phrase)

2.2.3.6. Patent Year (PPY)

Description:

The PPY field contains the year of publication or issue of a patent document.

Type of Indexing:

String (phrase)

2.2.3.7. CODEN (CO)

Description:

Journal titles have to be searched for using the Cassi Coden. A list of Coden of excerpted journals is part of the Appendix. Cassi Coden is 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. You can request a list of the journal titles and the corresponding six digit Coden excerpted by Beilstein if you use the LIST function in the Citation query input mask. The Coden can sort either by the journal titles or the list.

Tips and Hints:

Searches for journal titles can be carried out via the field Coden in the Citation mask or the Facts mask. Move the mouse cursor in the Citation mask to the field Coden and press LIST to verify valid search terms. The pop up window allows you to view the list of Coden and journal titles sorted according to either the Coden or the titles. You can scroll through the list and select the desired journal, whereupon the Coden is entered automatically into the search field.

Example:

Search for substances published in the journal Tetrahedron.

Field Name	Value
CO	TETRAB

Type of Indexing:

String (phrase)

Related Information:

AU, PAG, LA, VL, NB, PY

2.2.3.8. Journal Title (JT)

Description:

The title of the journal is present in this field if the journal could be assigned a CODEN. Journal titles without Coden are stored in the JTW field.

Type of Indexing:

String (phrase)

2.2.3.9. Journal/Review without CODEN (JTW)

Description:

If the Journal or review was unable to be assigned a coden, its title will be stored in this field.

Type of Indexing:

String (phrase)

2.2.3.10. ISBN (ISB)

Description:

The ISBN is stored in this field. This field is only visible but not searchable.

Type of Indexing:

String (phrase)

2.2.3.11. Country Code (CC)

Description:

The country code of the country issuing the Citation is stored in the CC field. The Country Code comprises patents, journals, book review and secondary references.

Type of Indexing:

String (phrase)

2.2.3.12. Language Code (LA)

Description:

The Language Code is a two-character String that provides information about the language of the original publication. The following codes are examples of codes used:

EN	English
FR	French
GE	German
JP	Japan
RU	Russian

Tips and Hints:

All data in the Beilstein database are in English. This field will tell you the language of the original article. It is not present for all references.

Example:

Search for all substances reported in English language publications

Query Input in the Facts search mask:

Field Name	Value
LA	EN

Type of Indexing:

String (phrase)

Related Information:

AU, CO, PAG, VL, NB, PY

2.2.3.13. Editor (EDT)

Description:

The name of editor is present in this field. This field is only visible but not searchable.

Type of Indexing:

String (wordwise)

2.2.3.14. Publisher (PUB)

Description:

The name of publisher is present in this field. This field is only visible but not searchable.

Type of Indexing:

String (wordwise)

2.2.3.15. Location of Publication (LO)

Description:

The location of publisher field contains the town or city where the publisher resides. The field is not standardized.

Type of Indexing:

String (phrase)

2.2.3.16. Volume (VL)

Description:

The Volume field contains information about the volume of a journal in which the substance has been reported. Most journals (however not all) count volumes per year and use numbers to distinguish between monthly or further issues. Some journals use the term volume to distinguish between the numbers they publish every year. Some volume descriptions contain letters.

Tips and Hints:

The field VL is not a typical search field. Its main use is to provide information to assist in finding the original articles. Nevertheless it is possible to search for volumes in the Facts and the Citation mask. Since it has been indexed as a String it is not possible to search for ranges.

Example:

Search for substances in Volume 46 of the journal Tetrahedron.

Query input in the Facts mask:

Operator	Field Name	Value
	CO	TETRAB
PROXIMITY	VL	46

Type of Indexing:

String (phrase)

2.2.3.17. Article Number (NB)

Description:

The numbers are the issues of journals within a volume. Usually the number ranges from 1 to 12. In many cases sub-numbers are issued. Since these numbers (6, 1.2, 1-6) are written in many different ways, the field has been indexed as a string.

This field also contains the CA article number.

Tips and Hints:

The field NB is not a typical search field. Its main use is to provide information to assist in finding the original articles. Nevertheless it is possible to search for numbers in the Facts and the Citation mask. Since it has been indexed as String it is not possible to search for ranges.

Example:

Search for compounds published in the journal Tetrahedron, Volume 46, Number 5

Query input in the Facts mask:

Operator	Field Name	Value
	CO	TETRAB
PROXIMITY	VL	46
PROXIMITY	NB	5

Type of Indexing:

String (phrase)

Related Information:

AU, CO, LA, PAG, VL, PY

2.2.3.18. Publication Year (PY)

Description:

The content of the Publication Year field is the publication year of the journal. It should not be confused with the entry date.

Example:

Search for all substances reported in 1990 in the journal Liebigs Ann. Chem.

Query input in the Facts mask:

Operator	Field Name	Value
	CO	LACHDL
PROXIMITY	PY	1990

Type of Indexing:

String (phrase)

Related Information:

AU, CO, LA, PAG, VL

2.2.3.19. Page (PAG)

Description:

The field Page contains the number of the page or the range of pages of the original article in which the information about the substance was published.

Tips and Hints:

The field PAG is not a typical search field. Its main use is to provide information to assist in finding the original articles. Nevertheless it is possible to search for pages in the Facts and the Citation mask. Since it has been indexed as String no Numeric ranges can be searched for. To find a particular page range it is best to extract the indexed String from the index.

Example:

Search for all substances in the article published in 1990 in Tetrahedron, volume 46, number 7 on pages 2483-2494.

Query input:

Operator	Field Name	Value
	PY	1990
PROXIMITY	CO	TETRAB
PROXIMITY	VL	46
PROXIMITY	NB	7
PROXIMITY	PAG	2483-2494

Type of Indexing:

String (phrase)

2.2.3.20. Citation (Unresolved) (URES)

Description:

Those citations that could not be resolved into the above fields are stored in the URES field.

Type of Indexing:

String (phrase)

2.2.4. Abstracts

2.2.4.1. Abstract Title (TI)

Description:

The content of the title field is taken from the organic chemistry literature from 1980 to the present.

Tips and Hints:

The Boolean Operators AND, OR, NOT can be used to find occurrences of the indicated terms anywhere in the title. In the case of PROXIMITY the entire title is considered as information unit. Therefore, the PROXIMITY Operator works like AND.

For terms containing special characters (e.g. Greek letters), look in the index for spelling.

Example:

Search for all documents where a relationship between the structure of a compound and its odor has been published:

ti=structure* and ti=odor*

Type of Indexing:

String (wordwise)

2.2.4.2. Abstract (AB)

Description:

The content of the abstract field is taken from the organic chemistry literature from 1980 to the present.

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.

For terms containing special characters (e.g. Greek letters), look in the index for spelling.

Example:

Search for all documents containing information about the synthesis of epibatidine:

ab=synthesis* and ab=epibatidine

Type of Indexing:

String (wordwise)

2.2.4.3. Abstract Language (ALA)

Description:

The Abstracts Language Code is a two-character String that provides information about the language in which an article being abstracted is written. The following codes are examples of codes used:

EN	English
FR	French
GE	German

Example:

Search for all abstracts written in English: Ala = en

Type of Indexing:

String (phrase)

2.2.4.4. Keywords (AB.KW)

Description:

This field contains keywords, index headings or similar items which are present in an article.

Type of Indexing:

String (wordwise)

2.3. Substance Identification (IDE)

Description:

IDE is a group code in the hierarchy of the Beilstein database. Fields belonging to the group IDE contain information, which is necessary or useful to identify compounds.

List of fields:

Beilstein Registry Number (BRN)

Beilstein Preferred RN (BPR)

CAS Registry Number (RN)

Chemical Name (CN)

Chemical Name Segment (CNS)

Autoname (AUN)

Linear Structure Formula (LSF)

Fragment Molecular Formula (FMF)

Molecular Formula (MF)

Search MF Range (MOFO)

Charge (CHA)

Element Count (ELC)

Number of Atoms (NA)

Number of Elements (NE)

Number of Fragments (NF)

Molecular Weight (MW)

Fragment BRN (FBRN)

Lawson Number (LN)

Structure Keyword (STR.KW)

Type of Substance (STYPE)

Constitution ID (CONSID)

Tautomer ID (TAUTID)

Composition: Comp. BRN (CCBRN)

Composition: Comp. Name (CCN)

Composition: Comp. Conc. (CCC)

Beilstein Reference (SO)

Entry Date (ED)

Update Date (UPD)

2.3.1. Beilstein Registry Number (BRN)

Description:

The Beilstein Registry Number (BRN) is assigned when a compound is registered for the first time in the Beilstein Information System. In general the registration procedure is based on the available structural information for a substance, which is included in the connection table. Exceptions are biomolecules, mixtures and polymers. Both the BRN and the structure of a substance are unambiguous identifiers of substances. The Beilstein Registry Number is the accession number of the substance record in Cross Fire and in the Beilstein Online database. It is an integer, which does not contain further information.

Example:

Search for information about the substance with the Beilstein Registry Number 227659

Field Name	Value
BRN	227659

Type of Indexing:

Numeric

Related Information:

IDE, ABRN

2.3.2. Beilstein Preferred (BPR)

Description:

The Beilstein Preferred RN is the single CAS Registry Number that has been selected as the best choice for a compound from the one or more RNs that may be present in the database. The BPR is, however, not always present and is selected according to the following criteria:

1. If there is only one RN available from all sources, this will also be BPR.
2. Some compounds have one or more Registry Numbers that have been assigned by CAS in Columbus. If Beilstein has one of these Registry Numbers on record in its file, this RN will be the BPR. If, however, Beilstein has different Registry Numbers in its file, the compound will not be given a BPR and only the CAS supplied numbers will appear in the RN field.

3. If a compound has not received a Registry Number from CAS and Beilstein has several RNs in its file, these RNs will appear in the compound record, but no BPR will be given.

Tips and Hints:
When searching for CAS Registry Numbers, it is recommended to first use the BPR field, which contains unique Registry Numbers. If the search results in no hits, then one should search in the RN field.

Type of Indexing:
String (phrase)

2.3.3. CAS Registry Number (RN)

Description:

The CAS Registry Number present in CrossFire database has either been extracted from the abstracted primary literature or from a match between database structures and the CAS Registry file. These different sources sometimes result in more than one Registry Number being present.

Example:

Search for information about the substance with the CAS Registry Number 100429-35-4.

Field Name	Value
RN	100429-35-4

Tips and Hints:

The field RN provides the means for cross-referencing to other databases or to printed media containing the Registry Number. When searching for CAS Registry Numbers, it is recommended to first use the BPR field, which contains unique Registry Numbers. If the search results in no hits, then one should search in the RN field.

Type of Indexing:

String (phrase)

2.3.4. Chemical Name (CN)

Description:

The field Chemical Name contains complete chemical names from various sources: the preferred name (the IUPAC based name used in the Beilstein Handbook) names from the original publication names generated by the program AutoNom Additionally compounds can have multiple entries for chemical names such as systematic, trivial and tradenames.

The names are indexed as phrases. You can search for name segments by using the left, right or middle truncation. You can use either of the wildcard symbols" ? " (One character) or " ***** " (any number of characters) in any position or combination. However, it is recommended to do chemical name segments searching in the CNS field.

Tips and Hints:

Name searches are not recommended to identify compounds, because names are ambiguous or non-systematic in many cases. You can also use unambiguous, systematic names generated by AUTONOM. In some cases name fragments might be useful to search for substance classes or substitution patterns, however there are more powerful methods available such as structure or substructure searches or the Lawson Number LN.

Example1:

Search for benzoic acid

Field Name	**Value**
CN	benzoic acid

Example 2:

Search for the trivial name nifedipine

Field Name	**Value**
CN	nifedipine

Type of Indexing:

String (phrase)

2.3.5. Chemical Name Segment (CNS)

Description:

The field Chemical Name Segment uses the same sources like 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 substitution patterns.

Example:

Search for compounds containing the name terms dihydroxy, chromen and pyran.

Operator	Field Name	Value
	CNS	dihydroxy
AND	CNS	chromen
AND	CNS	pyran

Type of Indexing:

String (wordwise)

2.3.6. Autoname (AUN)

Description:

For this compound an IUPAC based, unambiguous systematic name has been generated by using the program AUTONOM at Beilstein. The algorithm developed for AUTONOM analyzes the compound's structure diagram (Connection Table). When the program is not able to generate a correct name, no name is given.

However not all compounds have been processed by AUTONOM. In some cases name fragments might be useful to search for substance classes or substitution patterns, however there are more powerful methods available such as structure or substructure searches or the Lawson Number LN.

This field is only visible but not searchable as AUN. Autonames are part of the Chemical Name Index.

Type of Indexing:

String (wordwise)

2.3.7. Linear Structure Formula (LSF)

Description:

The LSF field contains the molecular formula in Hill order or in linearized format. The LSF field is always present for ionic structures and isotopically labeled compounds with the exception of Deuterium and Tritium. It may contain

- Charges
- Isotopes
- The formula of an organic compound
- The formula of an inorganic fragment in multifragment compounds in linearized format.

For multifragment compounds the molecular formulae of the individual fragments are separated from one another by asterisks (*). Stoichiometric multipliers need not to be integers.

Use this field to search for compounds with isotopes or charges, or for multifragment compounds in which the stoichiometric multipliers are not integers.

Tips and Hints:

Searches for compounds with isotopes or charges, or multifragment compounds with their reported stoichiometric multipliers can be carried out in this field.

Type of Indexing:

String (phrase)

2.3.8. Fragment Molecular Formula (FMF)

Description:

The field FMF Fragment Molecular Formula contains the molecular formula of a fragment calculated from the chemical structure in Hill order****** with no charge information. This field is searchable but not displayable.

****Arrangement of Fragment Formulas:**

Fragment formulas are arranged as follows:

Carbon containing compounds come first

Number of carbon atoms

Number of hydrogen

Alphabetical order of elements

Non carbon containing compounds follow

Alphabetical order of elements

Examples:

$C_6H_3N_3O_7$ * C_5H_5N

$2C_6H_7N$ * $C_6H_6Cl_6$ * 2ClH

Tips and Hints:

Since molecular or multifragment compounds may contain stoichiometric factors the field FMF is recommended as the search field. You need not take into account whether you are searching for a singlefragment or multifragment compound. The sorting of the index does not depend on leading factors.

Type of Indexing:

String (phrase)

2.3.9. Molecular Formula (MF)

Description:

The Molecular Formula field contains the complete molecular formula for single- and multifragment compounds. It is calculated from the chemical structure in Hill order**, with no charge or isotope information. For multifragment compounds the molecular formulae corresponding to the individual fragments are separated from another by an asterisk and have normalized stoichiometric multipliers. E.g.: $2C_8H_{11}N$ * $C_2HF_3O_2$.

****Arrangement of Fragment Formulas in the MF-Field**

Fragment formulas are arranged as follows:

Carbon containing compounds come first

Number of carbon atoms

Number of hydrogen

Alphabetical order of elements

Non carbon containing compounds follow

Alphabetical order of elements

Examples:

$C_6H_3N_3O_7$ * C_5H_5N

$2C_6H_7N$ * $C_6H_6Cl_6$ * 2ClH

Tips and Hints:

Searches for multifragment compounds with known stoichiometric multipliers and on the basis of the smallest common denominator should be carried out in this field. If isotopes or charges are relevant the Linear Structure Formula field should be used. The molecular formula is very useful to refine search strategies. Positional isomers can be searched for very effectively when the molecular formula is combined with a Lawson Number (LN).

Example:

Search for structural isomers with the molecular formula $C_6H_5NO_2$.

Field Name	Value
MF	C6H5NO2

Type of Indexing:

String (phrase)

2.3.10. Search MF Range (MOFO)

Description:

The MOFO field is a non-display field that allows the searching of ranges with molecular formula. It is not possible to have a look at this field via the expand command, because it is calculated during the search "on the fly".

Tips and Hints:

You can search for derivatives of a certain carbon skeleton by typing an asterisk at the end of a value. (see example (c)) 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 (b). If you want to restrict searches to compounds with a specific number of fragments it is necessary to combine the query with restrictions in the field NF.

Examples:

$C_{(2-4)}$ $H_{(4-8)}$

C_2 $H_{(4-5)}$ $O_{(4-99)}$

C_8 H_7 *

Type of Indexing:

String (phrase)

2.3.11. Charge (CHA)

Description:

The field CHA contains the charge of a fragment. The data for this field is taken from the field LSF. CHA will not always be equivalent to the total number of charges (this is particularly true for multifragment compounds). This field is indexed numerically and is not displayable.

Example:

Search for compounds with a total charge of -2 or more

Field Name	Value
CHA	<-2

(The input ">" is interpreted as ">=")

Tips and Hints:

Information about charges on single or multifragment compounds is displayed in the field LSF (Linear Structure Formula). It is possible to search for specifically charged fragments of multifragment compounds in the field LSF by using extensive truncation.

Type of Indexing:

Numeric

2.3.12. Element Counts (ELC)

Description:

The Element Count field contains the element counts for a fragment. The data for this field is taken from FMF. An element count is defined as the element symbol and the number of its occurrences per fragment. This field is indexed as a String and is not displayable. Since data are taken from FMF there is no stoichiometric factor taken into account.

Tips and Hints:

The Element Count must not be confused with the Number of Atoms (NA) or the Number of Elements (NE). NA and NE are single Numeric values as totals for a fragment. Element Counts are strings containing the type of atom and the number of occurrences in a fragment. Element Counts can be used to restrict searches on the basis of numbers of elements. It is possible to exclude elements by ELC search combinations using the Boolean NOT-Operator. This is convenient method to exclude deuterium and tritium.

Example1: Search for substances with 5 chlorine atoms

Field Name	Value
ELC	Cl5

Example2: Exclude Deuterium and Tritium from a given Hitset

Operator	Field Name	Value
	.Q01	
NOT	ELC	D*
NOT	ELC	T*

Type of Indexing:

String (phrase)

2.3.13. Number of Atoms (NA)

Description:

The field NA contains the number of atoms present in a fragment. The data for this field is taken from field FMF. Thus NA will be multiple for multifragment compounds. This field is indexed numerically and is not displayable.

Tips and Hints:

The Number of Atoms must not be confused with the Number of Elements (NE) or the Element Count (ELC). It is Numeric values that can be searched for with exact values or open and closed ranges.

Example:

Search for compounds with 20 to 30 atoms.

Field Name	Value
NA	20-30

Type of Indexing:

Numeric

2.3.14. Number of Elements (NE)

Description:

The field NE contains the number of different elements present in a fragment. The data for this field is taken from field FMF. Thus NE will be multiple for multifragment compounds. This field is indexed numerically and is not displayable. Isotopes, except deuterium and tritium, are not treated as different elements.

Tips and Hints:

The Number of Elements must not be confused with Element Count or the Number of Atoms. Since it is a Numeric value it is possible to search for exact values, open ranges and closed ranges.

Example:

Search for compounds with more than 5 different elements.

Field Name	Value
NE	>5

Type of Indexing:

Numeric

2.3.15. Number of Fragments (NF)

Description:

The field NF contains the number of different fragments present in a multifragment compound. The data for this field is taken from field FMF. Thus NF will not always be the total number of fragments. This field is indexed numerically and is not displayable.

$C_{10}H_8ClNO$ NF = 1

$C_{17}H_{23}ClN_2S * 2ClH$ NF = 2

$2C_6H_7N * C_6H_6Cl_6 * 2ClH$ NF = 3

Tips and Hints:

The NF field can be very useful in combination with the other Molecular Formula fields.

Example:

Search for compounds with five carbon atoms in three-fragment compounds.

Operator	Field Name	Value
	ELC	C5
AND	NF	3

Type of Indexing:

Numeric

2.3.16. Molecular Weight (MW)

Description:

The molecular weight is defined as the sum of the relative atomic masses of all atoms in a molecule. The Beilstein definition of the molecular weight is related to single fragments. Thus for multi-fragment compounds a MW is stored for each fragment. The content of this field is the relative molecular mass calculated from the molecular formula and the relative atomic masses of the elements for each fragment. The precision of the indexed value is 2 digits after the decimal point (e.g. 14.01).

Tips and Hints:

Searches with exact values require the input of the digits behind the point, e.g. 14.01 (not 14). If you search for ranges you may enter 144-169 if you wish to retrieve compounds from 145.00 to 169.99.

Example:

Search for compounds with a molecular weight greater than 300.

Field Name	Value
MW	>300

Type of Indexing:

Numeric

2.3.17. Fragment BRN (FBRN)

Description:

The Fragment BRN is an unambiguous identifier for the different fragments present in a multifragment compound.

It is also the accession number of a substance record in CrossFire.

This field is not searchable.

Type of Indexing:

Numeric

2.3.18. Lawson Number (LN)

Description:

The Lawson Number is a special feature related to the Beilstein Handbook registration system. Using the Lawson Number, it is possible to browse the database in terms of organic structures without involving the Structure Search System. The Lawson numbers are calculated by algorithmically segmenting the structure, whereby each fragment is automatically assigned a Lawson Number based on its structural characteristics. Usually there is more than one Lawson Number for each structure registered.

Tips and Hints:

CrossFire offers an opportunity to study the power of searching with the Lawson Number. Since a Lawson Number range defines a structural similarity it is easy to restrict search results to particular substance classes without carrying out complex substructure searches.

Searching with Lawson Numbers

Sometimes a controlled relaxation of precision in searching the database is desirable and advantageous: the experienced chemist knows that many types of information can be transferred from the particular reported case to other analogous cases. For instance, preparative methods are often equally applicable to classes of compounds, and certain physical data can be used as a starting point for estimating of missing data in the same class of compounds.

For this reason Beilstein databases are equipped with a retrieval tool for classification of structures, the LN. This number enables the searcher to investigate a family of structures; in particular the family referred to as "positional isomers". In general it is neither easy nor quick to retrieve positional isomers with traditional substructure searching, thus the LN can be regarded as an additional help to existing tools, not as a substitute.

The LN is a two-byte unsigned integer, which can take any value in the range 9 - 32759. Any particular compound may possess several LNs, one for each "chemically significant" fragment in the molecule. In general, most compounds have 2-3 LNs. An analysis of the Beilstein Database gave the following distribution:

25.1 % have 1 LN
39.4 % have 2 LNs
24.0 % have 3 LNs
8.5 % have 4 LNs
3.0 % have > 4 LNs

Thus the LN is an economical (but non-unique) Description of structural properties, since each structure is characterized by less than 5 bytes on average.

Example1:

You have found the hit pyridine-2-carboxylic acid (LN: 26332) and wish to locate positional isomers.

Operator	Field Name	Value
	LN	26332
AND	MF	C6H5NO2

The Lawson Number is a browsing tool and as with all other browsing methods false drops sometimes occur. Thus the user is sometimes confronted with a spattering of unexpected ring systems. (For instance a query based on pyridines might possibly contain a few methyl pyrroles, among the otherwise sensible hits, which would then be considered as false drops)Note that these can sometimes be filtered out by combining the search with nomenclature terms, but nomenclature alone is rarely capable of retrieving positional isomers in a dependable fashion, because of the non-systematic usage encountered in even the best of databases. For instance, not all the hits of the example above necessarily contain the nomenclature term "pyridine", since "nicotinic acid" and "isonicotinic acid" are perfectly acceptable names.

Example2:

You have found a dibenzocyclooctenone oxime (LN: 7525) and would like to find similar compounds

Operator	Field Name	Value
	LN	7525
AND	MOFO	C16*
AND	ELC	N1

Type of Indexing:

Numeric

2.3.19. Structure Keyword (STR.KW)

Description:

This field contains further information about the identity of a substance, in particular about stereochemical isomers and tautomers. The content has a controlled vocabulary. The following phrases are allowed:

- And cyclic tautomers
- And tautomers
- And valence tautomers
- And or tautomers
- Or tautomers
- Racemate
- Relative configuration
- Stereo compound
-

Type of Indexing:

String (phrase)

2.3.20. Type of Substance (STYPE)

Description:

The Type of Substance field contains the keywords from the following list of controlled terms

- aycclic
- isocyclic
- heterocyclic
- polymer (monomers given)
- polymer (monomers not given)
- biomolecule
- mixture (composition completely given)
- mixture (composition partially given)
- mixture (composition completely not given)

Type of Indexing:

String (phrase)

2.3.21. Constitution ID (CONSID)

Description:

Each stereoisomer of a compound has its own BRN. But all stereoisomers of a compound have the same Constitution ID. This will allow an easier search of all stereoisomers.

E.G.: You find a BRN, which has the Structure Keyword "Stereo Compound". To get a quick overview of the other stereoisomers in the Beilstein database you formulate a query with the Constitution ID.

Type of Indexing:

Numeric

2.3.22. Tautomer ID (TAUDID)

Description:

Each tautomer of a compound has its own BRN. But all tautomers of a compound have the same Tautomer ID.

This will allow an easier search of all tautomers.

E.G.: You want to know all sorts of tautomers of a specific BRN. To get a quick overview of the other tautomers in the Beilstein database you formulate a query with the Tautomers ID.

Type of Indexing:

Numeric

2.3.23. Composition: Comp. Name (CCN) / Composition: Comp. BRN (CCBRN)

Description:

These fields give information on composition of mixtures (composition completely or partially given), or polymer (monomers given). The hyperlinked BRNs of components, or monomers, including their related chemical names are given in the corresponding fields.

These fields are only displayable, not searchable

Type of Indexing:

String (Phrase) / Numeric

2.3.24. Composition: Comp.Conc (CCC)

Description:

For mixtures whose composition is either completely, or partially given, there is quantitative information on the concentrations of their components in mass percent or volume percent.

This field is only displayable, not searchable

Type of Indexing:

String (phrase)

2.3.25. Beilstein Reference (SO)

Description:

The field SO contains the Handbook reference of the substance if it is already published in the Beilstein Handbook. In some cases the SO field refers to Handbook volumes in print which are not published (Supplementary Series V or VI). The Beilstein Citation format consists of a four-part number:

a-bb-cc-ddddd

Example:

5-20-02-00523

A	Series	Supplementary Series EV
Bb	Volume	Volume 20
Cc	Subvolume	Subvolume 2
Ddddd	Page	Page 523

Tips and Hints:

The Beilstein Citation allows you to find information already published in the Handbook. If there is an entry without any page e.g. 6 – 17, this compound is probably not published in the Handbook. With the help of truncation Operators it is possible to select particular series, volumes, subvolumes or pages.

Type of Indexing:

String (phrase)

2.3.26. Entry Date (ED)

Description:

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

Type of Indexing:

String (phrase)

2.3.27. Update Date (UPD)

Description:

The Update Date field contains the date (year.month.day) when the last update of this compound was entered into the database.

Type of Indexing:

String (phrase)

2.4. Chemical Properties

Description:
The group Chemical Data contains information about:

Field Code	Name
RX	Reaction
RX	Reaction Details
RSTR	Related Structure
INP	Isolation From Natural Products
CDER	Derivative
PUR	Purification

Tips and Hints:
The Reactions (formally preparations and chemical behaviors) are stored in the facts Reaction Identification Data and Reaction Details. These reactions have been registered and hence assigned a Reaction Identification Number.

However, it is important to know that searches performed in the area of Reaction Identification Data and Reaction Details will result in a list of reactions.

Which methods of preparation are indexed?

Chemical or biochemical methods are only recorded when they are suitable for large-scale preparations. Preparative methods that are complicated or have low yields are acceptable only if they are new and have preparative usefulness.

A preparative method is also recorded if there is only one general method given which is applicable to the preparation of several compounds. If a preparative method has a back reference it need not be recorded if it is clear that the same compound has been prepared before by the same method. If it is suspected that the back reference relates only to an analogous preparation of another compound or a general method then the preparation is indexed. The field Reaction Classification (RX.CL) will contain the entry "Preparation".

Which other reactions (chemical behavior) are indexed?

For a reaction to be included and hence classified as "Chemical Behavior" one of the following criteria must be met.

1. There are quantitative results pertaining to the course of a reaction; at least one of the attributes presented should be listed in the field "Subject Studied" (RX.SUB).

2. The investigation of the chemical behavior of the compound is given as the object of the investigation or forms a major part of the publication (this can usually be determined from the abstract of the paper).

If the investigation of a new type of reaction forms the basis of the publication and a number of compounds were investigated and the results tabulated only the prototypes are recorded and not higher homologues or substituted compounds. This restriction applies only to qualitative results; quantitative results (e.g. kinetics) are recorded for all the compounds investigated.

Multistage Syntheses

Multistage syntheses are often reported in which the isolation and purification of the intermediate products is not described e.g. in short communicationsIf the structures of the intermediates are unambiguous the multistage preparation is split into several single step preparations so that each separate synthetic step can be searched for in the database. The intermediates get their own BRNs and structures.

Intermediates such as arynes, ozonides, Grignard-compounds, etc. do not get their own structure if the only attribute to be recorded is the preparation.

Two cases can be distinguished:

Full or complete reactions:

Educts and products are characterised by BRN's. In general structure representations are available. Only in special case (e.g. biomoleculs, polymers) structures are missing and chemical names are available instead.

Half reactions:

If not all educts or products are characterised by a BRN the reaction has the accompanying commentary "Half Reaction"

2.4.1. Reaction (RX)

Description:

The Reaction Identification Data are stored in 6 fields. These contain the keys to the unchanging structural information that has been used to register the reaction. Reactants and Products can be searched for by name or by BRN. The Reaction Identification Number is the registry number of the reaction and is hence unique.

The parameter data, such as solvent, temperature and further conditions, belonging to a particular variation of a reaction is stored in the fact Reaction Details. For any registered reaction there can be several variations present in the database whose total number is given in the field "Number of Reaction Details"

Reaction Identification Fields:

Field Code	Full Name	Type of Indexing
RX.ID	Reaction ID	Numeric
RX.RBRN	Reactant BRN	Numeric
RX.RCT	Reactant	String (phrase)
RX.PBRN	Product BRN	Numeric
RX.PRO	Product	String (phrase)
RX.NVAR	Number of Reaction Details	Numeric
RX.BCODE	Reaction Code (broad)	Numeric
RX.MCODE	Reaction Code (medium)	Numeric
RX.NCODE	Reaction Code (narrow)	Numeric
RX.ED	Reaction Entry Date	String (phrase)
RX.UPD	Reaction Update Date	String (phrase)

2.4.1.1. Reaction ID (RX.ID)

Description:

The Reaction ID is assigned when a reaction is registered for the first time in the MDL Information System. The Reaction ID is an unambiguous identifiers of a reaction. The Reaction ID is the accession number of the reaction record in Cross Fire. It is an integer, which does not contain further information.

Type of Indexing:

Numeric

2.4.1.2. Reactant BRN (RX.RBRN)

Description:

Reactants (starting materials) are defined as compounds that add at least one carbon atom to the skeleton of the products, e.g. CH_3OH in the preparation of esters or Ac_2O in an acetylation. Organic starting materials are usually registered compounds and are therefore present as title compounds with structures and data. If the starting material has no further chemical, physical or physiological data, it will still be present in the database but only have minimal "identification" data in addition to the structure.

Starting materials are searchable either by names (in the RX.RCT field) or, if present, by BRN (in the RX.RBRN field).

If a compound acts simultaneously as a starting material and a solvent, it is entered as a starting material.

Example:

Search for compounds that have been prepared from acetone (BRN unknown).

Step I

- Query input in the structure query editor

- (Structure exact)

- Display of Identification Data including the BRN

Step II

- Query input in the Facts search mask

Field Name	Value
RX.RBRN	635680

Type of Indexing:

Numeric

2.4.1.3. Reactant (RX.RCT)

Description:

Reactants (starting materials) are defined as compounds that add at least one carbon atom to the skeleton of the products, e.g. CH_3OH in the preparation of esters or Ac_2O in an acetylation. Organic starting materials are usually registered compounds and are therefore present as title compounds with structures and data. If the starting material has no further chemical, physical or physiological data, it will still be present in the database but only have minimal "identification" data in addition to the structure.

Starting materials are searchable either by names (in the RX.RCT field) or, if present, by BRN (in the RX.RBRN field).

If a compound acts simultaneously as a starting material and a solvent, it is entered as a starting material.

Type of Indexing:

String (phrase)

2.4.1.4. Product BRN (RX.PBRN)

Description:

Reaction products are usually registered compounds and are therefore present as title compounds with structures and data. If the product has no further chemical, physical or physiological data, it will still be present in the database but only have minimal "identification" data in addition to the structure.

Information on reaction products is given in form of the hyperlinked BRN numbers (RX.BRN) together with the related chemical names (RX.PRO).

Type of Indexing:

Numeric

2.4.1.5. Product (RX.PRO)

Description:

Reaction products are usually registered compounds and are therefore present as title compounds with structures and data. If the product has no further chemical, physical or physiological data, it will still be present in the database but only have minimal "identification" data in addition to the structure.

Information on reaction products is given in form of the hyperlinked BRN numbers (RX.BRN) together with the related chemical names (RX.PRO).

Type of Indexing:

String (phrase)

2.4.1.6. No. Of Reaction Details (RX.NVAR)

Description:

This field gives the information of the number of reaction details.

Type of Indexing:
Numeric

2.4.1.7. Reaction Class Codes

Broad Class Code (RX.BCODE)

Medium Class Code (RX.MCODE)

Narrow Class Code (RX.NCODE)

Description:

Reactions in Beilstein Database are processed with InfoChem's Reaction Classfication Algorithm "CLASSIFY". CLASSIFY categorizes reactions according to the type of chemical transformation they represent.

The indexing is based on changes occurring at atoms and bonds involved in the reaction (reaction center) and the immediate vicinity (alpha and beta atoms) and is expressed as a hashcode (ClassCode).

Two reactions are analyzed and get the same ClassCodes:

- Reaction ClassCode "Broad" when only reaction centers are same
- Reaction ClassCode "Medium" when reaction centers and alpha atoms and bonds are same
- Reaction ClassCode "Narrow" when reaction centers and alpha + beta atoms and bonds are same

The resulting reaction "ClassCodes" may be used to:

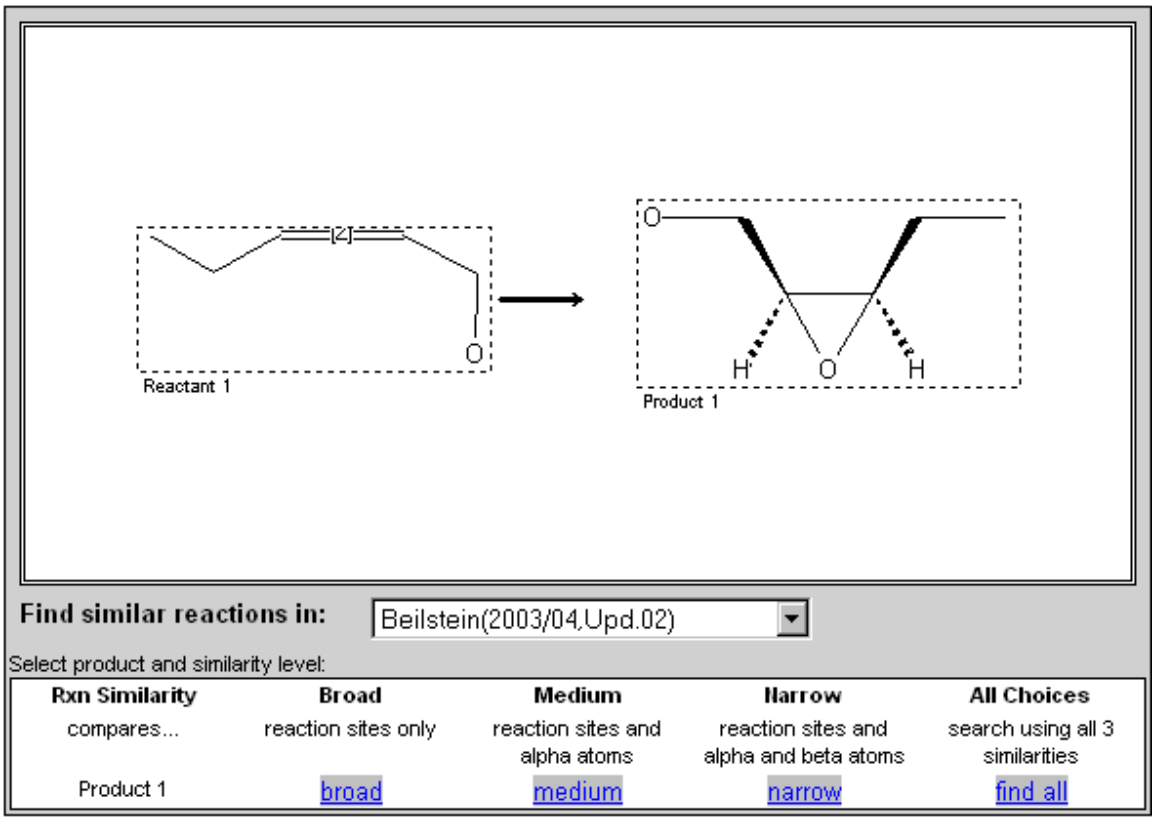
- Clustering reactions of the same type
- Post-management of large hitlists
- Facilitating query formulation (Transformation Searches)
- Linking to reactions in other MDL reaction databases like IMRW or Beilstein, which also have InfoChem ClassCodes

Type of Indexing:

Numeric

Hint:

In general, the class code search is not done by a numerical search, but by using a hyperlink within the results view:



2.4.1.8. Reaction Entry Date (RX.ED)

Description:

The search field Reaction Entry Date contains the date (year/month/day) when the reaction was first entered into the database. Dates have to be searched with a fixed format: yyyy/mm/dd.

Type of Indexing:

String (phrase)

2.4.1.9. Reaction Update Date (RX.UPD)

Description:

The search field Reaction 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)

2.4.2. Reaction Details (RX)

Reaction Detail Fields:

Field Code	Full Name	Type of Indexing	Unit
RX.CL	Reaction Classification	String (phrase)	
RX.YD	Yield	String (phrase)	
RX.NYD	Yield Numeric	Numeric (range)	
RX.SNR	No. of Stages	Numeric	
RX.RGT	Reagent	String (phrase)	
RX.CAT	Catalyst	String (phrase)	
RX.SOL	Solvent	String (phrase)	
RX.RCS	Index Reagents/Catalysts/Solvents	String (phrase)	
RX.TIM	Time	String (phrase)	
RX.T	Temperature	Numeric (range)	°C
RX.P	Pressure	Numeric (range)	Torr
RX.PH	pH-Value	Numeric (range)	
RX.COND	Other Conditions	String (wordwise)	
RX.SUB	Subject Studied	String (phrase)	
RX.TYP	Reaction Type	String (phrase)	
RX.PRT	Prototype Reaction	String (phrase)	
RX.DED	Entry Date	String (phrase)	

2.4.2.1. Reaction Classification (RX.CL)

Description:

A reaction in the Beilstein database is classified either as “Preparation" or "Chemical behavior" depending on whether the preparative methods of a specific compound or its chemical behaviors are the aim of the investigation.

Multistage reactions are a special type of preparations. The details for several reaction steps are given.

A further classification is between reactions and "Half reactions".

Reactions are defined by the fact, that all reactants (educts and products) are characterized by the BRN.

Half reactions are defined by the fact, that either only educts or only products are characterized by a BRN.

Type of Indexing:

String (phrase)

2.4.2.2. Yield (RX.YD)

Description:

The yields of products are stored in this field. Only the yield for the pure product quoted by the author is accepted (no crude yields). With ranges e.g. 70-85% the highest value (85%) is given. The yields must always refer to the registered starting material. Beside the relative yields in percent (% input, % turnover and % spectr.) also absolute yields (mg, g, kg) are included.

Type of Indexing:

String (phrase)

2.4.2.3. Yield Numeric (RX.NYD)

Description:

The yields of products are stored in this field. Only the yield for the pure product quoted by the author is accepted (no crude yields). With ranges e.g. 70-85% the highest value (85%) is given. The yields must always refer to the registered starting material. Beside the relative yields in percent (% input, % turnover and % spectr.) also absolute yields (mg, g, kg) are included.

From within this fields Numeric yield search is possible. This allows better refinements of reaction searching.

Example:

Search for the preparation of 4-bromo-benzyl bromide (BRN=606498) with the restriction to reactions with 70 to 100% yield.

Operator	Field Name	Value
	RX.PBRN	606498
AND	RX.NYD	70-100

Type of Indexing:

Numeric (range)

2.4.2.4. No. of Stages (RX.SNR)

Description:

This field gives the number of stages in case of a multistage reaction.

Type of Indexing:

Numeric

2.4.2.5. Reagent (RX.RGT)

Description:

Reagents are compounds, which take part in the reaction but do not contribute to the carbon skeleton of the product, e.g. halogenating agents (NBS), reducing agents ($LiAlH_4$), or oxidizing agents ($Pb(OAc)_4$). If a compound acts simultaneously as a reagent and a solvent it is entered as a reagent. It is often difficult to decide whether a substance acts as a reagent (RX.RGT) or as a catalyst (RX.CAT), thus it is recommended to search in both of the fields. If a series of experiments, e.g. oxidizing agents is tried during an investigation only the one with the highest yield is indexed.

Type of Indexing:

String (phrase)

2.4.2.6. Catalyst (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. If it is not clear from the publication whether the compound is used as a reagent or a catalyst it is entered as a reagent. In investigations involving different catalysts the same procedure may be followed as with reagents.

Type of Indexing:

String (phrase)

2.4.2.7. Solvent (RX.SOL)

Description:

This field contains information on the solvent or the solvent mixture used in the reaction. If a compound acts simultaneously as a reactant (starting material) and a solvent, it is entered as a starting material, and not as a solvent.

Type of Indexing:

String (phrase)

2.4.2.8. Index Reagents/Catalysts/Solvent (RX.RCS)

Description:

This is a common index concerning reagents (RX.RGT), catalysts (RX.CAT) and solvents (RX.SOL). Searching this common index is useful to be comprehensive in your search results. It is often difficult to decide whether a substance acts as a reagent or as a catalyst or as solvent, thus it is recommended to search in both of the fields.

Type of Indexing:

Word and phrase

2.4.2.9. Time (RX.TIM)

Description:
The time taken for the reaction is entered in this field.

Type of Indexing:

String (phrase)

2.4.2.10. Temperature (RX.T)

Description:
The temperature at which the reaction took place is entered in this field.

Type of Indexing:

Numeric (range)

2.4.2.11. Pressure (RX.P)

Description:
The pressure (range) at which the reaction took place is entered in this field.

Type of Indexing:

Numeric (range)

2.4.2.12. pH-Value (RX.PH)

Description:
The pH-value at which the reaction took place is entered in this field.

Type of Indexing:

Numeric (range)

2.4.2.13. Other Conditions (RX.COND)

Description:

Entries in the field Other Conditions are only given when there is important information that cannot be input in the other parameter fields, e.g. heating, UV-irradiation. Particularly in the Description of biochemical methods of preparation the biologically active materials (e.g. fungi, ferments, etc.) are entered in this field. If the preparation is a multi-step reaction which cannot be broken down into its constituent steps then the reaction conditions for each step are given here in a condensed form.

Type of Indexing:

String (wordwise)

2.4.2.14. Subject Studied (RX.SUB)

Description:

This field is present for the reaction classification "Chemical behavior".

The list contains the following attributes:

- Rate constant
- Product distribution
- Equilibrium constant
- Quantum yield
- Kinetics
- Mechanism
- Thermodynamic data
- Reactivity
- Activation energy
- G-values
- Enzyme kinetics

The attributes thermodynamic data, equilibrium constant, enzyme kinetics, product distribution, and kinetics are accepted as keywords if quantitative results are available.

Type of Indexing:

String (phrase)

2.4.2.15. Reaction Type (RX.TYP)

Description:

This field contains information on the reaction types assigned to a reaction, e.g. alkylation, esterification or name reactions such as Mannich Reaction, Clemmensen Reduction.

Type of Indexing:

String (phrase)

2.4.2.16. Prototype Reaction (RX.PRT)

Description:

This field is in use for the reaction classification "Chemical behavior". It indicates that the recorded reaction conditions (solvent, temperature, pH-value) refer to the prototype reaction of a series of experiments. Further variations of the reaction conditions are entered in this field.

Type of Indexing:

String (wordwise)

2.4.2.17. Entry Date (RX.DED)

Description:

The search field Reaction Entry Date contains the date (year/month/day) when the reaction details were first entered into the database. Dates have to be searched with a fixed format: yyyy/mm/dd.

Type of Indexing:

String (phrase)

2.4.3. Related Structure (RSTR)

Description:

The Related Structure field contains the Beilstein Registry Numbers (BRN) assigned to substances when a new investigation of the cited compound yields different results, e.g. regarding stereochemistry. The entry contains information about the earlier literature reference and a note as to whether the constitution or configuration assigned to the title compound is wrong or doubtful.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
RSTR.PB	Referenced BRN	Numeric
RSTR.PA	Referenced Compound	String (wordwise)

Type of Indexing:

String (wordwise)

2.4.4. Isolation from Natural Product (INP)

Description:

The Isolation from Natural Product field contains names of the source in nature (plant, fungus, animal etc.) or an industrial grade natural product from which compounds have been isolated. Sources are only recorded when a compound has been isolated. The identification of well-known compounds by instrumental methods (e.g. GLC, TLC) as components of natural or synthetic products is not recorded here (e.g. the identification of pentan-2-one in tobacco smoke or limonene in the ethereal oils of a rare plant or saccharose as a component of a tree-bark extract). Terms do not belong to a controlled vocabulary; specific names (e.g. the systematic name of the plant or animal) are used when they are available.

Example:

Search for substances, which have been isolated from iris.

Field Name	Value
INP	iris

Type of Indexing:

String (wordwise)

2.4.5. Derivative (CDER)

Description:

Characterization derivatives (hydrazones, oximes) and addition compounds (salts, complexes, adducts, associations, clathrates) are recorded as individual compounds with all their data if they fulfill the Criteria for the Acceptance of a compound given above.

In other cases, the Derivative field CDER contains chemical names and additional information about derivatives of the cited substance (e.g. salt names, salt molecular formulae, and melting point of derivatives). The Beilstein Registry Number of the derivative can be searched in the parameter field CDER.BRN.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
CDER.BRN	Derivative BRN	Numeric
CDER	Derivative	String (wordwise)

2.4.6. Purification (PUR)

Description:

The Purification field contains words and phrases that describe the method of purification of a substance.

Tips and Hints:

Comments on the purification of a compound are only accepted when the work, or a large section of it, contains unusual purification methods for the compound in question. Natural occurrence and isolation from natural products are entered under INP (Isolation from Natural Products). The resolution of racemates does not count as an independent preparation. This is entered under the Description of the preparation of the antipodes (via the racemate) as a method of purification.

Type of Indexing:

String (phrase)

2.5. Physical Properties (PHY)

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

Acceptance Criteria:
Data on compounds that are frequently met in the original literature will only be recorded if they are associated with precise measurements (the object of investigation) or if, according to the author, the measurements have been made for the first time.

Values which have been calculated by classical (not quantum mechanical) methods or which come from experimentally measured data have also been accepted, e.g. fundamental frequencies of vibrations, force constants, statistically calculated heat capacity, enthalpy of vaporization (calculated from vapour pressure), melting points extrapolated to 100 % purity etc.

In those cases where comparable calculated and experimentally determined values were mentioned in the abstracted article, the experimental values, or corresponding keywords have been recorded.

The Physical Properties group field is divided into two main categories:

Single-Component System (SCS)

Structure and Energy Parameters (SEP)

Physical State (SAG)

Transport Phenomena (TRA)

Thermochemical Data (THE)

Optical Properties (OPTP)

Spectroscopic Information (SPE)

Magnetic Properties (MAGP)

Electrical Properties (ELEP)

Electrochemical Behaviour (ECB)

Safety Data (SF)

Further Information (FINFO)

Multi-Component Systems (MCS)

Solution Behavior (MCS) (SOL)

Liquid/Vapour Systems (MCS) (LVS)

Liquid/Liquid Systems (MCS) (LLSM)

Liquid/Solid Systems (MCS) (LSSM)

Mechanical & Physical Properties (MCS) (MECM)

Transport Phenomena (MCS) (TRAM)

Energy Data (MCS) (ENEM)

Electrical Data (EDM)

Optical Data (ODM)

Boundary Surface Phenomena (MCS) (BSPM)

Adsorption (MCS) (ADSM)

Association (MCS) (ASSM)

2.5.1. Single-Component Systems (SCS)

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

2.5.1.1. Structure and Energy Parameter (SEP)

Description:

This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database concerned with structure and energy parameters.

Conformation (CNF)

Interatomic Distances and Angles (IDA)

Electrical Moment (EM)

Electrical Polarizability (ELP)

Molecular Deformation (DFM)

Energy Barriers (EBC)

Dissociation Energy (EDIS)

Ionization Potential (IP)

Electron Binding (CIP)

2.5.1.1.1. Conformation (CNF)

Description:

Conformations are defined as spatial arrangements of the atoms in a molecule, which can be interconverted by rotation about a single bond. You find associated information about thermochemical data in the field Object of Investigation (CNF.OBJ).

Type of Indexing:

String (phrase)

2.5.1.1.2. Interatomic Distances and Angles (IDA)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
IDA.KW	Description	String (phrase)

Type of Indexing:
Group Code

2.5.1.1.3. Interatomic Distances and Angles Description (IDA.KW)

Description:

The field IDA.KW contains the keywords from the following list of controlled terms:

- Electron distribution
- Interatomic distances and angles

Type of Indexing:

String (phrase)

2.5.1.1.4. Electrical Moment (EM)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
EM.KW	Description	String (phrase)
EM.T	Temperature	Numeric (range)
EM.MET	Method	String (phrase)
EM.SOL	Solvent	String (phrase)

Type of Indexing:
Numeric (range)

2.5.1.1.5. Electrical Moment Description (EM.KW)

Description:

This field contains the keywords from the following list of controlled terms:

- Bond moment
- Dipole moment
- Quadrupole moment
- Hexadecapole moment
- Octopole moment

Type of Indexing:

String (phrase)

2.5.1.1.6. Electrical Polarizability (ELP)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
ELP.KW	Description	String (phrase)

Type of Indexing:
Group Code

2.5.1.1.7. Electrical Polarizability Description (ELP.KW)

Description:

This field contains the keywords from the following list of controlled terms:

- Electron polarization
- Atom polarization
- Molar polarization
- Optical anisotropy
- Polarizability
- Hyperpolarizability

Type of Indexing:

String (phrase)

2.5.1.1.8. Molecular Deformation (DFM)

Description:
This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
DFM.KW	Description	String (phrase)

Type of Indexing:
String (phrase)

2.5.1.1.9. Molecular Deformation Description (DFM.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Fundamental vibrations
- Force constants
- Rotational constants
- Centrifugal distortion constant(s)
- Coriolis coupling constant(s)

Type of Indexing:
String (phrase)

2.5.1.1.10. Energy Barriers (EBC)

Description:

The Energy Barrier field contains the values for the amount of energy required to convert one conformation of a molecule to another where both conformations represent energy minima. Conformations are defined as spatial arrangements of the atoms in a molecule, which can be interconverted by rotation about a single bond. You can search for the associated information about the bond type using the parameter field code EBC.TYP.

Unit:
The default unit in the Beilstein database for this fact is J mol^{-1}.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
EBC.TYP	Barrier Type	String (phrase)
EBC.SOL	Solvent	String (phrase)

Type of Indexing:

Numeric (range)

2.5.1.1.11. Dissociation Energy (EDIS)

Description:

The dissociation energy is defined as the energy required breaking a specific bond in one mol of a compound to produce two fragments. You can search for the associated information about the bond type using the parameter field code EDIS.TYP.

Unit:
The default unit for this fact is J mol^{-1}.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
EDIS.TYP	Bond Type	String (phrase)

Example:

Field Name	Value
EDIS.TYP	N-H

Type of Indexing:

Numeric (range)

2.5.1.1.12. Ionization Potential (IP)

Description:

The ionization potential is defined as the energy per unit charge required to completely removing an electron from an atom or molecule to an infinite distance. The Ionization Potential search field contains the energy values and measurement methods. You can search for the associated information using the parameter field code IP.MET.

Unit:
The default unit in the Beilstein database for this fact is eV.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing
IP.MET	Method	String (phrase)

Example:

Field Name	Value
IP	9.77-11.22

Type of Indexing:

Numeric (range)

2.5.1.1.13. Electron Binding (CIP)

Description:

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
CIP.KW	Description	String (phrase)
CIP.ED	Entry Date	String (phrase)

Type of Indexing:
Group Code

2.5.1.1.14. Electron Binding Description (CIP.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Electron affinity
- Core IP

Type of Indexing:

String (phrase)

2.5.1.2. Physical State (SAG)

Description:

This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database concerned with the physical state, that is: crystals, liquids gases and other physical & mechanical properties.

Crystals (CRY)

Crystal Property Description: Colour & Other Properties (CPD)

Melting Point (MP)

Crystal Phase (CRYPH)

Decomposition (DP)

Sublimation (SP)

Triple Point (TP)

Transition Point(s) of Crystalline Modification(s) (CPTP)

Crystal System (CSYS)

Space Group (CSG)

Density Of Crystal (CDEN)

Liquids (LIQ)

Boiling Point (BP)

Liquid Phase (LIQPH)

Transition Point(s) of Liquid Modification(s) (LPTP)

Gases (GAS)

Critical Temperature (CRT)

Critical Pressure (CRP)

Critical Density (CRD)

Critical Volume (CRV)

Vapour Pressure (VP)

Gas Phase (GP)

Other Physical and Mechanical Properties (MECP)

Density of the Liquid (DEN)

Mechanical Properties (MEC)

Compressibility (COMP)

Sound Properties (SOUND)

Surface Tension (ST)

2.5.1.2.1. Crystals (CRY)

Description:

This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database concerned with crystallographic data.

Crystal Property Description (CPD)

Melting Point (MP)

Crystal Phase (CRYPH)

Decomposition (DP)

Sublimation (SP)

Triple Point (TP)

Transition Point(s) of Crystalline Modification(s) (CPTP)

Crystal System (CSYS)

Space Group (CSG)

Density of Crystal (CDEN)

Type of Indexing:

Group Code

2.5.1.2.1.1. Crystal Property Description (CPD)

Description:

The Crystal Property Description field contains terms that give a qualitative description of the outward appearance of crystalline materials such as the colour of the crystal and its shape. The crystal property description is searched using terms that describe the crystal.

Type of Indexing:

String (phrase)

2.5.1.2.1.2. Melting Point (MP)

Description:

The melting or freezing point of a pure substance is the temperature at which its crystals are in equilibrium with the liquid phase at atmospheric temperature. You can search for the associated information about the solvent from which the material whose melting point is mentioned was crystallized using the parameter field code MP.SOL.

Unit:

The default unit in the Beilstein database for this fact is ºC.

Type of Indexing:

Numeric (range)

Associated Parameter Field:

Field Code	Full Name	Type of Indexing
MP.SOL	Solvent	String (phrase)

Example:

Operator	Field Name	Value
	MP	150-170
PROXIMITY	MP.SOL	ethanol

Type of Indexing:

Numeric (range)

2.5.1.2.1.3. Crystal Phase (CRYPH)

Description:

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
CRYPH.KW	Description	String (phrase)	
CRYPH.T	Temperature	Numeric range	ºC

Type of Indexing:
Group Code

2.5.1.2.1.4. Crystal Phase Description (CRYPH.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Rate of crystallization
- Polymorphism
- Rate of transition
- Crystal habit
- Crystal growth
- Crystal morphology
- Crystal structure determination
- Interplanar spacing
- Association in the solid state
- Solid state structure properties
- Melting pressure
- Freezing point
- Glass transition temperature
- Phase diagram
- Long spacing
- Reorientation in the solid state

- Spin polarization
- Nuclear spin conversion
- Structure of the solid
- Dimensions of the unit cell

Type of Indexing:

String (phrase)

2.5.1.2.1.5. Decomposition (DP)

Description:

The decomposition point is the temperature at which a substance undergoes thermal decomposition at atmospheric pressure. You can search for the solvent in the associated parameter field DP.SOL.

Unit:
The default unit in the Beilstein database for this fact is ºC.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing
DP.SOL	Solvent	String (phrase)

Example:

Operator	Field Name	Value
	DP	150
PROXIMITY	DP.SOL	petroleum ether

Type of Indexing:
Numeric (range)

2.5.1.2.1.6. Sublimation (SP)

Description:
The sublimation point is defined as the temperature at which the vapour pressure above a solid is equal to a specified pressure. You can search for the associated information about the pressure at which the measurement was made using the parameter field code SP.P.

Unit:
The default unit is ºC.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
SP.P	Pressure	Numeric (range)	Torr

Example:

Operator	Field Name	Value
	SP	100-150
PROXIMITY	SP.P	0.001

Type of Indexing:
Numeric (range)

2.5.1.2.1.7. Triple Point (TP)

Description:
The triple point is the point in a phase diagram where three phases of a substance exist at equilibrium and is fully defined by the temperature and pressure at that point. The Triple Point field contains the temperature values for the substances.

Unit:
The default unit in the Beilstein database for this fact is ºC.

Type of Indexing:
Numeric (range)

2.5.1.2.1.8. Transition Point(s) of Crystalline Modification(s) (CPTP)

Description:
The Transition Point of Crystalline Modification field contains the temperature at which two crystal phases (cubic, hexagonal, tetragonal, monoclinic, triclinic, trigonal and rhombic) are in equilibrium at a specified pressure.

Unit:
The default unit in the Beilstein database for this fact is ºC.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing
CPTP.CM	Change of Modification	String (wordwise)

Type of Indexing:
Numeric (range)

2.5.1.2.1.9. Crystal System (CSYS)

Description:

The Crystal System field contains information on the seven crystal classes cubic, hexagonal, trigonal, tetragonal, monoclinic, triclinic and rhombic. You can search in the Crystal System field using the class name of the crystal system of interest.

Example:

Field Name	Value
CSYS	rhombic

Type of Indexing:

String (phrase)

2.5.1.2.1.10. Space Group (CSG)

Description:

The Space Group field contains information on the different crystal space groups using the relevant terms.

Type of Indexing:

String (phrase)

2.5.1.2.1.11. Density of the Crystal (CDEN)

Description:

The field contains the Numeric value of the density of the substance in the crystalline state at a particular temperature.

Unit:

The default unit in the Beilstein database for this fact is g cm^{-3}.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing
CDEN.T	Temperature	Numeric (range)

Type of Indexing:

Numeric (range)

2.5.1.2.2. Liquids (LIQ)

Description:

This field identifier is a group code for Field Availability searches concerned with the properties of liquids in the hierarchical system of the Beilstein database.

- Boiling Point (BP)
- Liquid Phase (LIQPH)
- Transition Point(s) of Liquid Modification(s) (LPTP)

Type of Indexing:

Group Code

2.5.1.2.2.1. Boiling Point (BP)

Description:

The boiling point is defined as the temperature at which the vapour pressure of a liquid is equal to a specified pressure. Because of the dependence of the boiling point on the pressure, boiling points with undefined statements about pressure and with inexact qualifiers have not been entered. The pressures can be searched for in the BP.P parameter field.

Unit:

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

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
BP.P	Pressure	Numeric (range)	Torr

Example:

Operator	Field Name	Value
	BP	150-170
PROXIMITY	BP.P	760

Type of Indexing:

Numeric (range)

2.5.1.2.2.2. Liquid Phase (LIQPH)

Description:

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
LIQPH.KW	Description	String (phrase)

Type of Indexing:
Group Code

2.5.1.2.2.3. Liquid Phase Description (LIQPH.KW)

Description:

This field contains keywords from a list of controlled terms:

- Rate of evaporation
- Supercoolability
- Structure of the liquid
- Radial distribution function
- Association in the liquid state
- Self-association in solution
- Relaxation time for reorientation
- Rotational correlation time
- Liquid-crystalline properties
- Rotational correlation function of the liquid
- Correlation function of the liquid
- Order parameter
- Liquid-crystalline transition temperatures

Type of Indexing:

String (phrase)

2.5.1.2.2.4. Transition Point(s) of Liquid Modification(s) (LPTP)

Description:

The temperature at which compounds undergo phase transition in the liquid phase is called the liquid phase transition point. The LPTP field contains the temperature values for the substances. The names of the phases (i.e. nematic, isotropic, crystalline, cholesteric, etc.) are given in the note field.

Unit:

The default unit in the Beilstein database for this fact is ºC.

Type of Indexing:

Numeric (range)

2.5.1.2.3. Gases (GAS)

Description:

This field identifier is a group code for Field Availability searches concerned with the characteristic behaviour of gases, in the hierarchical system of the Beilstein database.

- Critical Temperature (CRT)
- Critical Pressure (CRP)
- Critical Density (CRD)
- Critical Volume (CRV)
- Vapour Pressure (VP)
- Gas Phase (GP)

Type of Indexing:

Group Code

2.5.1.2.3.1. Critical Temperature (CRT)

Description:

The critical temperature is the temperature above which a gas cannot be liquefied by pressure. The Critical Temperature field contains the values of the critical temperature for the substance.

Unit:

The default unit in the Beilstein database for this fact is ºC.

Type of Indexing:

Numeric (range)

2.5.1.2.3.2. Critical Pressure (CRP)

Description:

The critical pressure is the minimum pressure required liquefying a gas at its critical temperature. The Critical Pressure field contains the value of the critical pressure for the substance.

Unit:

The default unit in the Beilstein database for this fact is Torr.

Example:

Field Name	Value
CRP	290000-300000

Type of Indexing:

Numeric (range)

2.5.1.2.3.3. Critical Density (CRD)

Description:

The Critical Density field contains the Numeric value for the density of a substance measured at its critical temperature and pressure.

Unit:

The default unit in the Beilstein database for this fact is g cm^{-3}.

Type of Indexing:

Numeric (range)

2.5.1.2.3.4. Critical Volume (CRV)

Description:

The Critical Volume field contains values for the molar volumes of substances measured at their critical pressures and critical temperatures.

Unit:

The default unit in the Beilstein database for this fact is cm^3 mol^{-1}.

Type of Indexing:

Numeric (range)

2.5.1.2.3.5. Vapour Pressure (VP)

Description:

The vapour pressure of a pure liquid or solid is the pressure of the vapour that is in equilibrium with it at a given temperature. You can search for the associated temperature using the parameter field code VP.T.

Unit:

The default unit in the Beilstein database for this fact is Torr.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
VP.T	Temperature	Numeric (range)	ºC

Example:

Operator	Field Name	Value
	VP	>300
PROXIMITY	VP.T	80-85

Type of Indexing:

Numeric (range)

2.5.1.2.3.6. Gas Phase (GP)

Description:

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
GP.KW	Description	String (phrase)

Type of Indexing:

Group Code

2.5.1.2.3.7. Gas Phase Description (GP.KW)

Description:

This field contains keywords from a list of controlled terms:

- Fugacity
- Rotational correlation function of the gas
- Neutron scattering of the gas
- Association in the gas phase

Type of Indexing:

String (phrase)

2.5.1.2.4. Other Physical and Mechanical Properties (MECP)

Description:

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

- Density of the Liquid (DEN)
- Mechanical Properties (MEC)
- Compressibility (COMP)
- Sound Properties (SOUND)
- Surface Tension (ST)

Type of Indexing:

Group Code

2.5.1.2.4.1. Density of the Liquid (DEN)

Description:

Density is defined as mass per unit volume at a particular temperature and pressure. The Density field contains values for the crystal density at 1 atm or below and liquid density at 1 atm when below normal boiling point, at saturation pressure at and above normal boiling point. Because the density varies with the temperature, you can search for the associated measurement temperature and reference temperature in the parameter fields DEN.T and DEN.RT.

Unit:
The default unit in the Beilstein database for this fact is g cm^{-3}.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
DEN.RT	Reference Temp.	Numeric (range)	ºC
DEN.T	Measurement Temp.	Numeric (range)	ºC

Example:

Operator	Field Name	Value
	DEN	0.8-0.9
PROXIMITY	DEN.T	20

Type of Indexing:
Numeric (range)

2.5.1.2.4.2. Mechanical Properties (MEC)

Description:
This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
MEC.KW	Description	String (phrase)

Type of Indexing:
Group Code

2.5.1.2.4.3. Mechanical Properties Description (MEC.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Specific volume
- Volume change on melting
- PVT relationship
- Virial coefficients of the equation of state
- Internal pressure
- Elasticity constants
- Compressibility

- Viscosity
- Molar volume
- Second virial coefficient of the equation of state
- Third virial coefficient of the equation of state
- Fourth virial coefficient of the equation of state

Type of Indexing:
String (phrase)

2.5.1.2.4.4. Compressibility (COMP)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
COMP.KW	Description	String (phrase)

Type of Indexing:
Group Code

2.5.1.2.4.5. Compressibility Description (COMP.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Adiabatic compressibility
- Isothermal compressibility
-

Type of Indexing:

String (phrase)

2.5.1.2.4.6. Sound Properties (SOUND)

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

Search fields:

Field Code	Full Name	Type of Indexing
SOUND.KW	Description	String (phrase)

Type of Indexing:
Group Code

2.5.1.2.4.7. Sound Properties Description (SOUND.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Velocity of sound
- Sound absorption
- Acoustic relaxation
- Ultrasonic properties
- Ultrasonic velocity
- Hypersonic velocity
- Ultrasonic absorption
- Hypersonic absorption

Type of Indexing:

String (phrase)

2.5.1.2.4.8. Surface Tension (ST)

Description:

Surface tension is the force per unit length required to create a new unit area of gas-liquid interface. You can search for information about the associated temperature using the parameter field code ST.T.

Unit:
The default unit in the Beilstein database for this fact is g s^{-2}.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
ST.T	Temperature	Numeric (range)	°C

Example:

Field Name	Value
ST	10-20

Type of Indexing:
Numeric (range)

2.5.1.3. Transport Phenomena (TRA)

Description:

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

- Viscosity (VIS)
- Self-diffusion (SDIF)
- Transport Data (TD)

Type of Indexing:

Group Code

2.5.1.3.1. Viscosity (VIS)

Description:

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

- Dynamic Viscosity (DV)
- Kinematic Viscosity (KV)
- Bulk Viscosity (BV)

Type of Indexing:

Group Code

2.5.1.3.1.1. Dynamic Viscosity (DV)

Description:

Dynamic viscosity is the ratio of the shearing stress to the rate of shear. 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 DV.T.

Unit:

The default unit in the Beilstein database for this fact is g . cm^{-1} s^{-1}.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
DV.T	Temperature	Numeric (range)	ºC

Type of Indexing:

Numeric (range)

2.5.1.3.1.2. Kinematic Viscosity (KV)

Description:

Kinematic viscosity is a coefficient defined as the ratio of the dynamic viscosity of a fluid to its density. The values are given at specified temperatures. These temperatures can be searched using the associated parameter field code KV.T.

Unit:

The default unit in the Beilstein database for this fact is cm^2 s^{-1}.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
KV.T	Temperature	Numeric (range)	ºC

Type of Indexing:

Numeric (range)

2.5.1.3.1.3. Bulk Viscosity (BV)

Description:

Bulk viscosity is the force per unit area required to maintain unit difference of velocity between two layers 1 cm apart. The values are given at the measurement temperatures and can be searched using the associated parameter field code BV.T.

Unit:

The default unit in the CrossFire database for this fact is g cm^{-1} s^{-1}.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
BV.T	Temperature	Numeric (range)	ºC

Type of Indexing:

Numeric (range)

2.5.1.3.2. Self-Diffusion (SDIF)

Description:

Self-diffusion is defined as the mutual diffusion caused by a concentration gradient (autodiffusion). The values are given at specified temperatures. You can search for this associated information using the parameter field code SDIF.T.

Unit:

The default unit in the Beilstein database for this fact is cm^2 s^{-1}.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
SDIF.T	Temperature	Numeric (range)	ºC

Type of Indexing:

Numeric (range)

2.5.1.3.3. Transport Data (TD)

Description:
This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
TD.KW	Description	String (phrase)

Type of Indexing:
Group Code

2.5.1.3.4. Transport Data Description (TD.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Thermal conductivity
- Rotational diffusion constant(s)
- Thermal diffusion

Type of Indexing:

String (phrase)

2.5.1.4. Thermochemical Data (THE)

Description:

This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database, concerned with:

- Enthalpy (HEA)
- Heat Capacity (CAP)
- Other Thermochemical Data (OTHE)

Type of Indexing:

Group Code

2.5.1.4.1. Enthalpy (HEA)

Description:

This field identifier is a group code for Field Availability searches concerned with enthalpy data in the hierarchical system of the Beilstein database.

Enthalpy of Combustion (HCOM)

Enthalpy of Formation (HFOR)

Enthalpy of Hydrogenation (HHDG)

Enthalpy of Fusion (HFUS)

Enthalpy of Vaporization (HVAP)

Enthalpy of Sublimation (HSP)

Enthalpies of Other Phase Transitions (HPTP)

Type of Indexing:

Group Code

2.5.1.4.1.1. Enthalpy of Combustion (HCOM)

Description:

The enthalpy of combustion is the change in enthalpy, which occurs when one mol of a compound reacts completely with an excess of oxygen at atmospheric pressure and at room temperature, the products being in their natural physical state under these conditions. The values are given at specified temperatures and pressures. You can search for this associated information using the parameter field codes HCOM.T and HCOM.P. The default values are 25 centigrade at 760 Torr.

Unit:

The default unit in the Beilstein database for this fact is J mol^{-1}.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
HCOM.T	Temperature	Numeric (range)	ºC
HCOM.P	Pressure	Numeric (range)	Torr

Example:

Operator	Field Name	Value
	HCOM	-6000000 - 5000000
PROXIMITY	HCOM.T	25

Type of Indexing:

Numeric (range)

2.5.1.4.1.2. Enthalpy of Formation (HFOR)

Description:

The enthalpy of formation is the change in enthalpy, which occurs when one mol of the compound is formed from its elements each being in its natural state at ordinary temperature and pressure. The values are given at specific temperatures and pressures and can be searched using the parameter field codes HFOR.T and HFOR.P.

Unit: The default unit in the Beilstein database for this fact is J mol^{-1}.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
HFOR.T	Temperature	Numeric (range)	ºC
HFOR.P	Pressure	Numeric (range)	Torr

Example:

Operator	Field Name	Value
	HFOR	>50000
PROXIMITY	HFOR.T	25

Type of Indexing:

Numeric (range)

2.5.1.4.1.3. Enthalpy of Hydrogenation (HHDG)

Description:

Enthalpy of hydrogenation is defined as the change in enthalpy, which occurs when one mol of an unsaturated compound reacts with an excess of hydrogen to become fully saturated at atmospheric pressure and room temperature the reactants and products being in their natural states under these conditions. The values are given at specified temperatures. This field may be linked to associated chemical name or BRN of the saturated compound. You can search for this associated information using the parameter field codes HHDG.BRN, HHDG.CN and HHDG.T.

Unit: The default unit in the Beilstein database for this fact is J mol^{-1}.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
HHDG.BRN	Product BRN	Numeric	
HHDG.CN	Product Name	String (wordwise)	
HHDG.T	Temperature	Numeric (range)	ºC

Type of Indexing:

Numeric (range)

2.5.1.4.1.4. Enthalpy of Fusion (HFUS)

Description:

The enthalpy of fusion is the change in enthalpy, which occurs when one mol of solid is converted to a liquid at a constant temperature.

Unit:

The default unit in the Beilstein database for this fact is J mol^{-1}.

Example:

Field Name	Value
HFUS	40000 - 50000

Type of Indexing:

Numeric (range)

2.5.1.4.1.5. Enthalpy of Vaporization (HVAP)

Description:

The enthalpy of vaporization is the enthalpy change, which occurs when one mol of a liquid is converted to a vapour at a constant temperature. The values in this search field are cited at specified temperatures and pressures. You can search for this associated information using the parameter field codes HVP.T and HVP.P. If a temperature range has been given in the literature, the average value has been stored.

Unit:

The default unit in the Beilstein database for this fact is J mol^{-1}.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
HVAP.T	Temperature	Numeric (range)	ºC
HVAP.P	Pressure	Numeric (range)	Torr

Example:

Operator	Field Name	Value
	HVAP	50000 - 60000
PROXIMITY	HVAP.T	>100

Type of Indexing:

Numeric (range)

2.5.1.4.1.6. Enthalpy of Sublimation (HSP)

Description:

Sublimation is defined as the direct conversion of a solid into a gas at constant temperature and pressure. The enthalpy of sublimation is the change in enthalpy, which occurs when one mol of a substance sublimes at a specified temperature and pressure. The values for this field are given at the sublimation temperature. You can search for the associated information about the temperature using the parameter field code HSP.T.

Unit:

The default unit in the Beilstein database for this fact is J mol^{-1}.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
HSP.T	Temperature	Numeric (range)	ºC

Example:

Operator	Field Name	Value
	HSP	>100000
PROXIMITY	HSP.T	>20

Type of Indexing:

Numeric (range)

2.5.1.4.1.7. Enthalpies of Other Phase Transitions (HPTP)

Description:

The enthalpy of a phase transition is defined as the heat evolved when one gram-mol of a substance is converted from one phase to another at a specified temperature and pressure. The HPTP field contains the energy values for the substances.

Unit:

The default unit in the Beilstein database for this fact is J mol^{-1}.

Type of Indexing:

Numeric (range)

2.5.1.4.2. Heat Capacity (CAP)

Description:

This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database, concerned with different heat capacities:

Heat Capacity Cp (CP)

Heat Capacity Cp0 (CP0)

Heat Capacity Cv (CV)

Type of Indexing:

Group Code

2.5.1.4.2.1. Heat Capacity, Cp (CP)

Description:

The molar heat capacity at constant pressure is defined as the quantity of heat necessary to raise the temperature of 1 mol of the substance 1 degree at constant pressure. The Values are given at specified temperatures. The Heat Capacity CP field contains calorimetric determined values (see also Cp0). You can search for the associated information about the temperature using the parameter field code CP.T.

Unit:

The default unit in the Beilstein database for this fact is J mol^{-1} $^oC^{-1}$

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
CP.T	Temperature	Numeric (range)	^oC

Example:

Operator	Field Name	Value
	CP	100 - 200
PROXIMITY	CP.T	>50

Type of Indexing:

Numeric (range)

2.5.1.4.2.2. Heat Capacity CP0 (CP0)

Description:

The molar heat capacity CP0 is defined as the quantity of heat necessary to raise the temperature of 1 mol of the ideal gas 1 degree at constant pressure. The Heat Capacity CP0 field contains values for ideal gases obtained from statistical-thermodynamic calculations (see also CP). You can search for the associated information about the temperature using the parameter field code CP0.T.

Unit:

The default unit in the Beilstein database for this fact is J mol^{-1} $^oC^{-1}$.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
CP0.T	Temperature	Numeric (range)	ºC

Example:

Operator	Field Name	Value
	CP0	<150
PROXIMITY	CP0.T	<30

Type of Indexing:

Numeric (range)

2.5.1.4.2.3. Heat Capacity CV (CV)

Description:

The molar heat capacity CV is defined as the quantity of heat necessary to raise the temperature of 1 mol of the substance 1 degree at constant volume. You can search for the associated information about the temperature using the parameter field code CV.T.

Unit:

The default unit in the Beilstein database for this fact is J mol^{-1}.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
CV.T	Temperature	Numeric (range)	ºC

Type of Indexing:

Numeric (range)

2.5.1.4.3. Other Thermochemical Data (OTHE)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
OTHE.KW	Description	String (phrase)

Type of Indexing:
Group Code

2.5.1.4.3.1. Other Thermochemical Data Description (OTHE.KW)

Description:

This field contains keywords from a list of controlled terms:

- Cryoscopic constant
- Ebullioscopic constant
- Enthalpy
- Heat of combustion at constant volume
- Enthalpy of self-association
- Thermodynamic properties
- Heat capacity
- Entropy
- Heat capacity ratio Cp/Cv
- Gibbs free energy

Type of Indexing:

String (phrase)

2.5.1.5. Optical Properties (OPTP)

Description:

This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database concerned with optical properties.

Refractive Index (RI)

Optics (OPT)

Optical Rotatory Power (ORP)

Mutarotation (MUT)

Circular Dichroism (CDIC)

Optical Rotatory Dispersion (ORD)

2.5.1.5.1. Refractive Index (RI)

Description:

The refractive index is the ratio of the velocity of light in a vacuum to its velocity in the substance. The ratio of the sine of the angle of incidence to the sine of the angle of refraction is the index of refraction of the second medium. The refractive index varies with the wavelength of the incident light, temperature and pressure.

The values are given at specified temperature and wavelength. You can search for this associated information using the parameter field codes RI.W and RI.T.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
RI.W	Wavelength	Numeric (range)	nm
RI.T	Temperature	Numeric (range)	ºC

Example:

Operator	Field Name	Value
	CN	*methyl*
AND	RI	1.44
PROXIMITY	RI.T	20

Type of Indexing:

Numeric (range)

2.5.1.5.2. Optics (OPT)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
OPT.KW	Description	String (phrase)

Type of Indexing:
Group Code

2.5.1.5.2.1. Optics Description (OPT.KW)

Description:

This field contains keywords from a list of controlled terms:

- Crystal refractive indices
- Natural birefringence
- Mechanical birefringence
- Magnetic birefringence (Cotton-Mouton effect)
- Electric birefringence (Kerr effect)
- Diffraction
- Reflection
- Rayleigh scattering
- Degree of depolarization of Rayleigh scattering
- Iso- & anisotropic components of Rayleigh scattering
- Plain curve
- Cotton Effect (abnormal curve)
- Magnetorotation
- Magnetic circular dichroism
- Thermochromism
- Photochromism

- Linear dichroism
- Mutarotation coefficient
- Optical properties
- Rayleigh-Brillouin scattering
- Verdet constant
- Flow birefringence

Type of Indexing:

String (phrase)

2.5.1.5.3. Optical Rotatory Power (ORP)

Description:
The optical rotatory power is the ability of a dissymmetric substance to refract and absorb right and left-polarized light to different extents. This results in continuous rotation of the plane of polarization. You can search for the associated information about the type, concentration, and length of path, solvent, wavelength and temperature using the parameter field codes ORP.TYP, ORP.C, ORP.LEN, ORP.SOL, ORP.W and ORP.T.

Unit: The default unit in the Beilstein database for this fact is degrees.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
ORP.TYP	Type	String (phrase)	
ORP.C	Concentration	String (phrase)	
ORP.LEN	Length of Path	Numeric	cm
ORP.SOL	Solvent	String (phrase)	
ORP.W	Wavelength	Numeric (range	nm
ORP.T	Temperature	Numeric (range	ºC

Example:

Operator	Field Name	Value
	ORP	-40
AND	CN	*methyl*

Type of Indexing:
Numeric (range)

2.5.1.5.4. Mutarotation (MUT)

Description:
Mutarotation is a change in optical rotation that takes place with time in solutions prepared freshly from optically active substances as a result of the reversible conversion of one isomeric form to another. The values are given at a specified wavelength. You can search for the associated information about the type, concentration, length of path, solvent, wavelength, temperature and time using the parameter field codes MUT.TYP, MUT.C, MUT.LEN, MUT.W, MUT.T and MUT.TIM.

Unit:
The default unit in the Beilstein database for this fact is degree.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
MUT.TYP	Type	String (phrase)	
MUT.C	Concentration	String (phrase)	
MUT.LEN	Length of Path	Numeric (range)	cm
MUT.SOL	Solvent	String (phrase)	
MUT.W	Wavelength	Numeric (range)	nm
MUT.T	Temperature	Numeric (range)	ºC
MUT.TIM	Time	String (phrase)	S

Example:

Operator	Field Name	Value
	MUT	-130 - -100
PROXIMITY	MUT.SOL	H2O

Type of Indexing:
Numeric (range)

2.5.1.5.5. Circular Dichroism (CDIC)

Description:
Optically active compounds absorb left and right polarized light unequally. When linearly polarized incident light passing through a substance becomes elliptically polarized the phenomenon is known as circular dichroism. The wavelength range over which this phenomenon has been measured is stored in the CDIC field. You can search for the solvent in the associated parameter field CDIC.SOL.

Unit:
The default unit in the Beilstein database for the wavelength range is nm.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing
CDIC.SOL	Solvent	String (phrase)

Example:

Operator	Field Name	Value
	CDIC	250 - 300
PROXIMITY	CDIC.SOL	methanol

Type of Indexing:
String (phrase)

2.5.1.5.6. Optical Rotatory Dispersion (ORD)

Description:
Optical rotatory dispersion is defined as the variation in optical rotation with the wavelength of light. The wavelength range over which this phenomenon has been measured is stored in the ORD field. You can search for the associated information about the solvent using the parameter field code ORD.SOL.

Unit:
The default unit in the Beilstein database for the wavelength range is nm

Associated Parameter Field:

Field Code	Full Name	Type of Indexing
ORD.SOL	Solvent	String (phrase)

Example:

Operator	Field Name	Value
	ORD	300 - 500
PROXIMITY	ORD.SOL	Pentane

Type of Indexing:
String (phrase)

2.5.1.6. Spectroscopic Information (SPE)

Description:

This field identifier is a group code for Field Availability searches concerned with spectral information in the hierarchical system of the Beilstein database.

NMR Spectroscopy (NMR)

ESR Spectroscopy (ESR)

NQR Spectroscopy (NQR)

Rotational Spectroscopy (ROT)

IR Spectroscopy (IR)

Raman Spectroscopy (RAMAN)

UV/VIS Spectroscopy (UV)

Luminescence Spectroscopy (LUM)

Fluorescence Spectroscopy (FLU)

Phosphorescence Spectroscopy(PHO)

Other Spectroscopic Methods (OSM)

Mass Spectrometry (MS)

Type of Indexing:

Group Code

2.5.1.6.1. NMR Spectroscopy (NMR)

Description:

This field identifier is a group code for Field Availability searches concerned with NMR (nuclear magnetic resonance) spectra in the hierarchical system of the Beilstein database.

The NMR Spectrum parameter fields are present when the publication contained individual chemical shift values from the NMR spectra for the substances. Some fields are very useful in combination with other queries to refine search strategies. You can search for this associated information using the parameter field codes see below.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
NMR.KW	Description	String (phrase)	
NMR.NUC	Nucleus	String (phrase)	
NMR.NUI	Coupling Nuclei	String (phrase)	
NMR.SOL	Solvent	String (phrase)	
NMR.T	Temperature	Numeric (range)	ºC
NMR.F	Frequency	Numeric (range)	MHz

Example:

Operator	Field Name	Value
	NMR.NUC	13C
AND	NMR.NUI	31P

Type of Indexing:
Group Code

2.5.1.6.1.1. NMR Description (NMR.KW)

Description:

This field contains keywords from a list of controlled terms:

- Spectrum
- Chemical shifts
- Dynamic NMR
- INDOR
- NMR with shift reagents
- Linewidth of NMR absorption
- NMR in liquid-crystal phase
- NOE
- Second moment of NMR absorption
- Spin-lattice relaxation time (T1)
- Spin-spin relaxation time (T2)
- 2D-NMR
- 3D-NMR

- Aromatic solvent induced shifts
- Radical contact shifts
- Double resonance
- Spin-rotation constant
- 1H-electron double resonance
- CIDNP
- NMR
- Spin-spin coupling constants

Type of Indexing:
String (phrase)

2.5.1.6.2. ESR Spectroscopy (ESR)

Description:
This field identifier is a group code for Field Availability searches concerned with ESR (electron spin resonance) data in the hierarchical system of the Beilstein database.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
ESR.KW	Description	String (phrase)	
ESR.NUI	Coupling Nuclei	String (phrase)	
ESR.SOL	Solvent	String (phrase)	
ESR.T	Temperature	Numeric (range)	ºC

Type of Indexing:
Group Code

2.5.1.6.2.1. ESR Description (ESR.KW)

Description:

This field contains keywords from a list of controlled terms:

- Spectrum
- Signals
- ENDOR (electron-nuclear double resonance)
- g-factor
- ESR linewidth

- ESR second moment
- Electron spin-lattice relaxation time
- Electron spin-spin relaxation time
- 1H-electron Overhauser effect
- CIDEP (chemically induced dynamic electron polarization)
- ELDOR (electron-electron double resonance)
- ESR
- ESR-hyperfine coupling constants
- Triplet state ESR spectrum
- Triplet state ESR
- Triplet state ESR g-factor
- Triplet state ESR hyperfine coupling constant(s)
- Triplet state ESR zero-field splitting parameter(s)

Type of Indexing:

String (phrase)

2.5.1.6.3. NQR Spectroscopy (NQR)

Description:
This field identifier is a group code for Field Availability searches concerned with NQR (nuclear quadrupole resonance) data in the hierarchical system of the CrossFire database.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
NQR.KW	Description	String (phrase)
NQR.NUC	Nucleus	String (phrase)

Type of Indexing:
Group Code

2.5.1.6.3.1. NQR Description (NQR.KW)

Description:

This field contains keywords from a list of controlled terms:

- Nuclear quadrupole resonance
- Nuclear quadrupole coupling constants
- Pure NQR

Type of Indexing:

String (phrase)

2.5.1.6.4. Rotational Spectroscopy (ROT)

Description:
This field identifier is a group code for Field Availability searches concerned with rotational spectra in the hierarchical system of the Beilstein database.

Search fields:

Field Code	Full Name	Type of Indexing
ROT.KW	Description	String (phrase)

Type of Indexing:
Group Code

2.5.1.6.4.1. Rotational Spectrum Description (ROT.KW)

Description:

This field contains keywords from a list of controlled terms:

- Microwave spectrum
- Rotational spectrum
- Intensity of microwave bands
- Stark effect
- Rotational-Raman spectrum
- Linewidth of microwave bands
- Intensity of rotational bands
- Linewidth of rotational bands

Type of Indexing:

String (phrase)

2.5.1.6.5. Infrared Spectroscopy (IR)

Description:
This field identifier is a group code for Field Availability searches concerned with Infrared spectra in the hierarchical system of the Beilstein database.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
IR.KW	Description	String (phrase)	
IR.SOL	Solvent	String (phrase)	
IR.T	Temperature	Numeric (range)	ºC

Type of Indexing:
Group Code

2.5.1.6.5.1. IR Description (IR.KW)

Description:

This field contains keywords from a list of controlled terms:

- Spectrum
- Bands
- Fine structure of IR bands
- Intensity of IR bands
- Polarization of IR bands
- Reflection spectrum
- Far IR spectrum
- Near IR spectrum
- Far IR bands
- Near IR bands
- Intensity of far IR bands
- Intensity of near IR bands

- Intensity of rotational lines of IR bands
- Linewidth of IR bands
- Linewidth of rotational lines of IR bands
- IR second moment
- IR-radiofrequency double resonance
- IR-microwave double resonance
- Vibrational relaxation
- Vibrational energy transfer
- Overtone spectrum
- Anisotropy of IR bands
- Fermi resonance
- IR

Type of Indexing:

String (phrase)

2.5.1.6.6. Raman Spectroscopy (RAMAN)

Description:
This field identifier is a group code for Field Availability searches concerned with Raman spectra in the hierarchical system of the Beilstein database.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
RAMAN.KW	Description	String (phrase)
RAMAN.SOL	Solvent	String (phrase)

Type of Indexing:
Group Code

2.5.1.6.6.1. Raman Description (RAMAN.KW)

Description:

This field contains keywords from a list of controlled terms:

- Spectrum
- Bands
- Degree of depolarization of Raman bands
- Hyper-Raman spectrum
- Linewidth of Raman bands
- Low frequency Raman bands
- Low frequency Raman spectrum
- Preresonance Raman spectrum
- Raman intensities
- Raman resonance effect
- Raman second moment
- Rotational fine structure of Raman bands
- Raman

Type of Indexing:

String (phrase)

2.5.1.6.7. UV/VIS Spectroscopy (UV)

Description:

This field identifier is a group code for Field Availability searches concerned with UV spectra in the hierarchical system of the Beilstein database.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
UV.KW	Description	String (phrase)
UV.SOL	Solvent	String (phrase)
UV.AM	Absorption Maxima	Numeric (range)
UV.EAC	Extinction/Absorption Coefficient	Numeric (range)

Type of Indexing:
Group Code

2.5.1.6.7.1. UV Description (UV.KW)

Description:

This field contains keywords from a list of controlled terms:

- Spectrum
- Absorption maxima
- Reflection spectrum
- Singlet-triplet band
- Solvatochromism
- Triplet-triplet band
- Vacuum-UV spectrum
- Absorption spectrum
- Absorption cross-section
- UV excited state absorption
- UV two-photon absorption
- Triplet-singlet absorption spectrum
- Opto-acoustic UV spectrum
- UV/VIS reflection maximum(a)
- X-ray absorption spectrum
- X-ray absorption cross-section
- Band anisotropy
- Oscillator strength
- UV/VIS

Type of Indexing:

String (phrase)

2.5.1.6.8. Luminescence Spectroscopy (LUM)

Description:
This field identifier is a group code for Field Availability searches concerned with Luminescence in the hierarchical system of the Beilstein database.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
LUM.KW	Description	String (phrase)

Type of Indexing:
Group Code

2.5.1.6.8.1. Luminescence Description (LUM.KW)

Description:

This field contains keywords from a list of controlled terms:

- Emission spectrum in the infrared region
- Radioluminescence
- Sonoluminescence
- Triboluminescence
- Thermoluminescence
- Electroluminescence
- Lasing properties
- Luminescence lifetime
- Luminescence quenching
- Degree of depolarization of luminescence
- Luminescence quantum yield
- Luminescence
- UV/VIS emission spectrum
- UV/VIS emission
- X-ray emission spectrum
- X-ray emission cross-section
- X-ray emission quantum yield

- Luminescence spectrum

Type of Indexing:

String (phrase)

2.5.1.6.9. Fluorescence Spectroscopy (FLU)

Description:
This field identifier is a group code for Field Availability searches concerned with Fluorescence spectra in the hierarchical system of the Beilstein database.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
FLU.KW	Description	String (phrase)	
FLU.SOL	Solvent	String (phrase)	
FLU.T	Temperature	Numeric (range)	ºC

Type of Indexing:
Group Code

2.5.1.6.9.1. Fluorescence Description (FLU.KW)

Description:

This field contains keywords from a list of controlled terms:

- Spectrum
- Maxima
- Fluorescence emission cross-section
- Fluorescence quantum yield
- Fluorescence lifetime
- Fluorescence decay kinetics
- Fluorescence self-quenching
- Fluorescence concentration quenching
- Fluorescence quenching
- Degree of polarization of fluorescence
- Excimer fluorescence
- Delayed fluorescence

- Intersystem crossing [singlet->triplet]
- Energy transfer from singlet state
- Fluorescence excitation spectrum
- Fluorescence intensity
- Fluorescence

Type of Indexing:

String (phrase)

2.5.1.6.10. Phosphorescence Spectroscopy (PHO)

Description:
This field identifier is a group code for Field Availability searches concerned with Phosphorescence in the hierarchical system of the Beilstein database.

Associated Parameter Fields

Field Code	Full Name	Type of Indexing	Unit
PHO.KW	Description	String (phrase)	
PHO.SOL	Solvent	String (phrase)	
PHO.T	Temperature	Numeric (range)	ºC

Type of Indexing:
Group Code

2.5.1.6.10.1. Phosphorescence Description (PHO.KW)

Description:

This field contains keywords from a list of controlled terms:

- Spectrum
- Maxima
- Phosphorescence lifetime
- Phosphorescence decay kinetics
- Phosphorescence quenching
- Degree of polarization of phosphorescence
- Excimer phosphorescence
- Delayed phosphorescence

- Triplet state energy
- Triplet state quantum yield
- Triplet state lifetime
- Triplet state decay kinetics
- Triplet state quenching
- Triplet state sublevel studies
- Energy transfer from triplet state
- Phosphorescence excitation spectrum
- Phosphorescence quantum yield
- Phosphorescence

Type of Indexing:

String (phrase)

2.5.1.6.11. Other Spectroscopic Methods (OSM)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
OSM.KW	Description	String (phrase)

Type of Indexing:
Group Code

2.5.1.6.11.1. Other Spectroscopic Methods Description (OSM.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Photoelectron spectrum
- ESCA
- Moessbauer effect
- Electronic state studies
- Electron impact spectrum

- Auger electron spectrum
- Multiple resonance studies

Type of Indexing:

String (phrase)

2.5.1.6.12. Mass Spectrometry (MS)

Description:
This field identifier is a group code for Field Availability searches concerned with Mass Spectrum in the hierarchical system of the Beilstein database

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
MS.KW	Description	String (phrase)

Type of Indexing:
Group Code

2.5.1.6.12.1. Mass Spectrometry Description (MS.KW)

Description:

This field contains keywords from the following list of controlled terms:

- spectrum
- chemical ionization (CI)
- collisional activation
- electron impact (EI)
- electrohydrodynamic ionization
- fast atom bombardment (FAB)
- field desorption
- field ionization
- fragmentation pattern
- high frequency spark
- hydrogen and carbon scrambling
- ion kinetic energy (spectrum) (IKE(S))

- ion current profiles
- laser desorption
- metastable ions
- mass ion kinetic energy (MIKE)
- negative ion spectroscopy
- negative secondary ions
- positive secondary ions
- charge exchange with rare gas ions
- collision-induced dissociation
- doubly charged ions
- ion-cyclotron resonance
- ion impact
- negative chemical ionization
- neutral impact
- Penning ionization
- photoelectron-photoion coincidence
- photoionization
- secondary ions
- charge exchange with negative ions
- neutral fragments
- surface ionization
- single ion monitoring (SIMS)
- liquid secondary ion mass spectrometry (LSIMS)
- neutralization-reionization mass spectrometry (NRMS)
- desorption chemical ionization (DCI)
- time-of-flight mass spectra (TOFMS)
- multiphoton ionization (MPI)
- resonance enhanced multiphoton ionization (REMPI)
- direct electron ionization (DEI)
- tandem mass spectrometry

- collisionally activated dissociation (CAD)
- appearance potentials
- charge exchange with positive ions

Type of Indexing:
String (phrase)

2.5.1.7. Magnetic Properties (MAGP)

Description:

This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database concerned with magnetic properties.

- Magnetic Susceptibility (MSUS)
- Magnetic Data (MAG)

Type of Indexing:

Group Code

2.5.1.7.1. Magnetic Susceptibility (MSUS)

Description:
Magnetic susceptibility is the ratio of magnetization to field strength. You can search for the associated information about the temperature using the parameter field code MSUS.T.

Unit:
The default unit in the Beilstein database for this fact is $cm^3\ mol^{-1}\ 10^{-6}$.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
MSUS.T	Temperature	Numeric (range)	ºC

Type of Indexing:
Numeric (range)

2.5.1.7.2. Magnetic Data (MAG)

Description:
This field identifier is a group code for Field Availability searches concerned with Magnetic Data in the hierarchical system of the Beilstein database

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
MAG.KW	Description	String (phrase)

Type of Indexing:
Group Code

2.5.1.7.2.1. Magnetic Data Description (MAG.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Anisotropy of magnetic susceptibility
- Magnetic moment
- Magnetic properties
- paramagnetic
- Volume susceptibility
- Rotational magnetic moment

Type of Indexing:
String (phrase)

2.5.1.8. Electrical Properties (ELEP)

Description:

This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database concerned with electrical properties.

Static Dielectric Constant (SDIC)

Dielectric Constant (DIC)

Electrical Data (ELE)

Type of Indexing:

Group Code

2.5.1.8.1. Static Dielectric Constant (SDIC)

Description:

For a given substance the static dielectric constant is the ratio of the capacity of a condenser with that substance as the dielectric medium to the capacity of the same condenser with a vacuum as the dielectric medium.

The dielectric constant is a function of temperature and frequency at which the alternating electric field varies.

The static dielectric constant is the dielectric constant at frequencies low enough that the equilibrium is maintained as the electric field varies

The values of the constant are given at specified temperatures. You can search for the associated temperature in the parameter fields SDIC.T.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
SDIC.T	Temperature	Numeric (range)	ºC

Example:

Operator	Field Name	Value
	SDIC	4.0 - 6.0
PROXIMITY	SDIC.T	20

Type of Indexing:

Numeric (range)

2.5.1.8.2. Dielectric Constant (DIC)

Description:

The dielectric constant is the ratio of the capacity of a condenser with that substance as the dielectric medium to the capacity of the same condenser in a vacuum. The values of the constant are given at specified temperatures and frequencies. You can search for the associated frequency and temperature in the parameter fields DIC.F and DIC.T.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
DIC.F	Frequency	Numeric (range)	Hz
DIC.T	Temperature	Numeric (range)	ºC

Example:

Operator	Field Name	Value
	DIC	80 - 90
PROXIMITY	DIC.T	20

Type of Indexing:
Numeric (range)

2.5.1.8.3. Electrical Data (ELE)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
ELE.KW	Description	String (phrase)

Type of Indexing:
Group Code

2.5.1.8.3.1. Electrical Data Description (ELE.KW)

Description:
This field contains keywords from the following list of controlled terms:

- Angle of dielectric loss
- Critical frequency (or wavelength)
- Dielectric anisotropy
- Dielectric increment
- Dielectric loss
- Dielectric relaxation time
- Dielectric saturation
- Relaxation frequency
- Cole-Cole diagram
- Piezoelectricity
- Thermoelectricity
- Photoelectricity (Becquerel effect)
- Electrical conductivity
- Photoconductivity
- Dielectric strength
- Electrical properties
- Photovoltaic effect

Type of Indexing:

String (phrase)

2.5.1.9. Electrochemical Behaviour (ECB)

Description:

This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database concerned with electrical properties.

Electrochemical Behaviour (ELCB)

Dissociation Exponent (DE)

Isoelectric Point pH (IEP)

Electrochemical Characteristics (POT)

Cross-Sections (XS)

Type of Indexing:

Group Code

2.5.1.9.1. Electrochemical Behaviour (ELCB)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
ELCB.KW	Description	String (phrase)
ELCB.ED	Entry Date	String (phrase)

Type of Indexing:
Group Code

2.5.1.9.1.1. Electrochemical Behaviour Description (ELCB.KW)

Description:

This topic contains the field ELCB.KW, which contains keywords from the following list of controlled terms:

- Autoprotolysis
- Enthalpy of dissociation (electrolytic) / protonation
- Kinetics of dissociation (electrolytic) / protonation
- Enthalpy of neutralization
- Proton affinity
- Electrolytic dissociation / protonation equilibrium
- Thermodynamic parameters for autoprotolysis
- Thermodynamic parameters for dissociation / protonation
- Volume change on dissociation
- Enthalpy of deprotonation
- Acidity
- Basicity
- Protonation
- Deprotonation
- pK(R+)
- pH of aqueous solutions
- Stability constant
- Electrochemical properties
- Polarography
- Degree of dissociation

Type of Indexing:

String (phrase)

2.5.1.9.2. Dissociation Exponent (pK) (DE)

Description:
The dissociation exponent is defined as the logarithm (base 10) of the reciprocal of the equilibrium constant. The Dissociation Exponent field contains the values for the dissociation exponents (pKa for acids, pKb for bases). You can search for the associated information about dissociation group, temperature, solvent, method and type using the parameter field codes DE.GRP, DE.T, DE.SOL, DE.MET and DE.TYP.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
DE.GRP	Dissociation Group	String (phrase)	
DE.T	Temperature	Numeric (range)	ºC
DE.SOL	Solvent	String (phrase)	
DE.MET	Method	String (phrase)	
DE.TYP	Type	String (phrase)	

Example:

Operator	Field Name	Value
	DE	1.5 - 2.0
PROXIMITY	DE.T	20

Type of Indexing:
Numeric (range)

2.5.1.9.3. Isoelectric Point, pH (IEP)

Description:
The isoelectric point is defined as the pH value at which a substance in a solution is electrically neutral. You can search for the associated information about the solvent using the parameter field code IEP.SOL.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing
IEP.SOL	Solvent	String (phrase)

Type of Indexing:
Numeric (range)

2.5.1.9.4. Electrochemical Characteristics (POT)

Description:
This field identifier is a group code for Field Availability searches concerned with electrochemical investigations in the hierarchical system of the Beilstein database.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
POT.KW	Description	String (phrase)	
POT.SOL	Solvent	String (phrase)	
POT.PH	pH Value	Numeric (range	
POT.T	Temperature	Numeric (range	ºC
POT.PBRN	Product BRN	Numeric	
POT.PRO	Product	String (wordwise)	

Type of Indexing:
Group Code

2.5.1.9.4.1. Electrochemical Characteristics Description (POT.KW)

Description:

This field contains keywords from the following list of controlled terms:

- cyclic voltammetry
- oxidation potential
- polarographic current/voltage curve
- polarographic half-wave potential
- redox potential
- reduction potential
- voltammetry
- photo-electrochemical half-wave potential

Type of Indexing:

String (phrase)

2.5.1.9.5. Cross-Sections (XS)

Description:
The Description field XS.KW contains keywords from the following list of controlled terms:

- Photoionization cross-section
- Electron ionization cross-section
- Proton ionization cross-section
- Ionization cross-section
- Collision cross-section

Type of Indexing:
String (phrase)

2.5.1.10. Safety Data (SAF)

Description:

This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database concerned with:

Flash Point (FLAP)

Autoignition (AUTI)

Explosion Limits (EXPL)

Type of Indexing:

Group Code

2.5.1.10.1. Flash Point (FLAP)

Description:
This is the lowest temperature of the liquid at which it gives off enough vapour to form an ignitable mixture of vapour and air immediately above the liquid surface.
A liquid is classified as flammable or combustible depending on its flash point. A flammable liquid has a flash point below 37.8 ºC while a combustible liquid has a flash point greater than 37.8 ºC.

Example:
Flash point of Acetone is –17.8 ºC and that of Aniline is 70.0 ºC.

The lower the Flash Point, the greater the potential fire hazards.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
FLAP	Temperature	Numeric (range)	ºC
FLAP.TYP	Type of Test	String (phrase)	

2.5.1.10.2. Autoignition (AUTI)

Description:

Autoignition or spontaneous combustion occurs when a substance reaches its ignition temperature without the application of external heat. This characteristic is particularly important to keep in mind in the storage and disposal of chemicals.

Associated Parameter Field:

Field Code	Full Name	Type of Indexing	Unit
AUTI.T	Temperature	Numeric (range)	ºC

Type of Indexing:

Group Code

2.5.1.10.2.1. Autoignition Temperature (AUTI.T)

Description:

The autoignition (or ignition) temperature of a substance -solid, liquid, or gas - is the minimum temperature required to initiate self- sustained combustion, in the absence of spark or flame. Some ignition temperatures can be quite low (for example, carbon disulfide at 90ºC (194F).

Type of Indexing:

Numeric (range)

2.5.1.10.3. Explosion Limits (EXPL)

Description:

The explosive range is the range between the lowest explosive limit (LEL) and the upper explosive limit (UEL).

The LEL is the lowest concentration of vapour in air, which will burn or explode upon contact with a source of ignition. Below the LEL, the mixture is to lean (i.e. there is insufficient fuel).

The UEL is the highest concentration of vapour in air, which will burn or explode upon contact with a source of ignition. Above the UEL, the mixture is too rich to burn (i.e. there is insufficient oxygen).

The LEL and UEL are usually indicated by the percentage by volume of vapour in air.

Example:
For diethyl ether, the LEL is 1.9% and the UEL is 36% by volume of air.
This range becomes wider with increasing temperature and in oxygen-rich atmospheres.

Type of Indexing:
Numeric (range)

2.5.1.11. Further Information (FINFO)

Description:

The field FINFO.KW contains references for rarely reported physical and chemical properties not covered in detail in the Beilstein database.

2.5.2. Multicomponent Systems (MCS)

Description:
This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database concerned with the physical properties of the title compound in a two or more component system.

Solution Behaviour (MCS) (SOL)

Solubility (MCS) (SLB)

Solubility Products (MCS) (SLBP)

Solution Behavior (MCS) (SOLM)

Critical Micelle Concentration (MCS) (CMC)

Henry Constant (MCS) (HEN)

Partition Octan-1-ol/Water (MCS) (POW)

Liquid/Vapour Systems (MCS) (LVS)

Liquid/Vapour Systems (MCS) (LVSM)

Azeotropes (MCS) (AZE)

Complex Phase Equilibria (CPEM)

Liquid/Liquid Systems (MCS) (LLSM)

Liquid/Solid Systems MCS (LSSM)

Mechanical & Physical Properties (MCS) (MECM)

Transport Phenomena (MCS) (TRAM)

Energy Data (MCS) (ENEM)

Electrical Data (EDM)

Optical Data (ODM)

Boundary Surface Phenomena (MCS) (BSPM)

Adsorption (MCS) (ADSM)

Association (MCS) (ASSM)

2.5.2.1. Solution Behaviour (MCS) (SOL)

Description:

This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database concerned with the physical properties of the title compound in a two or more component system.

Solubility (MCS) (SLB)

Solubility Products (MCS) (SLBP)

Solution Behaviour (MCS) (SOLM)

Critical Micelle Concentration (MCS) (CMC)

Henry Constant (MCS) (HEN)

Partition Octan-1-ol/Water (MCS) (POW)

2.5.2.1.1. Solubility (MCS) (SLB)

Description:
The solubility of one liquid or solid in another is the mass of a substance contained in a solution, which is in equilibrium with an excess of the substance at a specified temperature. You can search for the associated information about the saturation, the temperature, the solvent and the ratio of solvents using the parameter field codes SLB.SAT, SLB.T, SLB.SOL and SLB.RAT.

Unit: The default unit in the Beilstein database for this fact is g l^{-1}.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
SLB.SAT	Saturation	String (phrase)	
SLB.T	Temperature	Numeric (range)	ºC
SLB.SOL	Solvent	String (phrase)	
SLB.RAT	Ratio of Solvents	String (phrase)	

Type of Indexing:
Numeric (range)

2.5.2.1.2. Solubility Product (MCS) (SLBP)

Description:
The solubility product is the product of the concentrations of the ions of a substance in a saturated solution of the substance at a specified temperature. You can search for the associated information about the temperature, the solvent and the ratio of solvents using the parameter field codes SLBP.T, SLBP.SOL and SLBP.RAT.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
SLBP.T	Temperature	Numeric (range)	ºC
SLBP.SOL	Solvent	String (phrase)	
SLBP.RAT	Ratio of Solvents	String (phrase)	

Example:

Operator	Field Name	Value
	SLBP	1.0 - 2.0
PROXIMITY	SLBP.SOL	methanol

Type of Indexing:
Numeric (range)

2.5.2.1.3. Solution Behavior (MCS) (SOLM)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
SOLM.PB	Partner BRN	Numeric	
SOLM.PA	Partner	String (wordwise)	
SOLM.SOL	Solvent	String (phrase)	
SOLM.T	Temperature	Numeric (range)	ºC
SOLM.P	Pressure	Numeric (range)	Torr
SOLM.KW	Description	String (phrase)	

Type of Indexing:
Group Code

2.5.2.1.3.1. Solution Behaviour Description (MCS)(SOLM.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Dissolving capacity
- Miscibility
- Solubilizing
- Mutual solubility
- Rate of dissolution
- Solubility [Bunsen absorption coefficient]
- Solubility [Henry constant]
- Solubility [Ostwald absorption coefficient]

Type of Indexing:

String (phrase)

2.5.2.1.4. Critical Micelle Concentration (MCS) (CMC)

Description:
The critical micelle concentration is the concentration at which micelles begin to form in a system comprising solvent(s), surfactant(s), possibly other solutes and a defined physical environment. You can search for the associated temperature and solvent information in the parameter fields CMC.T and CMC.SOL.
Unit: The default unit in the CrossFire database for this fact is g l^{-1}.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
CMC.T	Temperature	Numeric (range)	ºC
CMC.SOL	Solvent	String (phrase)	

Example:

Operator	Field Name	Value
	CMC	<6.5
PROXIMITY	CMC.T	<30

Type of Indexing:
Numeric (range)

2.5.2.1.5. Henry Constant (MCS) (HEN)

Description:

The Henry constant is the ratio of the concentration of a chemical substance in air to the concentration in an aqueous solution at equilibrium. It can be used as a qualitative measure about the volatility of the substance and its whereabouts in nature.
You can search for the value of the constant or its decadic logarithm. Information on the related temperature and solvent is given in the parameter fields HEN.T and HEN.SOL.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
HEN	Henry Constant	Numeric	Pa m3 mol-1
HEN.LOG	Log Henry Constant	Numeric (range)	
HEN.T	Temperature	Numeric (range)	ºC
HEN.SOL	Solvent	String (phrase)	

2.5.2.1.6. Partition Octan-1-ol/Water (MCS)(POW)

Description:
The partition coefficient constant POW describes the equilibrium distribution of a substance between n-Octanol and water phases. The distribution coefficient is the quotient of two concentrations and is usually given in the form of the decadic logarithm (log POW). You can search for both values POW and log POW. Information on the related temperature is given in the parameter field POW.T.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
POW	Partition coefficient	Numeric (range)	
POW.LOG	Log Pow	Numeric (range)	
POW.T	Temperature	Numeric (range)	ºC

2.5.2.2. Liquid/Vapour Systems (MCS) (LVS)

Description:

This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database, concerned with the properties of liquid/vapour systems.

- Liquid/Vapour Systems (MCS) (LVSM)
- Azeotropes (MCS) (AZE)
- Complex Phase Equilibria (CPEM)

2.5.2.2.1. Liquid/Vapour Systems (MCS) (LVSM)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
LVSM.KW	Description	String (phrase)	
LVSM.PB	Partner BRN	Numeric	
LVSM.PA	Partner	String (wordwise)	
LVSM.SOL	Solvent	String (phrase)	
LVSM.T	Temperature	Numeric (range)	ºC
LVSM.P	Pressure	Numeric (range)	Torr

Type of Indexing:
Group Code

2.5.2.2.1.1. Liquid/Vapour Systems Description (MCS) (LVSM.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Liquid/vapour phase diagram
- Liquid/vapour equilibrium
- Boiling point diagram
- Boiling points of mixtures
- Vapour pressure diagram for the mixture
- Partial pressures of the components
- Critical data for mixtures
- Activity coefficients of the components in the mixture
- Vapour pressure
- Tricritical point
- Critical temperature
- Critical pressure
- Critical density

- Critical volume
- Fugacities

Type of Indexing:

String (phrase)

2.5.2.2.2. Azeotropes (MCS) (AZE)

Description:
The AZE field contains the names of the components of (chemical name fragment) azeotropic mixtures. These two or more substances in a liquid mixture behave like a single substance in that the vapour produced by partial evaporation of the liquid has the same composition as the liquid. In addition, temperature, pressure and concentration are present in parameter fields (AZE.T, AZE.P, AZE.C). You can also search for the Beilstein Registry Number BRN of these components in the parameter field AZE.PB.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
AZE.PB	Azeotrope BRN	Numeric	
AZE.PA	Azeotropes	String (wordwise)	
AZE.T	Temperature	Numeric (range)	ºC
AZE.P	Pressure	Numeric (range)	Torr
AZE.C	Concentrations	String (phrase)	

Example:

Field Name	Value
AZE.PA	toluene

Type of Indexing:
String (phrase)

2.5.2.2.3. Complex Phase Equilibria (CPEM)

Description:

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
CPEM.KW	Description	String (phrase)	
CPEM.PB	Partner BRN	Numeric	
CPEM.PA	Partner	String (wordwise)	
CPEM.SOL	Solvent	String (phrase)	
CPEM.T	Temperature	Numeric range	ºC
CPEM.P	Pressure	Numeric range	Torr
CPEM.ED	Entry Date	String (phrase)	

Type of Indexing:
Group Code

2.5.2.2.3.1. Complex Phase Equilibria Description (CPEM.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Solid-vapour phase equilibrium
- Liquid-solid-vapour phase diagram
- Liquid-solid-vapour phase equilibrium
- Triple point
- Quadruple point
- Phase equilibrium

Type of Indexing:

String (phrase)

2.5.2.3. Liquid/Liquid Systems (MCS) (LLSM)

Description:
This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database, concerned with the properties of liquid/liquid systems.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
LLSM.KW	Description	String (phrase)	
LLSM.PB	Partner BRN	Numeric	
LLSM.PA	Partner	String (wordwise)	
LLSM.SOL	Solvent	String (phrase)	
LLSM.T	Temperature	Numeric (range)	ºC
LLSM.P	Pressure	Numeric (range)	Torr

Type of Indexing:
Group Code

2.5.2.3.1. Liquid/Liquid Systems Description (MCS)(LLSM.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Liquid/liquid phase diagram
- Solution equilibrium
- Critical solution temperature
- Temperature of separation
- Equilibrium of liquid phases
- Distribution between solvent 1 + 2
- Solubility diagram
- Critical mixing temperature(s)
- Critical demixing temperature(s)

Type of Indexing:

String (phrase)

2.5.2.4. Liquid/Solid Systems (MCS) (LSSM)

Description:
This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database, concerned with the properties of liquid/solid systems.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
LSSM.KW	Description	String (phrase)	
LSSM.PB	Partner BRN	Numeric	
LSSM.PA	Partner	String (wordwise)	
LSSM.SOL	Solvent	String (phrase)	
LSSM.T	Temperature	Numeric	ºC
LSSM.P	Pressure	Numeric (range)	Torr

Type of Indexing:
Group Code

2.5.2.4.1. Liquid/Solid Systems Description (MCS)(LSSM.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Liquid/solid phase diagram
- Melting diagram
- Solidification diagram
- Solidification points of mixtures
- Eutectic
- Liquid-solid phase equilibrium
- Melting points
- Glass transition temperature(s)
- Phase transition temperature(s)

Type of Indexing:

String (phrase)

2.5.2.5. Mechanical & Physical Properties (MCS) (MECM)

Description:
This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database, concerned with mechanical and physical properties.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
MECM.KW	Description	String (phrase)	
MECM.PB	Partner BRN	Numeric	
MECM.PA	Partner	String (wordwise)	
MECM.SOL	Solvent	String (phrase)	
MECM.T	Temperature	Numeric (range)	°C
MECM.P	Pressure	Numeric (range)	Torr

Type of Indexing:
Group Code

2.5.2.5.1. Mechanical & Physical Properties Description (MCS)(MECM.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Volume change on mixing
- Partial molal volume
- PVT Relationship
- Virial coefficients
- Adiabatic compressibility
- Isothermal compressibility
- Excess partial molal volume
- Apparent molal volume
- Apparent specific volume
- Second virial coefficient(s) of the equation of state

- Third virial coefficient(s) of the equation of state
- Fourth virial coefficient(s) of the equation of state
- Ultrasonic velocity
- Hypersonic velocity
- Ultrasonic absorption
- Hypersonic absorption
- Acoustic relaxation time

Type of Indexing:
String (phrase)

2.5.2.6. Transport Phenomena (MCS) (TRAM)

Description:
This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database, concerned with transport phenomena.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
TRAM.PB	Partner BRN	Numeric	
TRAM.PA	Partner	String (wordwise)	
TRAM.SOL	Solvent	String (phrase)	
TRAM.T	Temperature	Numeric (range)	ºC
TRAM.P	Pressure	Numeric (range)	Torr
TRAM.KW	Description	String (phrase)	

Type of Indexing:

Group Code

2.5.2.6.1. Transport Phenomena Description (MCS)(TRAM.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Viscosity
- Diffusion
- Thermal diffusion

- Dynamic viscosity
- Kinematic viscosity
- Bulk viscosity
- Diffusion coefficient
- Binary diffusion coefficient
- Interdiffusion
- Thermal diffusion factor
- Thermal diffusion (Soret coefficient)
- Diffusion thermoeffect (Dufour effect)
- Thermal conductivity

Type of Indexing:

String (phrase)

2.5.2.7. Energy Data (MCS) (ENEM)

Description:
This field identifier is a group code for Field Availability searches in the hierarchical system of the Beilstein database, concerned energy with data.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
ENEM.KW	Description	String (phrase)	
ENEM.PB	Partner BRN	Numeric	
ENEM.PA	Partner	String (wordwise)	
ENEM.SOL	Solvent	String (phrase)	
ENEM.T	Temperature	Numeric (range)	ºC
ENEM.P	Pressure	Numeric (range)	Torr

Type of Indexing:
Group Code

2.5.2.7.1. Energy Data Description (MCS)(ENEM.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Enthalpy of solution
- Enthalpy of mixing
- Enthalpy of dilution
- Enthalpy of evaporation
- Heat capacity of mixtures
- Enthalpy of mixtures
- Entropy of mixtures
- Excess thermochemical parameter
- Thermodynamic properties of system with
- Partial molar enthalpy of mixing
- Heat capacity Cp
- Heat capacity Cv
- Excess heat capacity Cp
- Molar excess Gibbs free energy

Type of Indexing:

String (phrase)

2.5.2.8. Electrical Data (EDM)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
EDM.KW	Description	String (phrase)	
EDM.PB	Partner BRN	Numeric	
EDM.PA	Partner	String (wordwise)	

EDM.SOL	Solvent	String (phrase)	
EDM.T	Temperature	Numeric range	ºC
EDM.P	Pressure	Numeric range	Torr

Type of Indexing:
Group Code

2.5.2.8.1. Electrical Data Description (EDM.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Dielectric constant
- Dielectric loss
- Angle of dielectric loss

Type of Indexing:

String (phrase)

2.5.2.9. Optical Data (ODM)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
ODM.KW	Description	String (phrase)	
ODM.PB	Partner BRN	Numeric	
ODM.PA	Partner	String (wordwise)	
ODM.SOL	Solvent	String (phrase)	
ODM.T	Temperature	Numeric range	ºC
ODM.P	Pressure	Numeric range	Torr

Type of Indexing:
Group Code

2.5.2.9.1. Optical Data Description (ODM.KW)

Description:

This field contains keywords from the following list of controlled terms:

Kerr constant

Type of Indexing:

String (phrase)

2.5.2.10. Boundary Surface Phenomena (MCS) (BSPM)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
BSPM.PB	Partner BRN	Numeric	
BSPM.PA	Partner	String (wordwise)	
BSPM.SOL	Solvent	String (phrase)	
BSPM.T	Temperature	Numeric (range)	ºC
BSPM.P	Pressure	Numeric (range)	Torr
BSPM.KW	Description	String (phrase)	

Type of Indexing:
Group Code

2.5.2.10.1. Boundary Surface Phenomena Description(MCS)(BSPM.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Surface tension
- Surface potential
- Surface moment
- Pressure-surface isotherm
- Spreading pressure
- Interfacial tension

- Contact angle with compound
- Boundary surface phenomena
- Micellar weight
- Further surface properties

Type of Indexing:

String (phrase)

2.5.2.11. Adsorption (MCS) (ADSM)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
ADSM.PB	Partner BRN	Numeric	
ADSM.PA	Partner	String (wordwise)	
ADSM.SOL	Solvent	String (phrase)	
ADSM.T	Temperature	Numeric (range)	ºC
ADSM.P	Pressure	Numeric (range)	Torr
ADSM.KW	Description	String (phrase)	

Type of Indexing:
Group Code

2.5.2.11.1. Adsorption Description (MCS)(ADSM.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Adsorption
- Adsorption isotherm
- Chemisorption
- Enthalpy of adsorption
- Further physical properties of the adsorbed molecule
- Desorption

- Adsorption and desorption isotherms
- Rate of adsorption
- Desorption isotherm(s)
- Rate of desorption

Type of Indexing:

String (phrase)

2.5.2.12. Association (MCS) (ASSM)

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

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing	Unit
ASSM.PB	Partner BRN	Numeric	
ASSM.PA	Partner	String (wordwise)	
ASSM.SOL	Solvent	String (phrase)	
ASSM.T	Temperature	Numeric (range)	ºC
ASSM.P	Pressure	Numeric (range)	Torr
ASSM.KW	Description	String (phrase)	

Type of Indexing:
Group Code

2.5.2.12.1. Association Description (MCS)(ASSM.KW)

Description:

This field contains keywords from the following list of controlled terms:

- Association with compound
- Stability constant of the complex with ...
- Enthalpy of association
- Dipole moment of the complex
- Spectrum of the complex
- Further physical properties of the complex

- Exciplex formation
- IR spectrum of the complex
- NMR spectrum of the complex
- UV/VIS spectrum of the complex

Type of Indexing:

String (phrase)

2.6. Pharmacological and Ecological Data (PED)

Description:

Information on the influence of chemical substances and their behavior in the environment (man, animal, plant) is of vital importance in drug research as well as in the protection of the environment. For example it helps to plan the synthesis and evaluation of new therapeutic agents more efficiently with regard to health and environmental effects.

The influence of chemical substances on the living species can have desired therapeutic effects as well as adverse toxic results. This property is described in Pharmacological Data and Ecotoxicology. Their behavior in the non-living ecosystems such as air, soil and water are rather more complex and must be described in several properties of Ecological Data.

This field PED is a group code for Field Availability searches in the hierarchical system of the Beilstein database concerned with pharmacology, ecological chemistry and use.

Pharmacological data (PHARM)

Ecological data (ECO)

Ecotoxicology (ECT)

Exposure (EXP)

Exposure assessment (ECA)

Concentrations in the environment (ECC)

Mobility (MOBIL)

Transport and distribution (ECTD)

Bioaccumulation, biomagnification and biomonitoring (BIO)

Transformation and degradation (DEG)

Biodegradation (BIOD)

Abiotic degradation, hydrolysis (ECDH)

Abiotic degradation, photolysis (ECDP)

Stability in soil (ECS)

Oxygen demand (EOD)

Use (USE)

Laboratory Use and Handling (USE.LH)

Use Pattern (USE.PT)

2.6.1. Pharmacological Data (PHARM)

Description:
Pharmacological Data focus on human and mammalian pharmacology and toxicology, i.e. both therapeutic and toxic effects of chemical substances as well as studies on pharmacodynamics and pharmacokinetics are included. Examinations with bacteria or enzymes concerning human pathology are also regarded.

Associated Parameter Fields:

Field Code	**Full Name**	**Type of** Indexing
PHARM.E	Effect	String (phrase)
PHARM.EP	Endpoint	String (phrase)
PHARM.SP	Species or Test-System	String (phrase)
PHARM.S	Sex	String (phrase)
PHARM.RA	Route of Application	String (phrase)
PHARM.C	Concentration	String (phrase)
PHARM.KD	Kind of Dosing	String (wordwise)
PHARM.EX	Exposure Period	String (phrase)
PHARM.MR	Method	String (wordwise)
PHARM.FD	Further Details	String (wordwise)
PHARM.H	Half-life Time	String (phrase)
PHARM.TY	Type	String (phrase)
PHARM.V	Value of Type	String (phrase)
PHARM.RE	Results	String (wordwise)
PHARM.BRN	Metabolite BRN	Numeric
PHARM.META	Metabolite	String (wordwise)
PHARM.COM	Comment	String (wordwise)

2.6.1.1. Endpoint of Effect (PHARM.EP)

Description:
The investigation endpoint at which the effect was recorded is entered in this field. It is an observable or measurable biological or chemical event used as an index of the effect on a cell, tissue, organ, organism, etc.

Type of Indexing:

String (phrase)

2.6.1.2. Effect (PHARM.E)

Description:
This field contains effects from the areas of pharmacodynamics, pharmacokinetics and human toxicology. Both therapeutic and adverse effects are concerned. The entries are either keywords taken from a list or free-texts corresponding to original author's designations.
Type of Indexing:

String (phrase)

2.6.1.3. Species or Test-System (PHARM.SP)

Description:
Species or Test-Systems in Pharmacological Data are in general mammals, human or their isolated organs or cells. Microorganisms or enzymes concerning human pathology are also considered. Species are entered by means of the systematic (Latin) names and, if available, the English trivial name. For the entry of a test system the author's designation is used.
Type of Indexing:

String (phrase)

2.6.1.4. Sex (PHARM.S)

Description:

Information on the sex of the test species is entered in this field.

Type of Indexing:

String (phrase)

2.6.1.5. Route of Application (PHARM.RA)

Description:
This field provides information relating to the method of application of the substances under investigation such as per oral, subcutaneous, intravenous, etc.
Type of Indexing:

String (phrase)

2.6.1.6. Concentration (PHARM.C)

Description:
The administered test concentration or starting concentration is entered in this field.

Type of Indexing:

String (phrase)

2.6.1.7. Kind of Dosing (PHARM.KD)

Description:
This field contains special or explanatory information on the dosing, e.g. twice daily for the first 2 days then once daily for the following 3 days.
Type of Indexing:

String (wordwise)

2.6.1.8. Exposure Period (PHARM.EX)

Description:
This field generally describes the whole period of examination starting from the time-point of administration of the test substance. Other time-periods like incubation times, pre- or post-observation times, if available, are entered in the field "Method".
Type of Indexing:

String (phrase)

2.6.1.9. Method (PHARM.MR)

Description:
This field contains a comprehensive summary of the test procedure. It gives details about the method of investigation (e.g. hot plate test, Ames test, Western Blot) as well as explanatory information on test parameters such as number of animals exposed, age, weight, housing and feeding conditions, etc. If measurements were carried out according to EC, OECD, ISO or DIN guidelines or to Good Laboratory Practice regulations (GLP), this information is also included.

Type of Indexing:
String (wordwise)

2.6.1.10. Further Details (PHARM.FD)

Description:
This field offers further details about the investigated effect, test method as well as explanations for abbreviations used in other free-text fields.
Type of Indexing:
String (wordwise)

2.6.1.11. Half-life Time (PHARM.H)

Description:
The time required for the initial concentration of a test substance present in an organism to decrease by one-half through biological processes such as metabolism and excretion.
Type of Indexing:

Numeric (range)

2.6.1.12. Type (PHARM.TY)

Description:
This field contains specific dose designations derived from dose-response curves like LD_{50}, EC_{50}, LOEC, etc. Such Numeric parameters are particularly useful for comparing the potency of different substances causing the same effect on the same species or the potency of the same substance on different species.
LD_{50}: the quantity of a substance that causes the death of 50% of the subjects examined (lethal dose/ kg weight).
EC_{50}: the concentration of a substance (measured in air or water) that causes a specific effect/reaction on 50% of the subjects examined.
LOEC: abbreviation for "lowest observed effect concentration". It indicated the lowest concentration at which an effect is observable.
Type of Indexing:

String (phrase)

2.6.1.13. Value of Type (PHARM.V)

Description:
The Numeric value of the corresponding type is entered in this field.

Type of Indexing:

String (phrase)

2.6.1.14. Results (PHARM.RE)

Description:
Results which are not available in Numeric form, or other information related to Numeric entries are entered as free-text in this field. If there were no effects detected from the investigation this (negative) result is entered in the field "Comment".
Type of Indexing:
String (wordwise)

2.6.1.15. Metabolite BRN (PHARM.BRN)

Description:
Information on Metabolites from pharmacokinetic studies is given in form of the hyperlinked BRN numbers (PHARM.BRN) together with the related chemical names (PHARM.META).
Type of Indexing:

Numeric

2.6.1.16. Metabolite (PHARM.META)

Description:
Information on Metabolites from pharmacokinetic studies is given in form of the hyperlinked BRN numbers together with the related chemical names.
Type of Indexing:
String (wordwise)

2.6.1.17. Comment (PHARM.COM)

Description:
Data of the properties Biological Function (BF) and Toxicity (TOX) of the previous data-structure are stored in this field. Their indexing and searchability remain the same as before despite the new arrangement of the data-structure.
Type of Indexing:
String (wordwise)

2.6.2. Ecological Data (ECO)

Description:
Ecological Data are concerned with effects and interactions of chemical substances, especially environmental chemicals, with living and non-living nature. The influences of a substance on the ecosystems like air, soil and water are estimated by measurement of its toxic effects (ecotoxicology) on specific indicator species such as birds, earthworms and fish. Its behaviors in the environment for instance its distribution, accumulation potentials and transformation are also focal points of research in the ecological chemistry.
This field ECO is a group code for Field Availability searches in the hierarchical system of the Beilstein database. It comprises the following sub-topics:

Associated Parameter Fields:

Full Name	Field Code
Ecotoxicology	ECT
Exposure	EXP
Mobility	MOBIL
Transformation and Degradation	DEG

Refer to the hierarchical listing, which you can request with the LIST function for information on fields included in this group code.

Type of Indexing:
Group Code

2.6.2.1. Ecotoxicology (ECT)

Description:
Ecotoxicology is a sub-division of toxicology. It concentrates on the toxic effects of chemical substances on organisms, which are indicators for the degree of pollution in an ecosystem (air, soil, and water). Typical species are fish and daphnia for water, earthworms for soil and birds for air. Its aim is to reveal structural and functional changes in the ecosystems due to the effects of chemical substances.
Ecotoxicological Data are stored in the following fields:

Field Code	Full Name	Type of Indexing
ECT.E	Effect	String (phrase)
ECT.EP	Endpoint of Effect	String (phrase)
ECT.SP	Species or Test-System	String (phrase)
ECT.S	Sex	String (phrase)
ECT.RA	Route of Application	String (phrase)
ECT.C	Concentration	String (phrase)

ECT.KD	Kind of Dosing	String (wordwise)
ECT.EX	Exposure Period	String (phrase)
ECT.MR	Method	String (wordwise)
ECT.FD	Further Details	String (wordwise)
ECT.TY	Type	String (phrase)
ECT.V	Value of Type	String (phrase)
ECT.RE	Results	String (wordwise)
ECT.BRN	Metabolite BRN	Numeric
ECT.META	Metabolite	String (wordwise)

2.6.2.1.1. Effect (ECT.E)

Description:
This field contains toxic effects from the area of ecotoxicology. The entries are either keywords taken from a list or free-texts corresponding to original author's designations.
Type of Indexing:

String (phrase)

2.6.2.1.2. Endpoint of Effect (ECT.EP)

Description:
The investigation endpoint at which the effect was recorded is entered in this field. It is an observable or measurable biological or chemical event used as an index of the effect on a cell, tissue, organ, organism, etc.
Type of Indexing:

String (phrase)

2.6.2.1.3. Species or Test-System (ECT.SP)

Description:
Species or Test-Systems in Ecotoxicology are aquatic, terrestrial and aerial non-mammalian representatives of the food chain, which are used as indicators for the pollution degree of ecosystems. Typical species are fish and daphnia for water, earthworms for soil and birds for air. Also included are plants and microorganisms like ground bacteria or sludge inoculi.
Species are entered by means of the systematic (Latin) names and, if available, the English trivial name. For the entry of a test system such as cells, isolated organs the author's designation is used.
Type of Indexing:

String (phrase)

2.6.2.1.4. Sex (ECT.S)

Description:
Information on the sex of the test species is entered in this field.
Type of Indexing:

String (phrase)

2.6.2.1.5. Route of Application (ECT.RA)

Description:
This field provides information relating to the method of application of the substance under investigation such as per oral, skin absorption, inhalation, etc.
Type of Indexing:

String (phrase)

2.6.2.1.6. Concentration (ECT.C)

Description:
The administered test concentration or starting concentration is entered in this field.
Type of Indexing:

String (phrase)

2.6.2.1.7. Kind of Dosing (ECT.KD)

Description:
This field contains special or explanatory information on the dosing, e.g. test substance dissolved in corn oil, administered twice daily for the first 2 days then once daily for the following 3 days.
Type of Indexing:

String (wordwise)

2.6.2.1.8. Exposure Period (ECT.EX)

Description:
This field generally describes the whole period of examination starting from the time-point of administration of the test substance. Other time-periods like incubation times, pre- or post-observation times, if available, are entered in the field "Method" (ECT.MR).
Type of Indexing:

String (phrase)

2.6.2.1.9. Method (ECT.MR)

Description:
This field contains a comprehensive summary of the test procedure. It gives details about the method of investigation (e.g. spray test, Microtox test, ELISA) as well as explanatory information on test parameters such as number of animals exposed, housing conditions, water or soil parameters (type, pH, temperature), etc. If measurements were carried out according to EC, OECD, ISO or DIN guidelines or to Good Laboratory Practice regulations (GLP), this information is also included.

Type of Indexing:
String (wordwise)

2.6.2.1.10. Further Details (ECT.FD)

Description:
This field offers further details about the investigated effect, test method as well as explanations for abbreviations used in other free-text fields.

Type of Indexing:
String (wordwise)

2.6.2.1.11. Type (ECT.TY)

Description:
This field contains specific dose designations derived from dose-response curves like LD_{50}, EC_{50}, LOEC, etc. Such Numeric parameters are particularly useful for comparing the potency of different substances causing the same effect on the same species or the potency of the same substance on different species.

LD_{50}: the quantity of a substance that causes the death of 50% of the subjects examined (lethal dose/ kg weight).

EC_{50}: the concentration of a substance (measured in air or water) that causes a specific effect/reaction on 50% of the subjects examined.

LOEC: abbreviation for "lowest observed effect concentration". It indicated the lowest concentration at which an effect is observable.

Type of Indexing:

String (phrase)

2.6.2.1.12. Value of Type (ECT.V)

Description:
The Numeric value of the corresponding type is entered in this field.

Type of Indexing:

String (phrase)

2.6.2.1.13. Results (ECT.RE)

Description:
Results given in non-numerical form or other information related to Numeric entries are entered as free-text in this field.
Type of Indexing:
String (wordwise)

2.6.2.1.14. Metabolite BRN (ECT.BRN)

Description:
Information on Metabolites from toxicocokinetic studies is given in form of the hyperlinked BRN numbers (ECT.BRN) together with the related chemical names (ECT.META).
Type of Indexing:

Numeric

2.6.2.1.15. Metabolite (ECT.META)

Description:
Information on Metabolites from toxicocokinetic studies is given in form of the hyperlinked BRN numbers together with the related chemical names.
Type of Indexing:
String (wordwise)

2.6.2.2. Exposure (EXP)

Description:
Living organisms or individuals may come into contact with hazardous chemicals through air, soil, water and consumer products, including occupational or workplace exposure. To determine the degree of pollution knowledge or observations about distribution and release of chemicals from contamination sources (exposure assessment) as well as their concentrations in the environment are required.
This field EXP is a group code for Field Availability searches in the hierarchical system of the Beilstein database. It comprises the following sub-topics:

Full Name	Field Code
Exposure Assessment	ECA
Concentrations in the Environment	ECC

Refer to the hierarchical listing, which you can request with the LIST function for information on fields included in this group code.
Type of Indexing:
Group Code

2.6.2.2.1. Exposure Assessment (ECA)

Description:
The property Exposure Assessment describes the spread of pollution originating from natural or synthetic substances or sources, e.g. the contamination of chicken feed with dioxins and PCBs due to careless handling, or emission of volatile organic compounds from landfill sites into the atmosphere.
Exposure Assessment contains the following fields:

Field Code	Full Name	Type of Indexing
ECA.HE	Exposure	String (wordwise)
ECA.SO	Sources	String (wordwise)

2.6.2.2.1.1. Exposure (ECA.HE)

Description:

Knowledge or observations about distribution of substances in the environmental compartments (air, soil, water).

Type of Indexing:

String (wordwise)

2.6.2.2.1.2. Sources (ECA.SO)

Description:

Sources such as landfill sites, spoil heaps, factories, power stations, and environmental compartments such as air, soil, water from which pollution originates are entered in this field. If available also geographical locations and the name of the offenders are provided.

Type of Indexing:

String (wordwise)

2.6.2.2.2. Concentrations in the Environment (ECC)

Description:
This property gives information on the degree of pollution by hazardous chemicals in the living organisms or non-living environmental compartments.

Associated Parameter Fields:

Field Code	Full Name	Type of Indexing
ECC.SP	Species	String (phrase)

ECC.ME	Media	String (phrase)
ECC.LO	Location	String (phrase)
ECC.CC	Contamination Concentration	String (phrase)
ECC.BC	Background Concentration	String (phrase)
ECC.MR	Method, Remarks	String (wordwise)

2.6.2.2.2.1. Species (ECC.SP)

Description:

Species are entered by means of the systematic (Latin) names and, if available, the English trivial name.

Type of Indexing:

String (phrase)

2.6.2.2.2.2. Media (ECC.ME)

Description:

The medium could be an environmental compartment such as sediment, seawater, sewage sludge or contaminated food.

Type of Indexing:
String (phrase)

2.6.2.2.2.3. Location (ECC.LO)

Description:

The exact place where the investigation took place is entered in this field.

Type of Indexing:

String (phrase)

2.6.2.2.2.4. Contamination Concentration (ECC.CC)

Description:

This field contains the measured concentrations founded in the investigated species or medium as an indication for the degree of pollution.

Type of Indexing:

String (phrase)

2.6.2.2.2.5. Background Concentration (ECC.BC)

Description:

If a Numeric value for background pollution (normal pollution) is available, this field is filled out.

Type of Indexing:

String (phrase)

2.6.2.2.2.6. Method, Remarks (ECC.MR)

Description:

This field gives details about the method of investigation as well as additional information on species, location or media. If measurements were carried out according to EC, OECD, ISO or DIN guidelines or to Good Laboratory Practice regulations (GLP), this information is also included.

Type of Indexing:

String (wordwise)

2.6.2.3. Mobility (MOBIL)

Description:

The environmental impact of a substance is determined by its ability to move through the environment. This movement depends on the affinity of the chemical toward particular environmental compartments (e.g. soil, sediment) or certain parts of organisms (e.g. livers, tissues). The spread of a substance in soil, air and aquatic systems by way of physical processes like absorption, desorption, dispersion are described in the property Transport and Distribution. Its accumulation potentials in the living organisms are entered in the property Bioaccumulation, Biomagnification and Biomonitoring.

This field MOBIL is a group code for Field Availability searches in the hierarchical system of the Beilstein database. It comprises the following

Field Code	Full Name
ECTD	Transport and Distribution
BIO	Bioaccumulation, Biomagnification and Biomonitoring

Refer to the hierarchical listing, which you can request with the LIST function for information on fields included in this group code.

Type of Indexing:

Group Code

2.6.2.3.1. Transport and Distribution (ECTD)

Description:
This property describes the transport and distribution of chemical substances, especially environmental chemicals, in the non-living environment (air, soil, water) by way of physical processes like absorption, desorption, dispersion, etc.
This property contains the following fields:

Field Code	Full Name	Type of Indexing
ECTD.TY	Type	String (phrase)
ECTD.ME	Media	String (phrase)
ECTD.RE	Results	String (wordwise)
ECTD.MR	Method, Remarks	String (wordwise)

2.6.2.3.1.1. Type (ECTD.TY)

Description:

This field is meant for entries such as adsorption, desorption, volatility, dispersion, etc.

Type of Indexing:

String (phrase)

2.6.2.3.1.2. Media (ECTD.ME)

Description:

This field gives information on which environmental compartments were involved in the transport and distribution processes, e.g. soil-air, water-air, or soil-water, etc.

Type of Indexing:
String (phrase)

2.6.2.3.1.3. Results (ECTD.RE)

Description:

Results concerning phase transitions and whereabouts of the investigated substance in each environmental compartment are entered in this field.

Type of Indexing:
String (wordwise)

2.6.2.3.1.4. Method, Remarks (ECTD.MR)

Description:

Information on the method of investigation or applied computer models is entered in this field. If measurements were carried out according to EC, OECD, ISO or DIN guidelines or to Good Laboratory Practice regulations (GLP), this information is also included.

Type of Indexing:
String (wordwise)

2.6.2.3.2. Bioaccumulation, Biomagnification and Biomonitoring (BIO)

Description:
This property contains bioaccumulation, biomagnification and biomonitoring data.

Bioaccumulation is the ability of organisms to concentrate substances within themselves. The bioaccumulation is a result of two processes: accumulation and elimination, whereby the rate of intake exceeds the organism's ability to remove the substance from the body. A characteristic measure is the Bioconcentration Factor (BCF).
Biomagnification is a sequence of processes in an ecosystem by which higher concentrations of chemical substances are attained in organisms at higher trophic level in the food chain (plants, herbivores, carnivores).
Biomonitoring has the objective that the appearance of substances (and their damaging influences) is comprehensively monitored. This is achieved by the use of bioindicators (birds, fish, lichens, etc.) or biomarkers (CYP1A induction, metallothioneine, DNA-adducts, etc.)
Bioaccumulation data are stored in several fields, whereas Biomagnification (BIO.MAG) and Biomonitoring (BIO.MON) are free-text fields.
Following fields are comprised in this property:

Field Code	Full Name	Type of Indexing	Unit
BIO.SP	Species	String (phrase)	
BIO.ME	Media	String (phrase)	
BIO.C	Concentration	String (phrase)	
BIO.E	Exposure Period	String (phrase)	
BIO.T	Temperature	Numeric (range)	°C
BIO.BC	Bioconcentration Factor (BCF)	Numeric	
BIO.LOG	Log BCF	Numeric	
BIO.A	Accumulation Half-life Time	String (phrase)	
BIO.AR	Accumulation Rate Constant	String (phrase)	
BIO.H	Elimination Half-life Time	String (phrase)	

BIO.ER	Elimination Rate Constant	String (phrase)	
BIO.MR	Method, Remarks	String (wordwise)	
BIO.MAG	Biomagnification	String (wordwise)	
BIO.MON	Biomonitoring	String (wordwise)	

2.6.2.3.2.1. Species (BIO.SP)

Description:

The organism's name for the bioaccumulative investigation is entered in this field. Species are entered by means of the systematic (Latin) names and, if available, the English trivial name. In the absence of the Latin name the author's designation is used.

Type of Indexing:

String (phrase)

2.6.2.3.2.2. Media (BIO.ME)

Description:

Media for the bioaccumulative investigation are reference compartments such as surrounding water, soil or contaminated food.

Type of Indexing:
String (phrase)

2.6.2.3.2.3. Concentration (BIO.C)

Description:

The starting concentration for the bioaccumulative investigation is entered in this field.

Type of Indexing:

String (phrase)

2.6.2.3.2.4. Exposure Period (BIO.E)

Description:

This field describes the whole period of the bioaccumulative study.

Type of Indexing:

String (phrase)

2.6.2.3.2.5. Temperature (BIO.T)

Description:

The temperature at which the bioaccumulative investigation took place is entered in this field.

Type of Indexing:

Numeric (range)

2.6.2.3.2.6. Bioconcentration Factor (BIO.BC)

Description:

Bioconcentration Factor is a measure for the characterization of the accumulation of a chemical in an organism. It is defined as the concentration of a chemical in an organism (plants, microorganisms, animals) divided by the concentration in a reference compartment (e.g. food, surrounding water).

Type of Indexing:

Numeric (range)

2.6.2.3.2.7. Log BCF (BIO.LOG)

Description:

The corresponding logarithmic form of the bioconcentration factor.

Type of Indexing:

Numeric (range)

2.6.2.3.2.8. Accumulation Half-life Time (BIO.A)

Description:

Bioaccumulation is a result of two processes: accumulation and elimination. The half-life time of the accumulation process of a chemical in an organism or part of an organism is entered in this field.

Type of Indexing:

Numeric (range)

2.6.2.3.2.9. Accumulation Rate Constant (BIO.AR)

Description: The corresponding rate constant of the accumulation process.

Type of Indexing:

String (phrase)

2.6.2.3.2.10. Elimination Half-life Time (BIO.H)

Description:

Bioaccumulation is a result of two processes: accumulation and elimination. The half-life time of the elimination process of a chemical from the body of an organism is entered in this field.

Type of Indexing:

String (phrase)

2.6.2.3.2.11. Elimination Rate Constant (BIO.ER)

Description:

The corresponding rate constant of the elimination process.

Type of Indexing:

String (phrase)

2.6.2.3.2.12. Method, Remarks (BIO.MR)

Description:

This field provides information on the measurement methods with the related conditions and/or parameters.

Type of Indexing:
String (wordwise)

2.6.2.3.2.13. Biomagnification (BIO.MAG)

Description:

A sequence of processes in an ecosystem by which higher concentrations of chemical substances are attained in organisms at higher trophic level in the food chain (plants, herbivores, carnivores).

Type of Indexing:

String (wordwise)

2.6.2.3.2.14. Biomonitoring (BIO.MON)

Description:

Biomonitoring has the objective that the appearance of substances (and their damaging influences) is comprehensively monitored. This is achieved by the use of bioindicators (birds, fish, lichens, etc.) or biomarkers (CYP1A induction, metallothioneine, DNA-adducts, etc.)

Type of Indexing:

String (wordwise)

2.6.2.4. Transformation and Degradation (DEG)

Description:

Transformation and Degradation of chemical substances, especially environmental chemicals, are processes of decomposition by chemical, photochemical or biological reactions. The chemical transformations due to oxidation, reduction or hydrolysis are described in the property Abiotic Degradation, Hydrolysis. Information on photolytic transformations is stored in the property Abiotic Degradation, Photolysis. The property Biodegradation characterizes the ability of microorganisms to metabolize xenobiotic compounds. Examinations on the persistence in soil or water are included in the property Stability in Soil or Oxygen Demand, respectively.

This field DEG is a group code for Field Availability searches in the hierarchical system of the Beilstein database. It comprises the following sub-topics:

Field Code	Full Name
BIOD	Biodegradation
ECDH	Abiotic Degradation, Hydrolysis
ECDP	Abiotic Degradation, Photolysis
ECS	Stability in Soil
EOD	Oxygen Demand

Refer to the hierarchical listing, which you can request with the LIST function for information on fields included in this group code.

Type of Indexing:

Group Code

2.6.2.4.1. Biodegradation (BIOD)

Description:
Biodegradation describes the degradation of an organic substance to smaller molecules or to inorganic substances by microorganisms. This can occur by means of aerobic (i.e. in the presence of molecular oxygen) or anaerobic degradation. In a complete microbial transformation a xenobiotic organic compound is mineralized to CO_2, H_2O, etc.
The property Biodegradation contains the following fields:

Field Code	Full Name	Type of Indexing	Unit
BIOD.TY	Type	String (phrase)	
BIOD.IN	Inoculum	String (phrase)	
BIOD.C	Concentration	String (phrase)	
BIOD.D	Degradation Rate	String (phrase)	%
BIOD.E	Exposure Period	String (phrase)	
BIOD.T	Temperature	Numeric (range)	°C
BIOD.H	Half-life Time	String (phrase)	
BIOD.BRN	Degradation Product BRN	Numeric	
BIOD.DP	Degradation Product	String (wordwise)	
BIOD.MR	Method, Remarks	String (wordwise)	

2.6.2.4.1.1. Type (BIOD.TY)

Description:

This field contains information on the type of biodegradation, e.g. aerobic, anaerobic.

Type of Indexing:

String (phrase)

2.6.2.4.1.2. Inoculum (BIOD.IN)

Description:

The microorganism culture used for carrying out experiments is entered in this field, e.g. activated sludge, sulfate reducing bacteria or Bacillus stearothermophilus BR325.

Type of Indexing:

String (phrase)

2.6.2.4.1.3. Concentration (BIOD.C)

Description:

The concentration at the beginning of the degradation process is entered in this field.

Type of Indexing:

String (phrase)

2.6.2.4.1.4. Degradation Rate (BIOD.D)

Description:

This field gives information on the measured degradation rate. It is the relative percentage of degradation referred to the starting concentration.

Type of Indexing:

String (phrase)

2.6.2.4.1.5. Exposure Period (BIOD.E)

Description:

The duration of the biodegradation process is stored in this field.

Type of Indexing:

String (phrase)

2.6.2.4.1.6. Temperature (BIOD.T)

Description:

The temperature at which the process took place is entered in this field.

Type of Indexing:

Numeric (range)

2.6.2.4.1.7. Half-life Time (BIOD.H)

Description:

The time at which the concentration has fallen to half of its starting value.

Type of Indexing:

Numeric (range)

2.6.2.4.1.8. Degradation Product BRN (BIOD.BRN)

Description:

Information on degradation products is given in form of the hyperlinked BRN numbers together with the related chemical names.

Type of Indexing:

Numeric

2.6.2.4.1.9. Degradation Product (BIOD.DP)

Description:

Information on degradation products is given in form of the hyperlinked BRN numbers together with the related chemical names.

Type of Indexing:

String (wordwise)

2.6.2.4.1.10. Method, Remarks (BIOD.MR)

Description:

This field gives details about the method of investigation as well as additional information on applied inoculum. If measurements were carried out according to EC, OECD, ISO or DIN guidelines or to Good Laboratory Practice regulations (GLP), this information is also included.

Type of Indexing:
String (wordwise)

2.6.2.4.2. Abiotic Degradation, Hydrolysis (ECDH)

Description:
The property Abiotic Degradation, Hydrolysis describes the degradation process via chemical reactions (oxidation, reduction, hydrolysis) without the participation of organisms.

This property contains the following fields:

Field Code	Full Name	Type of Indexing	Unit
ECDH.TY	Type	String (phrase)	
ECDH.C	Concentration	String (phrase)	
ECDH.D	Degradation Rate	String (phrase)	%
ECDH.E	Exposure Period	String (phrase)	

ECDH.T	Temperature	Numeric (range)	°C
ECDH.RC	Rate Constant	String (phrase)	
ECDH.PH	pH-Value	Numeric (range)	
ECDH.H	Half-life Time	String (phrase)	
ECDH.BRN	Degradation Product BRN	Numeric	
ECDH.DP	Degradation Product	String (wordwise)	
ECDH.MR	Method, Remarks	String (wordwise)	

2.6.2.4.2.1. Type (ECDH.TY)

Description:

This field contains information on the type of abiotic degradation via chemical reactions such as oxidation, reduction, and hydrolysis.

Type of Indexing:

String (phrase)

2.6.2.4.2.2. Concentration (ECDH.C)

Description:

The concentration at the beginning of the degradation process is entered in this field.

Type of Indexing:

String (phrase)

2.6.2.4.2.3. Degradation Rate (ECDH.D)

Description:

This field gives information on the measured degradation rate. It is the relative percentage of degradation referred to the starting concentration.

Type of Indexing:

String (phrase)

2.6.2.4.2.4. Exposure Period (ECDH.E)

Description:

The duration of the degradation process is stored in this field.

Type of Indexing:

String (phrase)

2.6.2.4.2.5. Temperature (ECDH.T)

Description:

The temperature at which the process took place is entered in this field.

Type of Indexing:

Numeric (range)

2.6.2.4.2.6. Rate Constant (ECDH.RC)

Description:

The rate constant of the degradation process is entered in this field.

Type of Indexing:

String (phrase)

2.6.2.4.2.7. pH-Value (ECDH.PH)

Description:

The pH value at which the process took place is entered in this field.

Type of Indexing:

Numeric (range)

2.6.2.4.2.8. Half-life Time (ECDH.H)

Description:

The time at which the concentration has fallen to half of its starting value.

Type of Indexing:

Numeric (range)

2.6.2.4.2.9. Degradation Product BRN (ECDH.BRN)

Description:

Information on degradation products is given in form of the hyperlinked BRN numbers together with the related chemical names.

Type of Indexing:

Numeric

2.6.2.4.2.10. Degradation Product (ECDH.DP)

Description:

Information on degradation products is given in form of the hyperlinked BRN numbers together with the related chemical names.

Type of Indexing:

String (wordwise)

2.6.2.4.2.11. Method, Remarks (ECDH.MR)

Description:

This field gives details about the method of investigation. If measurements were carried out according to EC, OECD, ISO or DIN guidelines or to Good Laboratory Practice regulations (GLP), this information is also included.

Type of Indexing:
String (wordwise)

2.6.2.4.3. Abiotic Degradation, Photolysis (ECDP)

Description:
The property Abiotic Degradation, Photolysis describes the degradation process via photochemical reactions such as photooxidation, photomineralisation without the participation of organisms.

This property contains the following fields:

Field Code	Full Name	Type of Indexing	Unit
ECDP.TY	Type	String (phrase)	
ECDP.C	Concentration	String (phrase)	
ECDP.D	Degradation Rate	String (phrase)	%
ECDP.E	Exposure Period	String (phrase)	
ECDP.T	Temperature	Numeric (range)	°C
ECDP.RC	Rate Constant	String (phrase)	
ECDP.PH	pH-Value	Numeric (range)	
ECDP.H	Half-life Time	String (phrase)	
ECDP.BRN	Degradation Product BRN	Numeric	
ECDP.DP	Degradation Product	String (wordwise)	
ECDP.MR	Method, Remarks	String (wordwise)	

2.6.2.4.3.1. Type (ECDP.TY)

Description:

This field contains information on the type of abiotic degradation via photochemical reactions, e.g. photooxidation, photoreduction, photomineralisation, etc.

Type of Indexing:

String (phrase)

2.6.2.4.3.2. Concentration (ECDP.C)

Description:

The concentration at the beginning of the degradation process is entered in this field.

Type of Indexing:

String (phrase)

2.6.2.4.3.3. Degradation Rate (ECDP.D)

Description:

This field gives information on the measured degradation rate. It is the relative percentage of degradation referred to the starting concentration.

Type of Indexing:

String (phrase)

2.6.2.4.3.4. Exposure Period (ECDP.E)

Description:

The duration of the degradation process is stored in this field.

Type of Indexing:

String (phrase)

2.6.2.4.3.5. Temperature (ECDP.T)

Description:

The temperature at which the process took place is entered in this field.

Type of Indexing:

Numeric (range)

2.6.2.4.3.6. Rate Constant (ECDP.RC)

Description:

The rate constant of the degradation process is entered in this field.

Type of Indexing:

String (phrase)

2.6.2.4.3.7. pH-Value (ECDP.PH)

Description:

The pH value at which the process took place is entered in this field.

Type of Indexing:

Numeric (range)

2.6.2.4.3.8. Half-life Time (ECDP.H)

Description:

The time at which the concentration has fallen to half of its starting value.

Type of Indexing:

Numeric (range)

2.6.2.4.3.9. Degradation Product BRN (ECDP.BRN)

Description:

Information on degradation products is given in form of the hyperlinked BRN numbers together with the related chemical names.

Type of Indexing:

Numeric

2.6.2.4.3.10. Degradation Product (ECDP.DP)

Description:

Information on degradation products is given in form of the hyperlinked BRN numbers together with the related chemical names.

Type of Indexing:

String (wordwise)

2.6.2.4.3.11. Method, Remarks (ECDP.MR)

Description:

This field gives details about the method of investigation. If measurements were carried out according to EC, OECD, ISO or DIN guidelines or to Good Laboratory Practice regulations (GLP), this information is also included.

Type of Indexing:
String (wordwise)

2.6.2.4.4. Stability in Soil (ECS)

Description:
The property Stability in Soil characterizes the resistance or stability of a substance in the soil. Standardized soils are often used for measurement of specific dissipation times, after which 50, 90 or x% of a substance in a particular soil has disappeared.

This property includes the following fields:

Field Code	Full Name	Type of Indexing
ECS.TY	Type	String (phrase)
ECS.C	Concentration	String (phrase)
ECS.5	Dissipation Time 50	String (phrase)
ECS.9	Dissipation Time 90	String (phrase)
ECS.D	Dissipation	String (phrase)
ECS.E	Exposure Period	String (phrase)
ECS.T	Temperature	Numeric (range)
ECS.PH	pH-Value	Numeric (range)
ECS.HU	Humidity	String (phrase)
ECS.OC	Organic Carbon	String (phrase)
ECS.CE	Cation Exchange Rate	String (phrase)
ECS.MB	Microbial Biomass	String (phrase)
ECS.MR	Method, Remarks	String (wordwise)

2.6.2.4.4.1. Type (ECS.TY)

Description:

This field contains information on the type of soil, e.g. sandy loam, loam, mud, etc.

Type of Indexing:

String (phrase)

2.6.2.4.4.2. Concentration (ECS.C)

Description:

The starting concentration of the substance under investigation is entered in this field.

Type of Indexing:

String (phrase)

2.6.2.4.4.3. Dissipation Time 50 (ECS.5)

Description:

The time at which 50 % of the test substance has disappeared.

Type of Indexing:

String (phrase)

2.6.2.4.4.4. Dissipation Time 90 (ECS.9)

Description:

The time at which 90 % of the test substance has disappeared.

Type of Indexing:

String (phrase)

2.6.2.4.4.5. Dissipation (ECS.D)

Description:

This field gives information on the relative percentage of dissipation referred to the starting concentration.

Type of Indexing:

String (phrase)

2.6.2.4.4.6. Exposure Period (ECS.E)

Description:

The duration of the process is stored in this field.

Type of Indexing:

String (phrase)

2.6.2.4.4.7. Temperature (ECS.T)

Description:

The temperature at which the investigation took place is entered in this field.

Type of Indexing:

Numeric (range)

2.6.2.4.4.8. pH-Value (ECS.PH)

Description:

The pH-value of the investigated soil is entered in this field

Type of Indexing:

Numeric (range)

2.6.2.4.4.9. Humidity (ECS.HU)

Description:

The humidity content of soil expressed as a percentage of the oven-dry mass of soil is entered in this field.

Type of Indexing:

String (phrase)

2.6.2.4.4.10. Organic Carbon (ECS.OC)

Description:

The of the mass of organic carbon expressed as a percentage of the mass of soil is entered in this field

Type of Indexing:

String (phrase)

2.6.2.4.4.11. Cation Exchange Rate (ECS.CE)

Description:

Cation exchange

The interchange between a cation in solution and another cation in the boundary layer between the solution and surface of negatively charged material such as clay or organic matter.

Cation exchange rate (synonym: cation exchange capacity (CEC))

The total of exchangeable cations that a soil can absorb at a specific pH value. It is usually expressed in centimoles of charge per kilogram of exchanger (cmol/kg) or milliequivalents per 100grams (meq/100 g) of soil

Type of Indexing:

String (phrase)

2.6.2.4.4.12. Microbial Biomass (ECS.MB)

Description:

The total mass of living microorganisms in a given volume or mass of soil.

Type of Indexing:
String (phrase)

2.6.2.4.4.13. Method, Remarks (ECS.MR)

Description:

This field gives details about the method of investigation as well as information on non-numerical coding of the investigated soil. If measurements were carried out according to EC, OECD, ISO or DIN guidelines or to Good Laboratory Practice regulations (GLP), this information is also included.

Type of Indexing:
String (wordwise)

2.6.2.4.5. Oxygen Demand (EOD)

Description:
Oxygen demand studies are performed to determine the degree of pollution in an effluent of a sewage plant or a body of inland water. Oxygen Demand is differentiated into biochemical oxygen demand (BOD, German: BSB) and chemical oxygen demand (COD, German: CSB).
Biochemical Oxygen Demand is a measure of the oxygen requirement in microbial oxidation of organic substances contained in water. Usually BOD5 (5 days continuous measurement at 20°C in the dark) is reported.Chemical Oxygen Demand is a measure of the amount of oxygen required to oxidize organic and oxidizable inorganic compounds in water and wastewater. The amount of oxygen is provided by the addition of potassium dichromate.

This property includes the following fields:

Field Code	Full Name	Type of Indexing	Unit
EOD.TY	Type	String (phrase)	
EOD.RE	Related to	String (phrase)	

EOD.C	Concentration	String (phrase)	
EOD.D	Oxygen Demand	String (phrase)	Mg O_2/l
EOD.RAT	Ratio BOD5/COD	Numeric	
EOD.MR	Method, Remarks	String (wordwise)	

2.6.2.4.5.1. Type (EOD.TY)

Description:

This field contains information on the type of oxygen demand, e.g. BOD5, COD, etc.

Type of Indexing:

String (phrase)

2.6.2.4.5.2. Related to (EOD.RE)

Description:

Information about whether the studied oxygen demand refers to the test substance (usual case) or to COD (Chemical Oxygen Demand) or DOC (Dissolved Organic Carbon).

Type of Indexing:

String (phrase)

2.6.2.4.5.3. Concentration (EOD.C)

Description:

The starting concentration of the substance under investigation is entered in this field.

Type of Indexing:

String (phrase)

2.6.2.4.5.4. Oxygen Demand (EOD.D)

Description:

The measured value of oxygen demand corresponding to the above type is entered in this field.

Type of Indexing:

Numeric (range)

2.6.2.4.5.5. Ratio BOD5/COD (EOD.RAT)

Description:

This Numeric value serves as a gross measure for the biological degradability of chemical substances.

Type of Indexing:

Numeric (range)

2.6.2.4.5.6. Method, Remarks (EOD.MR)

Description:

This field gives details about the method of investigation as well as results in non-numerical form. If measurements were carried out according to EC, OECD, ISO or DIN guidelines or to Good Laboratory Practice regulations (GLP), this information is also included.

Type of Indexing:

String (wordwise)

2.6.3. Use (USE)

Description:

The property Use describes the use, application or handling of a substance
It contains the following fields:

Field Code	Full Name	Type of Indexing
USE.LH	Laboratory Use and Handling	String (wordwise)
USE.PT	Use Pattern	String (wordwise)

2.6.3.1. Laboratory Use and Handling (USE.LH)

Description:

This field describes the use of a substance in the preparative chemistry, in the laboratory and information on safety aspects or the attainment of the desired effect such as phase transfer catalysis, reduction, ^{14}C marking, quenching, storage under a protective gas, do not bring into contact with water.

Type of Indexing:

String (wordwise)

2.6.3.2. Use Pattern (USE.PT)

Description:

Information on the categories of use for substances (not in the preparative chemistry), usually the product category such as dyestuff, cleaning agent, tabletting adjuvant, preservative for food, pharmaceuticals, insecticides, fungicides, bactericides, herbicides.

Type of Indexing:

String (wordwise)

3. Index

F

G

H

I

J

K

L

M

N

O

P

Q

R

S

T

U

V

X

Y