Aspen Physical Property System

Physical Property Data 11.1

Part Number: Aspen Physical Property System 11.1
September 2001

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Contents

About This Manual

This manual includes technical reference information and listings for all Aspen Physical Property System databanks, electrolytes data, group contribution method functional groups, and property sets. Much of this information is also available in online prompts and help.

For information on property option sets, property methods, models, and parameter estimation, see *Physical Property Methods and Models*.

An overview of the Aspen Physical Property System physical property system, and information about how to use its full range and power, is in the Aspen Plus and Aspen Properties *User Guides*, as well as in online help and prompts in Aspen Plus and Aspen Properties.

For More Information

Online Help The Aspen Physical Property System has a complete system of online help and context-sensitive prompts. The help system contains both context-sensitive help and reference information.

Physical Property Reference Manuals Aspen Physical Property System reference manuals provide detailed technical reference information about the physical property calculation system supplied with Aspen Plus and Aspen Properties.

Aspen Plus and Aspen Properties manuals Aspen Plus reference manuals provide background information about Aspen Plus and Aspen Properties.

The manuals are delivered in Adobe portable document format (PDF).

Technical Support

World Wide Web For additional information about AspenTech products and services, check the AspenTech World Wide Web home page on the Internet at: **http://www.aspentech.com/**

Technical resources AspenTech customers with a valid license and software maintenance agreement can register to access the **Online Technical Support Center** at **http://support.aspentech.com/**

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- Report product defects
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Registered users can also subscribe to our Technical Support e-Bulletins. These e-Bulletins are used to proactively alert users to important technical support information such as:

- Technical advisories
- Product updates and Service Pack announcements

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CHAPTER 1

Databanks

Overview

Physical property models require parameters to calculate properties. After you have selected the option set(s) to be used in a calculation, you must determine the parameter requirements and ensure that all required parameters are available. The required parameters can be retrieved from databanks, entered directly on the Properties Parameters forms, or estimated by the Aspen Physical Property System using the Property Constant Estimation System (PCES).

This chapter discusses:

- the Aspen Physical Property System databanks
- Use of the Data File Management System (DFMS) to manage databanks
- Databanks available in the Aspen Physical Property System
- Binary parameters for activity coefficient models
- Electrolytes model parameters

The use of the Properties Parameters forms to enter parameters and the use of parameter estimation are described in the Aspen Plus *User Guide*, Chapter 8 and in the Aspen Properties User Guide.

Aspen Physical Property System Databanks

Aspen Physical Property System physical property databanks are listed in Table 1.1. There are three categories of databanks: system, in-house, and user.

System databanks System databanks are part of the Aspen Physical Property System and are delivered with it. You can modify the system databanks to add your own components or parameters. But this practice is discouraged. If you have a large amount of data, use the in-house databank instead. System databanks are available for every Aspen Physical Property System calculation. Property parameters are retrieved automatically from the PURECOMP, SOLIDS, AQUEOUS, INORGANIC, and BINARY databanks. To retrieve parameters from other databanks, use the Components.Main form.

Tables 1.2 through 1.15 list the parameters available in: AQUEOUS, ASPENPCD, INORGANIC, PURE10, PURE856, PURE93,SOLIDS and COMBUST. See Databanks Available in the Aspen Physical Property System for descriptions of these databanks.

In-house databanks Use the in-house databanks when you have a large amount of in-house data to be used in the Aspen Physical Property System. These databanks are independent of the system databanks. Your system administrator for AspenTech software must create and activate in-house databanks. (See Using DFMS to Manage Databanks for information about creating in-house databanks.) Information on activation of in-house databanks is in *Aspen Plus System Management*.

User databanks User databanks are appropriate when certain data are not intended for all Aspen Physical Property System users. This may occur when the accuracy of the data is in question, or when data are of a proprietary nature. Use the Aspen Physical Property Data File Management System (DFMS) to create user databanks. (See Using DFMS to Manage Databanks.) These databanks can be used in any Aspen Physical Property System calculation.

Any in-house or user databanks you created using DFMS must also be installed on ModelManager (see *Aspen Plus System Management*, Chapter 6, for installation instructions).

Table 1.1 Aspen Physical Property System Physical Property Databanks

System Databanks

Databank Name	Password	Type	Maximum Parameters	Maximum Components	Maximum Pairs	Description
PURE11	PURE11	PP1	100	2500	—	Main pure component databank
ASPENPCD	ASPENPCD	PP1	40	1000	—	Aspen Physical Property System pure component databank
SOLIDS	SOLIDS	PP1	40	4000	—	Solid component databank
AQUEOUS	AQUEOUS	PP1	40	4000	—	Aqueous component databank
BINARY	BINARY	PP2	20	100	3000	Binary databank
COMBUST	COMBUST	PP1	40	4000	—	Combustion databank
ETHYLENE	ETYHYLENE	PP2	20	100	3000	Ethylene databank
INORGANIC	INORGANIC	PP1	25	2500	—	Inorganic component databank
PURE856	PURE856	PP1	100	2500	—	Pure component databank from release 8.5 – 6
PURE93	PURE93	PP1	100	2500	—	Pure component databank from release 9.3
PURE10	PURE10	PP1	100	2500	—	Pure component databank from version 10.2
AQU92	AQU92	PP1	40	4000		AQUEOUS databank for Release 9.2

In-House Databanks

Databank Name	Password	Type	Maximum Parameters	Maximum Components	Maximum Pairs	Description
INHSPCD	INHSPCD	PP1	40	1800	—	In-house pure component databank
INHSSOL	INHSSOL	PP1	25	2500	—	In-house SOLIDS databank
INHSAQUS	INHSAQUS	PP1	40	4000	—	In-house AQUEOUS databank
INHSBIN	INHSBIN	PP2	20	100	3000	In-house binary databank

User Databanks

Databank Name	Password †	Type	Maximum Parameters	Maximum Components	Maximum Pairs	Description
USRPP1A		PP1	40	500	—	User PP1 databank
USRPP1B		PP1	40	500	—	User PP1 databank
USRPP2A		PP2	20	100	3000	User PP2 databank
USRPP2B		PP2	20	100	3000	User PP2 databank

† Assigned by the user

See *Using DFMS to Manage Databanks*, this chapter, for an explanation of Type.

Using DFMS to Manage Databanks

DFMS is a system for creating and updating system, in-house, or user physical property databanks. The five major functions of DFMS are to:

- Create a new databank
- Add new data to an existing databank
- Delete data from an existing databank
- Copy data from one databank to another
- Print the contents of a databank

DFMS is a peripheral system of the Aspen Physical Property System. It has its own run procedure, which is different for each operating system. DFMS is described in *Aspen Plus System Management.*

Physical property databanks have directories of information about the type and location of data they contain. The directory structure reflects the databank type. Two types of databanks can be created and maintained by DFMS: Type 1 (or PP1 databank) and Type 2 (or PP2 databank).

Type 1 (PP1 databank) Has an unpacked structure. There is space for any combination of components and parameters. It resembles a grid, with all components listed on one axis and parameters on the other. There may be holes in the data file, if parameter values are missing (the file is not packed full). This type of databank uses only one parameter directory. Every component has the same parameters and the same structure. The grid and data structure are illustrated in Figure 1.1.

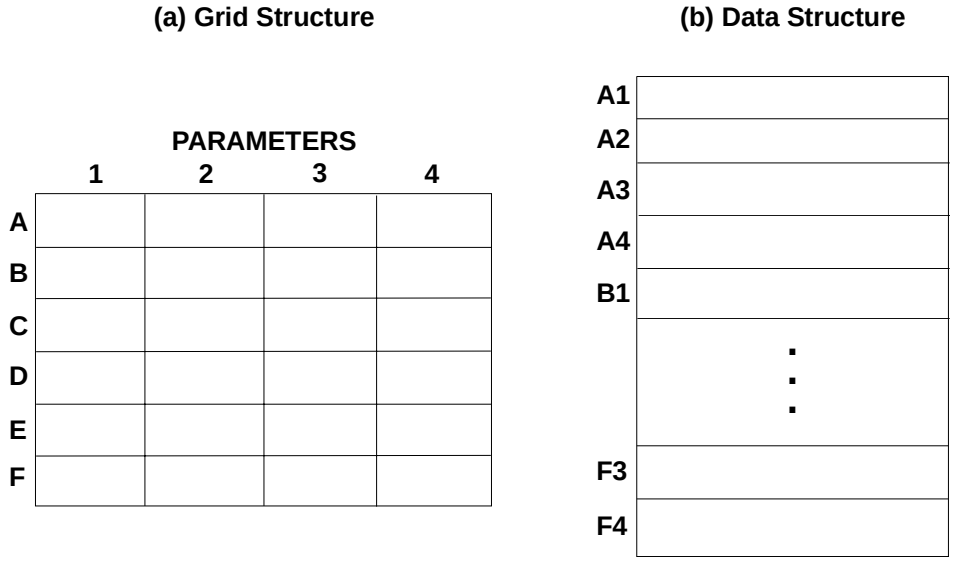

Figure 1.1 Unpacked Structure Databank

Type 2 (or PP2 databank) Has a packed structure, which differs from the unpacked structure in two ways:

- Each component has its own parameter directory and may have a unique set of parameters.
- Data are not stored positionally. Pointers track the data, so the file is packed full.

Figure 1.2 demonstrates how pointers are used in the PP2 databank structure.

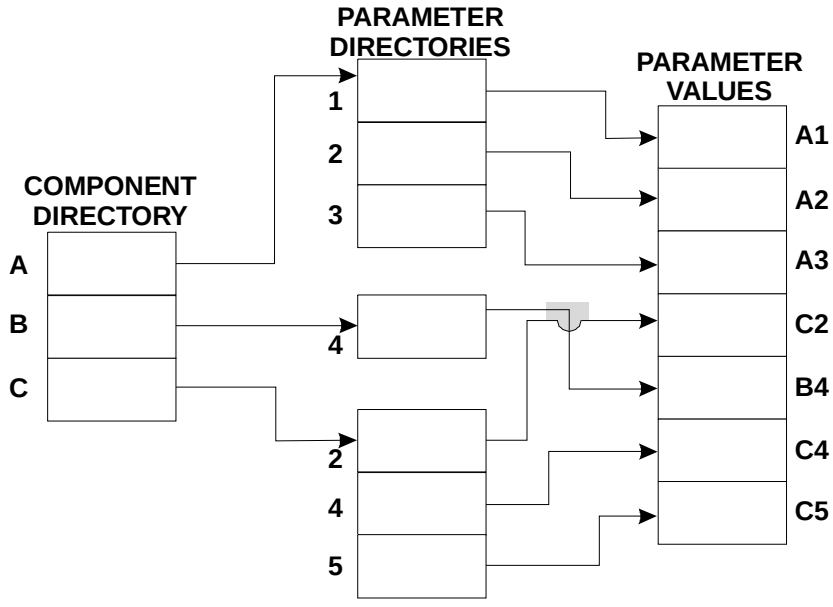

Figure 1.2 Packed Structure Databank

A PP2 databank uses space more efficiently than a PP1 databank, but the PP2 databank requires increased overhead when storing or retrieving data. The PP1 structure is appropriate when most of the

values are available for a relatively comprehensive set of parameters, common to all of the components included. The PP2 structure is intended for parameters not appropriate for a PP1 file. All binary pair parameters, for example, must be stored in PP2 databanks.

In addition to a type, all databanks have names and passwords. Table 1.1 lists the databanks recognized by DFMS. The passwords listed for system databanks and in-house databanks are recognized by DFMS. For user databanks, you must use input language to assign a password.

DFMS Input Language Conventions

For readers familiar with Aspen Plus input language, the DFMS input language is similar:

- Keywords are written in sentences and paragraphs.
- Only primary keywords start in column one.
- Titles are enclosed in single quotes.
- Descriptions are enclosed in double quotes.
- Binary pairs are enclosed in parentheses.
- The slash (/) is used to separate sentences.
- Comment lines are allowed. Each comment line must begin with
  a semicolon (;).

However, in DFMS input language:

- The sentence continuation character, the ampersand (&), is not needed.
- DFMS input is processed in two separate passes: first the TITLE, DESCRIPTION, FILE, and NO-ECHO commands are processed. On the second pass all remaining commands are processed.

The DFMS primary keywords are:

COPY	DESCRIPTION	NEW- COMP	PRINT-DIR
CLEAN-UP	END- INPUT	NEW- PROP	PROP- DATA
DELETE	FILE	NO-ECHO	TITLE
		PRINT-DATA	WRFILE

You can enter each primary keyword only once in a DFMS run. In addition, the following limitations apply:

Maximum	In a
32 Characters	Component name
12 Characters	Component alias
6 Characters	Parameter name
16 Elements	Unary parameter
8 Elements	Binary parameter
100 Paragraphs	Run
1000 Sentences	Paragraph
100 Arguments	Tertiary keyword

You may need to create several DFMS input files when building a large databank. Create the databank by making enough DFMS runs to use all the input files. The maximum number of components allowed in a databank and the maximum number of parameters per component are listed in Table 1.1.

DFMS Primary Keywords

There are four types of DFMS keywords:

Purpose	Keywords
General utility	TITLE, DESCRIPTION, CLEAN-UP, END-INPUT
Defining databank characteristics	FILE, WRFILE, NEW-COMP, NEW-PROP
Entering or deleting databank data	COPY, DELETE, PROP-DATA
Controlling databank reports	NO-ECHO, PRINT-DIR, PRINT-DATA

TITLE and DESCRIPTION

Your title is printed on each page of the DFMS report file, and your description is printed at the beginning of the report.

Input Language

```
TITLE    'up to 64 characters enclosed in single quotes'

DESCRIPTION     "any amount of text entered on any number
                 of lines
                 and enclosed in double quotes"
```

CLEAN-UP

CLEAN-UP compresses a databank file. Using CLEAN-UP is recommended after several deletions from a databank.

Input Language

```
CLEAN-UP
```

END-INPUT

END-INPUT must be the last keyword given to DFMS. It terminates DFMS, and any keywords that follow are ignored.

Input Language

```
END-INPUT
```

FILE

FILE is used to specify the databank names and passwords of all databanks used during a DFMS run. It also specifies whether the databank is old or newly created.

Input Language

```
                                        [NEW]
FILE     name     password              [OLD]      /
```

Input Language Description

name	Name of the databank obtained from Table 1.1.
password	Password for the system, in-house, and user databanks (see Table 1.1). A user-supplied password identical to the external file name is recommended, to avoid confusion. This password is also used to retrieve parameters from the databank in an Aspen Physical Property System calculation.
NEW	For a new databank
OLD	For an old databank (Default)

Example 1 Creating a user databank

A user PP1 databank USRPP1A is created. The password is XYZ. It references the ASPENPCD. The FILE paragraph required is:

```
FILE   USRPP1A   XYZ   NEW  /  ASPENPCD   ASPENPCD   OLD
```

WRFILE

WRFILE specifies that the databank can be written to. This command must precede the PROP-DATA, NEW-COMP, NEW-PROP, COPY, DELETE, and CLEAN-UP paragraphs.

You cannot have more than one WRFILE paragraph in a DFMS run.

Input Language

```
WRFILE     password     [auth]
```

Input Language Description

password	Password for the databank
auth	Optional authorization code. Needed only when you want to modify the built-in system databanks from the Aspen Physical Property System.

NEW-COMP

Use the NEW-COMP paragraph to add new components to a databank. If you use the COPY paragraph to copy data from another databank, the NEW-COMP paragraph is not required. No more than 1000 components can be added using NEW-COMP in a single DFMS run. Table 1.1 shows the maximum number of

components or component pairs allowed for each Aspen Physical Property System databank.

Input Language

To add components:

```
NEW-COMP     cname     calias  /  . . .
```

To add binary pairs:

```
(cname1  cname2)   (calias1   calias2)  /  . . .
```

Input Language Description

cname, cname1, cname2	Component name. If the component name contains embedded blanks, it must be enclosed in single quotes.
calias, calias1, calias2	Component alias. If the alias name contains embedded blanks, it must be enclosed in single quotes.

NEW-PROP

Use the NEW-PROP paragraph to add new property parameters to a databank. The NEW-PROP paragraph is not required if you use a COPY paragraph to copy data from another databank. Table 1.1 shows the maximum number of parameters per component that can be stored in each Aspen Physical Property System databank.

Input Language

```
NEW-PROP     paramname     nelem  /  . . .
```

Input Language Description

paramname	Parameter name
nelem	Number of elements in the parameter

Example 1 Adding parameters to a databank

The following parameters are added to a databank: TC, PC, CPIG, PLXANT, and MW. The number of elements for each parameter is 1, 1, 11, 9, and 1.

```
NEW-PROP  TC  1  /  PC 1  /  CPIG 11  /  PLXANT 9  / MW 1
```

COPY and DELETE

Use the COPY paragraph to copy information from one databank to another. Use the DELETE paragraph to delete information from a databank. You can copy or delete data for certain properties, all properties, or all components.

Input Language

```
COPY  password    COMPS=cname-list    PROPS=paramname-list
              [NEW-NAMES=cname-list]   /
        PAIRS=pair-list  PROPS=paramname-list
              [NEW-NAMES=cname-list]

DELETE    COMPS=cname-list    PROPS=paramname-list  /
        PAIRS=pair-list   PROPS=paramname-list
```

Input Language Description

password	Password of the databank from which data are copied
COMPS	List of component names or aliases to be copied or deleted. There is a limit of 100 components for a COPY or DELETE paragraph. If COMPS=ALL, all components are copied. COMP=ALL is used only with the copy paragraph. You must specify the component names or aliases if you use the DELETE paragraph or if there are more than 100 components in the databank.
PROPS	List of property names to be copied or deleted. To delete a component from the databank, specify PROPS=ALL (Default=ALL).
NEW-NAMES	Optional list of new component names; used for COPY only.
PAIRS	List of component pairs to be copied or deleted, in the form (cname1 cname2) (cname3 cname4), and so on. There is a limit of 50 pairs for a COPY or DELETE paragraph. If PAIRS=(ALL ALL), all component pairs are copied. You can use PAIRS=(ALL ALL) only with the COPY paragraph. You must specify the names or aliases of the component pairs if you use the DELETE paragraph, or if the databank contains more than 100 component pairs (as defined in the NEW-COMP paragraphs).

Example: Creating a User Databank Using COPY

A user databank is created by copying data from the ASPENPCD. The components are CH4, H2O, C6H6, and C2H6O-2. The properties to be copied for each component are MW, TC, PC, VC, CPIG, PLXANT, DHVLWT, and RKTZRA.

```
COPY  ASPENPCD   COMPS=CH4    H2O     C6H6     C2H6O-2
      PROPS=MW   TC  PC  VC  CPIG  PLXANT  DHVLWT  RKTZRA
```

Example: Deleting a Component

All data for methane are deleted from the databank in Example 1.

```
DELETE      COMPS=CH4
```

PROP-DATA

Use PROP-DATA to add parameter values to new or existing databanks. Eight sentences are associated with this command. Each sentence must start on a new line, but not in column one.

You can enter parameter values in one of two ways. The PROP-LIST form is more convenient when there are more parameters than components. The COMP-LIST form is more convenient when components outnumber parameters. You must enter all data in SI units, because DFMS does not perform units conversion. Only one PROP-DATA paragraph is allowed in each DFMS run.

Input Language

```
PROP-DATA
    PROP-LIST     paramname     srcode  /  . . .
    PVAL    cname     value-list  /  value-list  /  . . .

    PROP-LIST     paramname    srcode  /  . . .
    BPVAL   cname1  cname2  value-list / value-list / . . .

    COMP-LIST     cname-list
    CVAL    paramname   srcode   0   elemno   value-list  /
               elemno     value-list  /  . . .

    COMP-LIST     cname-list
    BCVAL   paramname  srcode 0 elemno cname1 value-list  /
              elemno     cname2     value-list /  . . .
```

Input Language Description

PROP-LIST	Used to enter parameter names and source code
paramname	Parameter name
srcode	Parameter source code. Use any integer value.
PVAL	Used to enter the PROP-LIST parameter values
cname	Component name or alias
value-list	List of parameter values. Enter one value for each element of the parameters listed in corresponding PROP-LIST sentences.
BPVAL	Used to enter the PROP-LIST binary parameter values
cname1	Component name or alias of first component of binary pair
cname2	Component name or alias of second component of binary pair

value-list	List of binary parameter values. Enter two values for each element of the binary parameters listed in the corresponding PROP-LIST sentence. The two values entered are for the cname1-cname2 and the cname2-cname1 pairs.
COMP-LIST	Used to enter component names or aliases; the COMP-LIST sentence cannot contain more than seven components.
cname-list	List of component names or aliases
CVAL	Used to enter the COMP-LIST parameter values
elemno	Parameter element number
value-list	List of parameter values. Enter one value for each component in the cname-list of the COMP-LIST sentence.
BCVAL	Used to enter the COMP-LIST binary parameter values
elemno	Parameter element number
cname1	Component name or alias of the component in the first row of the binary parameter matrix
cname2	Component name or alias of the component in the second row of the binary parameter matrix
value-list	List of binary parameter values. Enter one value for each component in the cname-list of the COMP-LIST sentence.

Example: Using PROP-LIST to Enter Data for Water

Enter TC, PC, and vapor pressure parameters for water (component H2O). PROP-LIST and PVAL are used, since there are more parameters than components.

```
PROP-DATA
    PROP-LIST     TC     1  /  PC     1  /  PLXANT 1
    PVAL    H2O   647.13  /  0.220550D8  /
                 73.6490    -7258.20  0.0    0.0   -7.3037
                 0.41653D-5    2.0    273.16   647.13
```

Example: Using COMP-LIST and CVAL

Add TC and vapor pressure parameters for H2O, C6H6, and CH4O. COMP-LIST and CVAL are used, since there are more components than parameters.

```
PROP-DATA
    COMP-LIST                H2O          C6H6         CH4O
    CVAL   TC      1  0 1   647.13       561.16       512.58  /
    CVAL   PLXANT  1  0 1   73.6490      78.050       109.93  /
                        2   -7258.20     -6275.50     -7471.30  /
                        3   0.0          0.0          0.0 /
                        4   0.0          0.0          0.0  /
                        5   -7.3037      -8.4443      -13.988  /
                        6   0.41653D-5   -0.626D-5    0.15281D-1 /
                        7   2.0          2.0          1.0  /
                        8   273.16       278.68       175.47  /
                        9   647.13       561.16       512.58
```

Example: Using COMP-LIST and BCVAL

Add binary parameters for many components. With BCVAL, DFMS expects all possible pairs to be defined. If the pair is not in the databank, it must appear in the NEW-COMP paragraph. In this example, six pairs must be defined (C1-C1, C1-C2, C1-C3, C2-C2, C2-C3, and C3-C3). Defining C1-C2 also defines C2-C1.

```
NEW-COMP
       (C1     C1)      (C1     C1)  /
       (C1     C2)      (C1     C2)  /
       (C1     C3)      (C1     C3)  /
       (C2     C2)      (C2     C2)  /
       (C2     C3)      (C2     C3)  /
       (C3     C3)      (C3     C3)
PROP-DATA
    COMP-LIST                C1       C2       C3
BCVAL  WILSON    1 0 2  C1  0.0      272.98   -267.60  /
                    2  C2  -393.58   0.0      503.60  /
                    2  C3  -764.31   887.28   0.0
```

Example: Using PROP-LIST and BPVAL

Enter the UNIQUAC binary parameters for acetone and water. The number of values entered in a BPVAL sentence is equal to twice the number of elements of the binary parameter. In this example, -190.72 is the GMUQB value for the acetone-water interaction and -56.19 is the value for the water-acetone interaction.

```
PROP-DATA
    PROP-LIST     GMUQB     1
    BPVAL     C3H6O    H2O      -190.72      -56.19
```

NO-ECHO

Use NO-ECHO to suppress the echo printing of the keyword input in the report file.

Input Language

```
NO-ECHO
```

PRINT-DIR and PRINT-DATA

Use PRINT-DIR and PRINT-DATA to print the databank's directories and parameter values, to verify that the databank was created correctly.

Input Language

```
PRINT-DIR      password

                                    [ cname - list ]
                                    [ pair - list  ]
PRINT-DATA     password             [ ALL          ]
```

Input Language Description

password	Password of the databank to be printed
ALL	Print all directories or data (Default)
cname-list	List of component names or aliases. Default is ALL.
pair-list	List of pair names or aliases. Default is ALL pairs

Example: Creating a User PP1 Databank

A user PP1 databank, USRPP1A, is created with password XYZ, by copying data from the ASPENPCD. The components included are: methane, water, benzene, and ethanol. The properties copied are: MW, TC, PC, VC, CPIG, PLXANT, DHVLWT, and RKTZRA. The databank directory and values of the parameters stored in this databank are printed.

```
TITLE     'CREATE A USER databank BY COPYING FROM THEASPENPCD'

FILE     USRPP1A     XYZ     NEW  /  ASPENPCD     ASPENPCD    OLD

WRFILE     XYZ

COPY   ASPENPCD     COMPS=CH4      H2O      C6H6     C2H6O-2
       PROPS=MW     TC     PC      VC      CPIG      PLXANT      DHVLWT     RKTZRA

PRINT-DIR     XYZ

PRINT-DATA     XYZ

END-INPUT
```

Example: Creating a User PP2 Databank

A user PP2 databank, USRPP2A, is created with the password MYDATA. This databank stores both the pure component parameters MW, DHVLWT, and the user binary parameter USRBIN. The components included are: water, benzene, and methanol. This example illustrates the use of NEW-PROP, NEW-COMP, and PROP-DATA. Both PROP-LIST and COMP-LIST sentences are used for data entry.

```
TITLE     'USE PROP-DATA TO ENTER DATA FOR A USER PP2 databank'
FILE    USRPP2A    MYDATA    NEW
WRFILE     MYDATA
NEW-PROP     MW     1  /  DHVLWT     5  /  USRBIN     1
NEW-COMP
    WATER                      H2O               /
    BENZENE                    C6H6              /
    METHANOL                   CH4O              /
    (WATER WATER)              (H2O H2O)         /
    (WATER BENZENE)            (H2O  C6H6)       /
    (WATER METHANOL)           (H2O  CH4O)       /
    (BENZENE BENZENE)          (C6H6 C6H6)       /
    (BENZENE METHANOL)         (C6H6  CH4O)      /
    (METHANOL METHANOL)        (CH4O  CH4O)
PROP-DATA
    COMP-LIST                   H2O            C6H6           CH4O
    CVAL     MW     1  0  1    18.015         78.114         32.042
PROP-LIST        DHVLWT     1
     PVAL     H2O    0.406831D+08   373.20   0.310646   0.0   273.20
     PVAL     C6H6   0.307814D+08   353.30   0.349117   0.0   278.70
     PVAL     CH4O   0.352780D+08   337.80   0.371655   0.0   175.50
COMP-LIST                             H2O         C6H6        CH4O
    BCVAL  USRBIN    1 0  1  H2O      0.0         200.        210.  /
                          1  C6H6     -100.       0.0         310.  /
                          1  CH4O     -120.       -130.       0.0
PRINT-DATA     MYDATA
END-INPUT
```

Databanks Available in the Aspen Physical Property System

The topics listed below describe the pure component databanks that are available in the Aspen Physical Property System. Each topic includes a table of the parameters available in the databank.

AQUEOUS Databank
AQU92 Databank
ASPENPCD Databank
INORGANIC Databank
PURE11 Databank
PURE10 Databank
PURE856 Databank
PURE93 Databank
SOLIDS Databank
COMBUST Databank
ETHYLENE Databank

AQUEOUS Databank

Contains parameters for 900 ionic species. It is used for electrolytes applications. The key parameters are the aqueous heat and Gibbs free energy of formation at infinite dilution and aqueous phase heat capacity at infinite dilution. See Aqueous Component Databanks for the parameters and components available in the databank.

AQU92 Databank

Contains parameters for 900 ionic species. This is the AQUEOUS databank for Aspen Plus Release 9.2. This databank has been retained for upward compatibility. See Aqueous Component Databanks for the parameters and components available in the databank.

ASPENPCD Databank

Contains parameters for 472 organic and some inorganic compounds. This databank has been superseded by the PURECOMP databank as the main source of pure component parameters. The ASPENPCD is retained for upward compatibility. See Pure Component Databanks for the parameters and components available in the PURE11 databank.

INORGANIC Databank

Contains thermochemical data for about 2450 (mostly inorganic) components. The key data are the enthalpy, entropy, Gibbs free energy, and heat capacity correlation coefficients. For a given component, there can be data for a number of solid phases, a liquid phase, and the ideal gas phase. The same set of parameters are used to calculate enthalpy, entropy, Gibbs free energy and heat capacity for a given phase over a given temperature range.

In order to achieve adequate accuracy of fit over a wide temperature range, multiple data ranges have been used for solid, liquid, and ideal gas phases:

Number of Data Ranges	Properties
7	Solid (CPSXP1 to CPSXP7)
2	Liquid (CPLXP1 and CPLXP2)
3	Ideal gas (CPIXP1 and CPIXP3)

In the case of the solid phase, the multiple ranges can also refer to different solid phases of different crystal structure, for the same species.

If a component has more than one solid phase, each solid phase is also defined as a separate component. For example, in addition to the component FE, there are components FE-A, FE-B, FE-C, and FE-D. Each component contains data for the different solid phases of FE. For these components, the same liquid and ideal gas parameters are used.

When modeling liquid metallurgical solutions, it is common to choose liquid reference state components. However, liquid solutions may have gaseous components as reference state materials. For example, oxygen, hydrogen, nitrogen, and sulfur dissolved in alloys and other phases would have ideal gas reference states. Additionally, the reference state may be monatomic (for example, 1/2 O2(g)) or polytomic (for example, S2(g)). The INORGANIC databank contains a number of components commonly used as reference state materials, such as 1/2 O2(g).

The reference state for enthalpy, entropy and Gibbs free energy used in the INORGANIC databank is the elements in their standard phase at 25°C and 1 atm. Standard enthalpy of formation at 25°C is used for enthalpy while standard Gibbs free energy of formation at 25°C is used in Gibbs free energy. Since this reference state is also used in ASPENPCD, PURECOMP, and other pure component databanks, it is possible to mix data from this with those from the other Aspen Physical Property System databanks. Note that this reference state is different from that used in the Barin Data Book (Barin, 1989) compilation where the enthalpy of formation and the absolute entropy at 25°C are used. Therefore, the Gibbs free energy and entropy values computed using the INORGANIC databank will be different from those tabulated in the Barin Data Book.

The INORGANIC databank is used for solids, pyrometallurgical, and electrolytes applications. See Inorganic Component Databank for the parameters and components available in the databank.

PURE11 Databank

Contains parameters for over 1727 (mostly organic) components. This is the main source of pure component parameters for the Aspen Physical Property System. The databank is based on the data developed by the AIChE DIPPR® data compilation project, parameters developed by AspenTech, parameters obtained from the ASPENPCD databank, and other sources. For most calculations, the PURE11 databank contains all the property parameters you need. The parameters stored in the databank can be categorized as:.

- Universal constants, such as critical temperature, and critical pressure
- Temperature and property of transition, such as boiling point and triple point
- Reference state properties, such as enthalpy and Gibbs free energy of formation
- Coefficients for temperature-dependent thermodynamic properties, such as liquid vapor pressure
- Coefficients for temperature-dependent transport properties, such as liquid viscosity
- Safety properties, such as flash point and flammability limits
- Functional group information for all UNIFAC models
- Parameters for RKS and PR equations of state
- Petroleum-related properties, such as API gravity, octane numbers, aromatic content, hydrogen content, and sulfur content

- Other model-specific parameters, such as the Rackett and UNIQUAC parameters

The content of the main pure component databank is continually updated, expanded, and improved. Therefore, from one release of the Aspen Physical Property System to the next, certain parameter values change. This change can cause differences in your calculation results if you use the new, updated databank.

To facilitate upward compatibility (that is, allowing you to obtain the same calculation results as in the previous release), the main pure component databank is named according to the major release of Aspen Plus or the Aspen Physical Property System. For example, the pure component databank from Release 8.5-6 is called PURE856 (see PURE856 databank). PURE93 and PURE10 are also available.

See Pure Component Databanks for the parameters and components available in the PURE11 databank.

PURE10 Databank

Contains parameters for over 1727 (mostly organic) components. It is the main pure component databank from Aspen Plus Version 10. This databank has been retained for upward compatibility. See PURE11 databank for detailed discussions.

See Pure Component Databanks for the parameters and components available in the PURE10 databank.

PURE856 Databank

Contains parameters for 1,212 components. It is the main pure component databank from Aspen Plus Release 8.5-6. This databank has been retained for upward compatibility. See PURE11 databank for detailed discussions.

See Pure Component Databanks for the parameters and components available in the PURE856 databank.

PURE93 Databank

Contains parameters for 1,550 components. It is the main pure component databank from Aspen Plus Release 9.3. This databank has been retained for upward compatibility. See PURE11 databank for detailed discussions.

See Pure Component Databanks for the parameters and components available in the PURE93 databank.

SOLIDS Databank

Contains parameters for 3314 solid components. This databank is used for solids and electrolytes applications. This databank is largely superceded by the INORGANIC databank, but is still essential for electrolytes applications.

See Solids Component Databank for the parameters and components available in the databank.

COMBUST Databank

The COMBUST databank is a special databank for high temperature, gas phase calculations. It contains parameters for 59 components typically found in combustion products, including free radicals. The CPIG parameters were determined from data in JANAF tables for temperatures up to 6000K (JANAF Thermochemical Tables, Dow Chemical Company, Midland, Michigan, 1979). Calculations using parameters in the ASPENPCD and PURECOMP are generally not accurate above 1500K.

You may use the COMBUST databank only for ideal gas calculations (IDEAL option set) and only in the following unit operation models: MIXER, FSPLIT, SEP, SEP2, HEATER, HEATX, MHEATX, RSTOIC, RYIELD, REQUIL, RGIBBS, RCSTR, RPLUG, RBATCH, COMPR, MCOMPR, DUPL and MULT. You must enter the option NPHASE=1 for each unit operation block for which it is applicable, and for each STREAM.

See Combust Component Databank for the parameters and components available in the databank.

ETHYLENE Databank

The new ETHYLENE databank contains pure component and binary interaction parameters required to model the typical ethylene process. The parameters are for the SRK property method which include the critical temperature, critical pressure, acentric factor and binary interaction parameters. The parameters are available for 85 components commonly encountered in the ethylene process. The ETHYLENE databank should be used with the PURE11 databank and the SRK property method.

See Ethylene Component Databank for the parameters and components available in the databank.

Binary Parameters for Activity Coefficient Models

The Aspen Physical Property System offers a comprehensive collection of built-in binary parameters for the following activity coefficient models: WILSON, NRTL, and UNIQUAC. Separate databanks are available for vapor-liquid and liquid-liquid applications. The Aspen Physical Property System also contains a large collection of Henry's law constants. These built-in parameters are used automatically when the appropriate property methods are used.

Binary Parameters for Vapor-Liquid Applications

There are four databanks for vapor-liquid applications: VLE_IG, VLE_RK, VLE_HOC, and VLE-LIT. Table 1.16 lists the characteristics of these databanks.

The databanks VLE_IG, VLE_RK, and VLE_HOC were developed by AspenTech using binary vapor liquid equilibrium data from the Dortmund databank. To the extent possible, only thermodynamically consistent data are used. In addition to the parameter values, the databanks contain the temperature, pressure, and composition limits of the data and the quality of the fits, such as average and maximum deviations.

The databank VLE_LIT contains binary parameters obtained from the literature.

Built-in Binary Parameters for Vapor Liquid Systems

These databanks	Are used with these property methods	Vapor phase model	Number of component pairs
VLE_IG	WILSON,NRTL, UNIQUAC	Ideal gas	3600
VLE_RK	WILS-RK,NRTL-RK, UNIQ-RK	Redlich-Kwong	3600
VLE_HOC	WILS-HOC,NRTL-HOC, UNIQ-HOC	Hayden-O'Connell	3600
VLE_LIT	WILSON,NRTL, UNIQUAC	Ideal gas	1200

Binary Parameters for Liquid-Liquid Applications

There are two databanks for liquid-liquid applications: LLE_ASPEN and LLE_LIT.

The LLE_ASPEN databank contains binary parameters for the NRTL and UNIQUAC models, and can be used with all NRTL and UNIQUAC property methods. This databank was developed by AspenTech using binary liquid-liquid equilibrium data from the Dortmund databank. The binary parameters are valid over a very wide temperature range. The systems in the databank include those exhibiting upper critical solution temperature, lower critical solution temperature, and closed loops.

The databank LLE_LIT contains binary parameters obtained from the literature for the UNIQUAC model. These binary parameters were determined from both binary and ternary liquid-liquid equilibrium data. They are valid for the temperature range 20 – 30°C.

For accurate representation of multicomponent liquid-liquid systems, binary parameters should be obtained from regression of binary and ternary LLE data in the operating range of the process. Use the Data Regression System to regress the parameters (see the *Aspen Plus User Guide*, Chapter 31 or the Aspen Properties User Guide).

Henry's Law Constants

There are two databanks of Henry's law constants: HENRY and BINARY. The HENRY databank is developed by AspenTech using gas-liquid equilibrium data from the Dortmund databank. It

contains over 1600 sets of Henry's constants for a wide variety of solutes in solvents. The solvents are not limited to water.

The BINARY databank contains Henry's constants obtained from the literature. It has data for about 60 solutes in water.

Electrolytes Model Parameters

The Aspen Physical Property System contains built-in parameters for the Pitzer and electrolyte NRTL models.

The Pitzer Parameter

Many binary Pitzer model parameters are available in the Aspen Physical Property System. This databank contains parameters for over 200 electrolyte pairs. All parameters were taken from the Pitzer series of papers. Only cation-anion parameters, cation-cation parameters, and anion-anion parameters are stored in the databank. There are no parameters for cation1-cation2-anion interaction, anion1-anion2-cation interaction, molecule-ion interaction, or molecule-molecule interaction.

If you do not enter the Pitzer parameters on a Properties.Parameters form, the Aspen Physical Property System automatically retrieves from the databank the necessary parameters for a specific ion-ion pair. If the parameters are unavailable, the default value of zero is used. The Pitzer parameters are available only on the Calculation Engine. They are not displayed on the Properties Parameters forms.

The Electrolyte NRTL Parameters

Electrolyte NRTL parameters are available in the Aspen Physical Property System. This databank contains the nonrandomness factor (GMELCN), and energy parameters (GMELCC, GMELCD, GMELCE) for many molecule-electrolyte and electrolyte-electrolyte pairs. The databank also contains the binary parameters (NRTL) for molecule-molecule interactions.

This databank is part of the electrolyte expert system and is searched automatically when the ELECNRTL property method is used. Parameters for a given pair are not retrieved if you enter the parameters on the Properties.Parameters form. You can access the electrolyte expert system using the Electrolyte Wizard button on the Components Specifications Selection sheet.

See Electrolytes Data for detailed information on the electrolytes systems used to develop the parameter databank, the solution chemistry used, the source of data, and the application ranges.

Barin, I. (1989). *Thermochemical Data of Pure Substances*. VCH Verlagsgesellschaft, FRG.

Pure Component Databanks

The tables below list the components present in the pure component databanks PURE11, PURE10, PURE93, PURE856, and ASPENPCD.

Components beginning with:

C1	C2	C3	C4	C5	C6	C7	C8	C9	C10
C11	C12	C13	C14	C15	C16	C17	C18	C19	C20
C21+	Al	B	Ca	Cl	Fe	H	K	N	Na
O	P	S	Si	Other elements		Heating Fluids			

Pure Component Databank Parameters

		Available in Databank				
Parameter Name	**Description**	**P11**	**P10**	**P93**	**P856**	**PCD**
AIT	Auto ignition temperature	X	X	X	X	
ANILPT	Aniline point	X	X	X		
API	Standard API gravity at 60°F	X	X	X		X
AROMATIC	Aromatic content (1=aromatic, 0=non-aromatic)	X				
ATOMNO	Vector containing the atom types (atomic numbers) for a given molecule (e.g., H=1, C=6, O=8). Must use the vector NOATOM to define the number of occurrences of each atom.	X	X	X	X	
CPDIEC	Dielectric constant	X	X	X		X
CPIG	Ideal gas heat capacity coefficients					X
CPIGDP	DIPPR ideal gas heat capacity coefficients	X	X	X	X	
CPLDIP	DIPPR liquid heat capacity coefficients	X	X	X	X	
CPSDIP	DIPPR solid heat capacity coefficients	X	X	X	X	
DCPLS	Difference between liquid and solid heat capacity at the Triple point	X	X	X		
DELTA	Solubility parameter at 298.2 K	X	X	X	X	X
DGFORM	Standard Gibbs free energy of formation; ideal gas at 298.2 K	X	X	X	X	X
DHFORM	Standard heat of formation; ideal gas at 298.2 K	X	X	X	X	X
DHLCVT	Cavett enthalpy departure parameter					X
DHVLB	Heat of vaporization at TB	X	X	X	X	X
DHVLDP	DIPPR heat of vaporization coefficients	X	X	X	X	

Parameter Name	Description	Available in Databank P11	P10	P93	P856	PCD
DHVLWT	Watson heat of vaporization parameters					X
DNLDIP	DIPPR liquid density coefficients	X	X	X	X	
DNSDIP	DIPPR solid density coefficients	X	X	X	X	
ENT	Absolute entropy of formation at 298.2 K	X	X	X	X	
FLML	Lower flammability limit	X	X	X	X	
FLMU	Upper flammability limit	X	X	X	X	
FP	Flash point	X	X	X	X	
FREEZEPT	Normal freezing point (see also TFP)	X				
GMUQQ	UNIQUAC area parameter	X	X	X	X	X
GMUQR	UNIQUAC volume parameter	X	X	X	X	X
HCOM	Standard enthalpy of combustion at 298.2 K	X	X	X	X	
HFUS	Enthalpy of fusion at melting point	X	X	X	X	
HYDROGEN	Hydrogen content (weight fraction)	X				
KLDIP	DIPPR liquid thermal conductivity coefficients	X	X	X	X	
KVDIP	DIPPR vapor thermal conductivity coefficients	X	X	X	X	
MOCTNO	Motor octane number	X	X	X		
MULAND	Andrade liquid viscosity coefficients					X
MULDIP	DIPPR liquid viscosity coefficients	X	X	X	X	
MUP	Dipole moment	X	X	X	X	X
MUVDIP	DIPPR vapor viscosity coefficients	X	X	X	X	
MW	Molecular weight	X	X	X	X	X
NAPHTHEN	Naphthene content (1=naphthenic, 0=non-naphthenic)	X				
NATOM	Vector containing numbers of C, H, O, N, S, F, Cl, Br, I, Ar, and He atoms					X
NOATOM	Vector containing the number of occurrences of each atom defined in ATOMNO for a given molecule. ATOMNO and NOATOM define the chemical formula of the molecule.	X	X	X	X	
NTHA	Nothnagel parameters	X	X	X		X
OLEFIN	Olefin content (1=olefin, 0=non-olefin)	X				
OMEGA	Pitzer acentric factor	X	X	X	X	X
OMGCTD	Acentric factor for the COSTALD model	X	X	X	X	X
OXYGEN	Oxygen content (weight fraction)	X				

Parameter Name	Description	Available in Databank				
		P11	P10	P93	P856	PCD
PARAFFIN	Paraffin content (1=paraffin, 0=non-paraffin)	X				
PC	Critical pressure	X	X	X	X	X
PLCAVT	Cavett vapor pressure coefficients					X
PLXANT	Extended Antoine vapor pressure coefficients	X	X	X	X	X
PRMCP	Mathias-Copeman parameters for PR equation of state	X	X	X		
PRSRP	Schwartzentruber-Renon parameters for PR equation of state	X	X	X		
RGYR	Radius of gyration	X	X	X	X	X
RI	Refractive index at 298.2 K	X	X	X	X	
RKSMCP	Mathias-Copeman parameters for RKS equation of state	X	X	X		
RKSSRP	Schwartzentruber-Renon parameters for RKS equation of state	X	X	X		
RKTZRA	Rackett liquid density parameter	X	X	X	X	X
ROCTNO	Research octane number	X	X	X		
SG	Standard specific gravity at 60°F	X	X	X		X
SIGDIP	DIPPR surface tension coefficients	X	X	X	X	
SULFUR	Sulfur content (weight fraction)	X				
SVRDIP	Second virial coefficient	X	X	X	X	
TB	Normal boiling point	X	X	X	X	X
TC	Critical temperature	X	X	X	X	X
TFP	Normal freezing point (see also FREEZEPT)		X	X	X	X
TOTAL-N2	Total nitrogen content (weight fraction)	X				
TPP	Triple point pressure	X	X	X	X	
TPT	Triple point temperature	X	X	X	X	
UFGRP	Functional group information for the UNIFAC model	X	X	X	X	X
UFGRPD	Functional group information for the Dortmund modified UNIFAC model	X	X	X		
UFGRPL	Functional group information for the Lyngby modified UNIFAC model	X	X	X		
VB	Liquid molar volume at TB	X	X	X	X	X
VC	Critical volume	X	X	X	X	X
VLCVT1	Scatchard-Hildebrand characteristic volume parameter	X	X	X		X
VLSTD	Standard liquid volume at 60°F	X	X	X	X	X

Parameter Name	Description	Available in Databank P11	P10	P93	P856	PCD
VSTCTD	Characteristic volume for the COSTALD model	X	X	X	X	X
WATSOL	Water solubility correlation coefficients	X	X	X		X
ZC	Critical compressibility factor	X	X	X	X	X

These parameters are not used in Aspen Plus models but can be accessed by user or in-house models: AIT, ENT, FLML, FLMU, SVRDIP, TPP

Vectors ATOMNO and NOATOM together form the chemical formula of the compound. They are used to compute molecular weight and are used in RGIBBS.

UFGRP, UFGRPD, UFGRPL contain functional group number and number of occurrences of each group.

P11 = PURE11 Databank

P10 = PURE10 Databank

P93 = PURE93 Databank

P856 = PURE856 Databank

PCD = ASPENPCD Databank

Pure Component Databanks: Al

Alias	Name	Available in Databank P11	P10	P93	P856	PCD
AL	ALUMINIUM	X	X	X	X	
AL(OH)3	ALUMINIUM-HYDROXIDE	X	X	X	X	
AL2(SO4)3	ALUMINIUM-SULFATE	X	X	X	X	
AL2O3	ALUMINIUM-OXIDE-ALPHA-CORUNDUM	X	X	X	X	
ALCL3	ALUMINIUM-CHLORIDE	X	X	X	X	
ALPO4-O	ALUMINIUM-PHOSPHATE-ORTHO	X	X	X	X	

Pure Component Databanks: B

Alias	Name	Available in Databank P11	P10	P93	P856	PCD
B2H6	DIBORANE	X	X	X	X	
B4H20NA2O17	BORAX	X	X	X	X	
BCL3	BORON-TRICHLORIDE	X	X	X	X	X
BF3	BORON-TRIFLUORIDE	X	X	X	X	X

Alias	Name	Available in Databank P11	P10	P93	P856	PCD
C	CARBON-GRAPHITE	X	X	X	X	
CBR2F2	DIBROMODIFLUOROMETHANE	X	X	X	X	
CBRCL3	BROMOTRICHLOROMETHANE	X	X	X	X	
CBRCLF2	BROMOCHLORODIFLUOROMETHANE	X	X	X	X	
CBRF3	TRIFLUOROBROMOMETHANE	X	X	X	X	X
CCL2F2	DICHLORODIFLUOROMETHANE	X	X	X	X	X
CCL2O	PHOSGENE	X	X	X	X	X
CCL3F	TRICHLOROFLUOROMETHANE	X	X	X	X	X
CCL4	CARBON-TETRACHLORIDE	X	X	X	X	X
CCLF3	CHLOROTRIFLUOROMETHANE	X	X	X	X	X
CCLN	CYANOGEN-CHLORIDE	X	X	X	X	
CF4	CARBON-TETRAFLUORIDE	X	X	X	X	X
CH2BR2	DIBROMOMETHANE	X	X	X	X	X
CH2BRCL	BROMOCHLOROMETHANE	X	X	X	X	
CH2CL2	DICHLOROMETHANE	X	X	X	X	X
CH2CLF	CHLOROFLUOROMETHANE	X	X			
CH2F2	DIFLUOROMETHANE	X	X	X	X	
CH2I2	DIIODOMETHANE	X	X	X	X	
CH2O	FORMALDEHYDE	X	X	X	X	X
CH2O2	FORMIC-ACID	X	X	X	X	X
CH3BR	METHYL-BROMIDE	X	X	X	X	X
CH3CL	METHYL-CHLORIDE	X	X	X	X	X
CH3F	METHYL-FLUORIDE	X	X	X	X	X
CH3I	METHYL-IODIDE	X	X	X	X	X
CH3NO	FORMAMIDE	X	X	X	X	
CH3NO2	NITROMETHANE	X	X	X	X	X
CH3SICL3	METHYL-TRICHLOROSILANE	X	X	X	X	
CH4	METHANE	X	X	X	X	X
CH4N2O	UREA	X	X	X	X	
CH4N2S	THIOUREA	X	X	X	X	
CH4O	METHANOL	X	X	X	X	X
CH4O3S	METHANESULFONIC-ACID	X	X	X	X	
CH4S	METHYL-MERCAPTAN	X	X	X	X	X
CH4SICL2	METHYL-DICHLOROSILANE	X	X	X	X	
CH5N	METHYL-AMINE	X	X	X	X	X
CH5SICL	METHYL-CHLOROSILANE	X	X	X	X	
CH6N2	METHYL-HYDRAZINE	X	X	X		X
CH6SI	METHYL-SILANE	X	X	X	X	
CHBR3	TRIBROMOMETHANE	X	X	X	X	
CHBRF2	BROMODIFLUOROMETHANE	X				
CHCL2F	DICHLOROMONOFLUOROMETHANE	X	X	X	X	X
CHCL3	CHLOROFORM	X	X	X	X	X
CHCLF2	CHLORODIFLUOROMETHANE	X	X	X	X	X
CHF3	TRIFLUOROMETHANE	X	X	X	X	
CHN	HYDROGEN-CYANIDE	X	X	X	X	X

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
CN4O8	TETRANITROMETHANE	X	X	X	X	
CO	CARBON-MONOXIDE	X	X	X	X	X
CO2	CARBON-DIOXIDE	X	X	X	X	X
COF2	CARBONYL-FLUORIDE	X	X	X	X	
COS	CARBONYL-SULFIDE	X	X	X	X	X
CS2	CARBON-DISULFIDE	X	X	X	X	X

Pure Component Databanks: C2

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C2BR2F4	1,2-DIBROMOTETRAFLUOROETHANE	X	X	X	X	
C2BRF3	BROMOTRIFLUOROETHYLENE	X	X	X	X	
C2CL2F4-1	1,1-DICHLORO-1,2,2,2-TETRAFLUORO	X	X	X		X
C2CL2F4-2	1,2-DICHLORO-1,1,2,2-TETRAFLUORO	X	X	X	X	X
C2CL3F3	1,2,2-TRICHLORO-1,1,2-TRIFLUOROE	X	X	X	X	X
C2CL3F3-D1	1,1,1-TRICHLOROTRIFLUOROETHANE	X				
C2CL4	TETRACHLOROETHYLENE	X	X	X	X	X
C2CL4F2	1,1,2,2-TETRACHLORO-1,2-DIFLUORO	X	X	X	X	X
C2CL4F2-D1	1,1,1,2-TETRACHLORODIFLUOROETHAN	X	X	X	X	
C2CL4O	TRICHLOROACETYL-CHLORIDE	X	X	X	X	
C2CL5F	PENTACHLOROFLUOROETHANE	X				
C2CL6	HEXACHLOROETHANE	X	X	X	X	
C2CLF3	CHLOROTRIFLUOROETHYLENE	X	X	X	X	
C2CLF5	CHLOROPENTAFLUOROETHANE	X	X	X	X	X
C2F4	PERFLUOROETHENE	X	X	X	X	X
C2F6	PERFLUOROETHANE	X	X	X	X	X
C2H2	ACETYLENE	X	X	X	X	X
C2H2BR4	1,1,2,2-TETRABROMOETHANE	X	X	X	X	
C2H2CL2-D1	1,1-DICHLOROETHYLENE	X	X	X	X	
C2H2CL2-D2	CIS-1,2-DICHLOROETHYLENE	X	X	X	X	
C2H2CL2-D3	TRANS-1,2-DICHLOROETHYLENE	X	X	X	X	
C2H2CL2O	CHLOROACETYL-CHLORIDE	X	X	X	X	
C2H2CL2O-D1	DICHLOROACETALDEHYDE	X	X	X	X	
C2H2CL2O2	DICHLOROACETIC-ACID	X	X	X	X	
C2H2CL3F	1,1,1-TRICHLOROFLUOROETHANE	X	X	X	X	
C2H2CL4-D1	1,1,1,2-TETRACHLOROETHANE	X	X	X	X	
C2H2CL4-D2	1,1,2,2-TETRACHLOROETHANE	X	X	X	X	
C2H2CLF3	2-CHLORO-1,1,1-TRIFLUOROETHANE	X	X			
C2H2F2	1,1-DIFLUOROETHYLENE	X	X	X	X	X
C2H2F4	1,1,1,2-TETRAFLUOROETHANE	X	X	X	X	
C2H2F4-D1	1,1,2,2-TETRAFLUOROETHANE	X	X	X		
C2H2F4O	BIS-DIFLUOROMETHYL-ETHER	X				
C2H2O	KETENE	X	X	X	X	X
C2H2O2	GLYOXAL	X	X	X	X	
C2H2O4	OXALIC-ACID	X	X	X	X	
C2H3BR	VINYL-BROMIDE	X	X	X	X	

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C2H3CL	VINYL-CHLORIDE	X	X	X	X	X
C2H3CL2F	1,1-DICHLORO-1-FLUOROETHANE	X	X	X		
C2H3CL3	1,1,2-TRICHLOROETHANE	X	X	X	X	X
C2H3CL3-D0	1,1,1-TRICHLOROETHANE	X	X	X	X	
C2H3CLF2	1-CHLORO-1,1-DIFLUOROETHANE	X	X	X	X	X
C2H3CLO	ACETYL-CHLORIDE	X	X	X	X	X
C2H3CLO-D0	CHLOROACETALDEHYDE	X	X	X	X	
C2H3CLO2	CHLOROACETIC-ACID	X	X	X	X	
C2H3CLO2-D1	METHYL-CHLOROFORMATE	X	X	X	X	
C2H3F	VINYL-FLUORIDE	X	X	X	X	X
C2H3F3	1,1,1-TRIFLUOROETHANE	X	X	X	X	X
C2H3F3-D1	1,1,2-TRIFLUOROETHANE	X				
C2H3N	ACETONITRILE	X	X	X	X	X
C2H3NAO2	SODIUM-ACETATE	X	X	X		
C2H3NO	METHYL-ISOCYANATE	X	X	X	X	X
C2H3NO-E1	HYDROXYACETONITRILE	X	X	X		
C2H3O2LI	LITHIUM-ACETATE	X				
C2H3SICL3	VINYLTRICHLOROSILANE	X				
C2H4	ETHYLENE	X	X	X	X	X
C2H4BR2	1,2-DIBROMOETHANE	X	X	X	X	
C2H4BR2-D1	1,1-DIBROMOETHANE	X	X	X	X	
C2H4CL2-1	1,1-DICHLOROETHANE	X	X	X	X	X
C2H4CL2-2	1,2-DICHLOROETHANE	X	X	X	X	X
C2H4CL2O	BIS-CHLOROMETHYL-ETHER	X	X	X	X	
C2H4F2	1,1-DIFLUOROETHANE	X	X	X	X	X
C2H4F2-D1	1,2-DIFLUOROETHANE	X	X	X	X	
C2H4N2	AMINOACETONITRILE	X	X	X		
C2H4N2O6	ETHYLENE-GLYCOL-DINITRATE	X	X	X		
C2H4N4	DICYANDIAMIDE	X	X	X		
C2H4O-1	ACETALDEHYDE	X	X	X	X	X
C2H4O-2	ETHYLENE-OXIDE	X	X	X	X	X
C2H4O2-1	ACETIC-ACID	X	X	X	X	X
C2H4O2-2	METHYL-FORMATE	X	X	X	X	X
C2H4O2S	THIOGLYCOLIC-ACID	X	X	X		
C2H4O3-D1	GLYCOLIC-ACID	X	X	X	X	
C2H4O3-D2	PERACETIC-ACID	X	X	X	X	
C2H4S	THIACYCLOPROPANE	X	X			
C2H5BR	ETHYL-BROMIDE	X	X	X	X	X
C2H5CL	ETHYL-CHLORIDE	X	X	X	X	X
C2H5CLO	2-CHLOROETHANOL	X	X	X	X	
C2H5CLO-D1	CHLOROMETHYL-METHYL-ETHER	X	X	X		
C2H5F	ETHYL-FLUORIDE	X	X	X	X	X
C2H5I	ETHYL-IODIDE	X	X	X	X	
C2H5N	ETHYLENE-IMINE	X	X	X	X	X
C2H5NO-D1	ACETAMIDE	X	X	X	X	

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C2H5NO-D2	N-METHYLFORMAMIDE	X	X	X	X	
C2H5NO-D3	ACETALDOXIME	X				
C2H5NO2	NITROETHANE	X	X	X	X	
C2H5NO2-D1	GLYCINE	X	X	X		
C2H6	ETHANE	X	X	X	X	X
C2H6ALCL	DIMETHYLALUMINUM-CHLORIDE	X	X	X	X	
C2H6O-1	DIMETHYL-ETHER	X	X	X	X	X
C2H6O-2	ETHANOL	X	X	X	X	X
C2H6O2	ETHYLENE-GLYCOL	X	X	X	X	X
C2H6O4S	DIMETHYL-SULFATE	X	X	X	X	
C2H6OS	DIMETHYL-SULFOXIDE	X	X	X	X	
C2H6OS-D1	2-MERCAPTOETHANOL	X	X	X		
C2H6S-1	ETHYL-MERCAPTAN	X	X	X	X	X
C2H6S-2	DIMETHYL-SULFIDE	X	X	X	X	X
C2H6S2	DIMETHYL-DISULFIDE	X	X	X	X	
C2H6S2-D1	1,2-ETHANEDITHIOL	X	X	X		
C2H6SICL2	DIMETHYLDICHLOROSILANE	X	X	X		
C2H7N-1	ETHYL-AMINE	X	X	X	X	X
C2H7N-2	DIMETHYLAMINE	X	X	X	X	X
C2H7NO	MONOETHANOLAMINE	X	X	X	X	X
C2H7NO2	AMMONIUM-ACETATE	X	X	X	X	
C2H7SICL	DIMETHYLCHLOROSILANE	X	X	X		
C2H8N2	ETHYLENEDIAMINE	X	X	X	X	X
C2H8N2O4	AMMONIUM-OXALATE	X	X	X	X	
C2H8P2O6	1,2-ETHANE-DIPHOSPHONIC-ACID	X	X	X		
C2H8SI	DIMETHYL-SILANE	X	X	X	X	
C2HBRCLF3	HALOTHANE	X	X	X	X	
C2HCL2F3-D1	1,1-DICHLORO-2,2,2-TRIFLUOROETHA	X	X	X		
C2HCL2F3-D2	1,2-DICHLORO-1,1,2-TRIFLUOROETHA	X	X	X		
C2HCL2F3-D3	2,2-DICHLORO-1,1,2-TRIFLUOROETHA	X				
C2HCL3	TRICHLOROETHYLENE	X	X	X	X	X
C2HCL3O	DICHLOROACETYL-CHLORIDE	X	X	X	X	
C2HCL3O-D1	TRICHLOROACETALDEHYDE	X	X	X	X	
C2HCL3O2	TRICHLOROACETIC-ACID	X	X	X	X	
C2HCL5	PENTACHLOROETHANE	X	X	X	X	
C2HCLF2	2-CHLORO-1,1-DIFLUOROETHYLENE	X	X	X	X	
C2HCLF4	2-CHLORO-1,1,1,2-TETRAFLUOROETHA	X	X	X		
C2HF3O2	TRIFLUOROACETIC-ACID	X	X	X	X	X
C2HF5	PENTAFLUOROETHANE	X	X	X	X	
C2N2	CYANOGEN	X	X	X	X	X

Alias	Name	Available in Databank P11	P10	P93	P856	PCD
C3CL2F6	1,3-DICHLOROHEXAFLUOROPROPANE	X	X			
C3F6	HEXAFLUOROPROPYLENE	X	X	X	X	
C3F6O	HEXAFLUOROACETONE	X	X	X	X	
C3F8	OCTAFLUOROPROPANE	X	X	X	X	
C3H10N2	1,2-PROPANEDIAMINE	X	X	X	X	
C3H10N2-D1	1,3-PROPANEDIAMINE	X				
C3H10SI	TRIMETHYL-SILANE	X	X	X	X	
C3H10SIO3	TRIMETHOXYSILANE	X				
C3H2F6	1,1,1,2,3,3-HEXAFLUOROPROPANE	X				
C3H2N2	MALONONITRILE	X	X	X	X	
C3H3CL	PROPARGYL-CHLORIDE	X	X	X	X	
C3H3F3	3,3,3-TRIFLUOROPROPENE	X				
C3H3F5	1,1,1,2,2-PENTAFLUOROPROPANE	X	X			
C3H3F5O	2-DIFLUOROMETHOXY-1,1,1-TRIFLURO	X				
C3H3N	ACRYLONITRILE	X	X	X	X	X
C3H3NO	OXAZOLE	X	X	X	X	
C3H4-1	PROPADIENE	X	X	X	X	X
C3H4-2	METHYL-ACETYLENE	X	X	X	X	X
C3H4CL2	2,3-DICHLOROPROPENE	X	X	X	X	
C3H4N2	PYRAZOLE	X	X			
C3H4O	ACROLEIN	X	X	X	X	X
C3H4O-D0	PROPARGYL-ALCOHOL	X	X	X	X	
C3H4O2-1	ACRYLIC-ACID	X	X	X	X	X
C3H4O2-2	VINYL-FORMATE	X	X	X	X	X
C3H4O2-D0	BETA-PROPIOLACTONE	X	X	X	X	
C3H4O3	ETHYLENE-CARBONATE	X	X	X	X	
C3H4O3-D1	PYRUVIC-ACID	X	X	X	X	
C3H4O4	MALONIC-ACID	X	X	X		
C3H5CL	ALLYL-CHLORIDE	X	X	X	X	X
C3H5CL-D0	2-CHLOROPROPENE	X	X	X	X	
C3H5CL3	1,2,3-TRICHLOROPROPANE	X	X	X	X	X
C3H5CLO	ALPHA-EPICHLOROHYDRIN	X	X	X	X	
C3H5CLO2	METHYL-CHLOROACETATE	X	X	X	X	
C3H5CLO2-D1	ETHYL-CHLOROFORMATE	X	X	X	X	
C3H5N	PROPIONITRILE	X	X	X	X	X
C3H5N3O9	NITROGLYCERINE	X	X	X	X	
C3H5NO	LACTONITRILE	X	X	X	X	
C3H5NO-D1	ACRYLAMIDE	X	X	X	X	
C3H5NO-D2	HYDRACRYLONITRILE	X	X	X	X	
C3H6-1	CYCLOPROPANE	X	X	X	X	X
C3H6-2	PROPYLENE	X	X	X	X	X
C3H6CL2	1,2-DICHLOROPROPANE	X	X	X	X	X
C3H6CL2-D1	1,1-DICHLOROPROPANE	X	X	X	X	
C3H6CL2-D2	1,3-DICHLOROPROPANE	X	X	X	X	
C3H6CL2O-D1	1,3-DICHLORO-2-PROPANOL	X				

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C3H6CL2O-D2	2,3-DICHLORO-1-PROPANOL	X				
C3H6N6	MELAMINE	X	X	X		
C3H6O-1	ACETONE	X	X	X	X	X
C3H6O-2	ALLYL-ALCOHOL	X	X	X	X	X
C3H6O-3	N-PROPIONALDEHYDE	X	X	X	X	X
C3H6O-4	PROPYLENE-OXIDE	X	X	X	X	X
C3H6O-5	VINYL-METHYL-ETHER	X	X	X	X	X
C3H6O-D0	1,3-PROPYLENE-OXIDE	X	X	X	X	
C3H6O2-1	PROPIONIC-ACID	X	X	X	X	X
C3H6O2-2	ETHYL-FORMATE	X	X	X	X	X
C3H6O2-3	METHYL-ACETATE	X	X	X	X	X
C3H6O2-D1	ACETOL	X	X	X		
C3H6O2-D2	2,3-EPOXY-1-PROPANOL	X	X	X		
C3H6O2S	3-MERCAPTOPROPIONIC-ACID	X	X	X	X	
C3H6O3	METHOXYACETIC-ACID	X	X	X	X	
C3H6O3-D1	LACTIC-ACID	X	X	X	X	
C3H6O3-D2	TRIOXANE	X	X	X	X	
C3H6O3-D3	DIMETHYL-CARBONATE	X	X	X		
C3H6S	TRIMETHYLENE-SULFIDE	X	X			
C3H6SICL2	METHYL-VINYL-DICHLOROSILANE	X				
C3H7BR-D1	1-BROMOPROPANE	X	X	X	X	
C3H7BR-D2	2-BROMOPROPANE	X	X	X	X	
C3H7CL-1	PROPYL-CHLORIDE	X	X	X	X	X
C3H7CL-2	ISOPROPYL-CHLORIDE	X	X	X	X	X
C3H7CLO2	3-CHLORO-1,2-PROPANEDIOL	X				
C3H7I-D1	ISOPROPYL-IODIDE	X	X	X	X	
C3H7I-D2	N-PROPYL-IODIDE	X	X	X	X	
C3H7N	ALLYLAMINE	X	X	X	X	
C3H7N-D1	PROPYLENEIMINE	X	X	X	X	
C3H7NO	N,N-DIMETHYLFORMAMIDE	X	X	X	X	
C3H7NO-D1	N-METHYLACETAMIDE	X	X	X	X	
C3H7NO2-D1	1-NITROPROPANE	X	X	X	X	
C3H7NO2-D2	2-NITROPROPANE	X	X	X	X	
C3H8	PROPANE	X	X	X	X	X
C3H8O-1	1-PROPANOL	X	X	X	X	X
C3H8O-2	ISOPROPYL-ALCOHOL	X	X	X	X	X
C3H8O-3	METHYL-ETHYL-ETHER	X	X	X	X	X
C3H8O2	2-METHOXYETHANOL	X	X	X	X	
C3H8O2-1	METHYLAL	X	X	X	X	X
C3H8O2-2	PROPANEDIOL-1,2	X	X	X	X	X
C3H8O2-3	1,3-PROPANEDIOL	X	X	X	X	X
C3H8O3	GLYCEROL	X	X	X	X	X
C3H8S	METHYL-ETHYL-SULFIDE	X	X	X		X
C3H8S-D1	ISOPROPYL-MERCAPTAN	X	X	X	X	
C3H8S-E1	N-PROPYLMERCAPTAN	X	X	X	X	

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C3H9AL	TRIMETHYLALUMINUM	X	X	X		
C3H9GA	TRIMETHYLGALLIUM	X	X	X		
C3H9N-1	N-PROPYL-AMINE	X	X	X	X	X
C3H9N-2	ISOPROPYL-AMINE	X	X	X	X	X
C3H9N-3	TRIMETHYL-AMINE	X	X	X	X	X
C3H9NO	METHYL-ETHANOLAMINE	X	X	X	X	
C3H9NO-D1	1-AMINO-2-PROPANOL	X	X	X	X	
C3H9NO-D2	3-AMINO-1-PROPANOL	X	X	X	X	
C3H9NO2	AMMONIUM-PROPIONATE	X				
C3H9O4P	TRIMETHYL-PHOSPHATE	X	X	X	X	
C3H9SICL	TRIMETHYLCHLOROSILANE	X	X	X		
C3HF7	1,1,1,2,3,3,3-HEPTAFLUOROPROPANE	X				

Pure Component Databanks: C4

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C4CL2F6	1,2-DICHLOROHEXAFLUOROCYCLOBUTAN	X	X			
C4CL4S	TETRACHLOROTHIOPHENE	X	X	X	X	
C4CL6	HEXACHLORO-1,3-BUTADIENE	X	X	X	X	
C4F10	DECAFLUOROBUTANE	X	X	X	X	
C4F8-D1	OCTAFLUORO-2-BUTENE	X	X	X	X	
C4F8-D2	OCTAFLUOROCYCLOBUTANE	X	X	X	X	
C4H10-1	N-BUTANE	X	X	X	X	X
C4H10-2	ISOBUTANE	X	X	X	X	X
C4H10N2	PIPERAZINE	X	X	X	X	
C4H10O-1	N-BUTANOL	X	X	X	X	X
C4H10O-2	2-BUTANOL	X	X	X	X	X
C4H10O-3	ISOBUTANOL	X	X	X	X	X
C4H10O-4	TERT-BUTYL-ALCOHOL	X	X	X	X	X
C4H10O-5	DIETHYL-ETHER	X	X	X	X	X
C4H10O-D1	METHYL-ISOPROPYL-ETHER	X	X	X	X	
C4H10O-D2	METHYL-N-PROPYL-ETHER	X	X	X		
C4H10O2	1,2-DIMETHOXYETHANE	X	X	X	X	X
C4H10O2-D1	1,3-BUTANEDIOL	X	X	X	X	
C4H10O2-D10	N-BUTYLHYDROPEROXIDE	X				
C4H10O2-D2	1,4-BUTANEDIOL	X	X	X	X	
C4H10O2-D3	T-BUTYL-HYDROPEROXIDE	X	X	X	X	
C4H10O2-D4	2-ETHOXYETHANOL	X	X	X	X	
C4H10O2-D5	2,3-BUTANEDIOL	X	X	X	X	
C4H10O2-D6	1,2-BUTANEDIOL	X	X	X		
C4H10O2-D7	PG-MONOMETHYL-ETHER	X	X	X		
C4H10O2-D8	2-METHYL-1,3-PROPANEDIOL	X	X	X		
C4H10O2-D9	2-METHOXY-PROPANOL-1	X	X			
C4H10O2S	THIODIGLYCOL	X	X	X		
C4H10O3	DIETHYLENE-GLYCOL	X	X	X	X	X

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C4H10O4S	DIETHYL-SULFATE	X	X	X	X	
C4H10OS	ETHYLTHIOETHANOL	X	X	X		
C4H10OS2	DIMERCAPTOETHYL-ETHER	X	X	X		
C4H10S	DIETHYL-SULFIDE	X	X	X	X	X
C4H10S-D1	N-BUTYL-MERCAPTAN	X	X	X	X	
C4H10S-D2	TERT-BUTYL-MERCAPTAN	X	X	X	X	
C4H10S-D3	METHYL-N-PROPYL-SULFIDE	X	X	X		
C4H10S-E1	SEC-BUTYL-MERCAPTAN	X	X	X	X	
C4H10S-E2	ISOBUTYL-MERCAPTAN	X	X	X	X	
C4H10S2	DIETHYL-DISULFIDE	X	X	X	X	X
C4H10SO3	DIETHYLSULFITE	X	X	X		
C4H11N-1	N-BUTYL-AMINE	X	X	X	X	X
C4H11N-2	ISOBUTYL-AMINE	X	X	X	X	X
C4H11N-3	DIETHYL-AMINE	X	X	X	X	X
C4H11N-D1	SEC-BUTYLAMINE	X	X	X	X	
C4H11N-D2	TERT-BUTYLAMINE	X	X	X	X	
C4H11NO	DIMETHYLETHANOLAMINE	X	X	X	X	
C4H11NO-D1	3-METHOXYISOPROPYLAMINE	X				
C4H11NO-D2	N,N-DIETHYLHYDROXYLAMINE	X				
C4H11NO2-1	DIETHANOLAMINE	X	X	X	X	X
C4H11NO2-2	DIGLYCOLAMINE	X	X	X	X	X
C4H12N2O	N-AMINOETHYL-ETHANOLAMINE	X	X	X	X	
C4H12SI	TETRAMETHYLSILANE	X	X	X	X	
C4H12SIO2	DIMETHYLDIMETHOXYSILANE	X	X			
C4H13N3	DIETHYLENE-TRIAMINE	X	X	X	X	
C4H2N2-D1	FUMARONITRILE	X	X			
C4H2N2-D2	MALEONITRILE	X	X			
C4H2O3	MALEIC-ANHYDRIDE	X	X	X	X	X
C4H4	VINYLACETYLENE	X	X	X	X	X
C4H4N2	SUCCINONITRILE	X	X	X	X	
C4H4N2-D1	PYRAZINE	X	X			
C4H4N2-D2	PYRIDAZINE	X	X			
C4H4N2-D3	PYRIMIDINE	X	X			
C4H4O	FURAN	X	X	X	X	X
C4H4O2	DIKETENE	X	X	X	X	
C4H4O3	SUCCINIC-ANHYDRIDE	X	X	X	X	
C4H4O4-D1	FUMARIC-ACID	X	X	X	X	
C4H4O4-D2	MALEIC-ACID	X	X	X	X	
C4H4S	THIOPHENE	X	X	X	X	X
C4H5CL	CHLOROPRENE	X	X	X	X	
C4H5N	METHACRYLONITRILE	X	X	X	X	
C4H5N-1	ALLYL-CYANIDE	X	X	X	X	X
C4H5N-2	PYRROLE	X	X	X	X	X
C4H5N-E1	TRANS-CROTONITRILE	X	X	X	X	
C4H5N-E3	CIS-CROTONITRILE	X	X	X	X	

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C4H5N3	2,2-IMINOBIS-ACETONITRILE	X	X	X		
C4H5NO	ACROLEIN-CYANOHYDRIN	X	X			
C4H5NO2	METHYL-CYANOACETATE	X	X	X	X	
C4H6-1	1-BUTYNE	X	X	X	X	X
C4H6-2	2-BUTYNE	X	X	X	X	X
C4H6-3	1,2-BUTADIENE	X	X	X	X	X
C4H6-4	1,3-BUTADIENE	X	X	X	X	X
C4H6CL2	1,4-DICHLORO-TRANS-2-BUTENE	X	X	X	X	
C4H6CL2-E1	1,3-DICHLORO-TRANS-2-BUTENE	X	X	X	X	
C4H6CL2-E2	3,4-DICHLORO-1-BUTENE	X	X	X	X	
C4H6CL2-E3	1,4-DICHLORO-CIS-2-BUTENE	X	X	X	X	
C4H6O	2,5-DIHYDROFURAN	X	X	X	X	
C4H6O-D1	TRANS-CROTONALDEHYDE	X	X	X	X	
C4H6O-D2	DIVINYL-ETHER	X	X	X	X	
C4H6O-D3	METHACROLEIN	X	X	X	X	
C4H6O-D4	2,3-DIHYDROFURAN	X	X			
C4H6O2-1	VINYL-ACETATE	X	X	X	X	X
C4H6O2-2	METHYL-ACRYLATE	X	X	X	X	X
C4H6O2-D1	2-BUTYNE-1,4-DIOL	X	X	X	X	
C4H6O2-D2	GAMMA-BUTYROLACTONE	X	X	X	X	
C4H6O2-D3	CIS-CROTONIC-ACID	X	X	X	X	
C4H6O2-D4	TRANS-CROTONIC-ACID	X	X	X	X	
C4H6O2-D5	METHACRYLIC-ACID	X	X	X	X	
C4H6O2S	SULFOLENE		X	X		
C4H6O3	ACETIC-ANHYDRIDE	X	X	X	X	X
C4H6O3-D1	PROPYLENE-CARBONATE	X	X	X		
C4H6O4-1	DIMETHYL-OXALATE	X	X	X		X
C4H6O4-2	SUCCINIC-ACID	X	X	X	X	X
C4H6O5	DIGLYCOLIC-ACID	X	X	X	X	
C4H6O5-D1	MALIC-ACID	X	X	X	X	
C4H6O6	TARTARIC-ACID	X	X	X	X	
C4H7CLO2	ETHYLCHLOROACETATE	X	X	X		
C4H7N	BUTYRONITRILE	X	X	X	X	X
C4H7N-D0	ISOBUTYRONITRILE	X	X	X	X	
C4H7NO-D1	ACETONE-CYANOHYDRIN	X	X	X	X	
C4H7NO-D2	2-PYRROLIDONE	X	X	X	X	
C4H7NO-E1	2-METHACRYLAMIDE	X	X	X	X	
C4H7NO-E2	3-METHOXYPROPIONITRILE	X	X	X	X	
C4H8-1	1-BUTENE	X	X	X	X	X
C4H8-2	CIS-2-BUTENE	X	X	X	X	X
C4H8-3	TRANS-2-BUTENE	X	X	X	X	X
C4H8-4	CYCLOBUTANE	X	X	X	X	X
C4H8-5	ISOBUTYLENE	X	X	X	X	X
C4H8CL2	1,4-DICHLOROBUTANE	X	X	X	X	
C4H8CL2-D1	1,2-DICHLOROBUTANE	X	X	X		

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C4H8CL2-D2	2,3-DICHLOROBUTANE	X	X	X		
C4H8CL2O	DICHLOROETHYL-ETHER	X				
C4H8O	1,2-EPOXYBUTANE	X	X	X	X	
C4H8O-1	N-BUTYRALDEHYDE	X	X	X	X	X
C4H8O-2	ISOBUTYRALDEHYDE	X	X	X	X	X
C4H8O-3	METHYL-ETHYL-KETONE	X	X	X	X	X
C4H8O-4	TETRAHYDROFURAN	X	X	X	X	X
C4H8O-5	VINYL-ETHYL-ETHER	X	X	X	X	X
C4H8O-D1	1,2-EPOXY-2-METHYLPROPANE	X	X	X		
C4H8O2-1	N-BUTYRIC-ACID	X	X	X	X	X
C4H8O2-2	1,4-DIOXANE	X	X	X	X	X
C4H8O2-3	ETHYL-ACETATE	X	X	X	X	X
C4H8O2-4	ISOBUTYRIC-ACID	X	X	X	X	X
C4H8O2-5	METHYL-PROPIONATE	X	X	X	X	X
C4H8O2-6	N-PROPYL-FORMATE	X	X	X	X	X
C4H8O2-D1	ACETALDOL	X	X	X		
C4H8O2-D2	CIS-2-BUTENE-1,4-DIOL	X	X	X	X	
C4H8O2-D3	TRANS-2-BUTENE-1,4-DIOL	X	X	X	X	
C4H8O2-D4	1,3-DIOXANE	X	X	X		
C4H8O2-D5	3-HYDROXY-2-METHYL-PROPIONALDEHY	X	X	X		
C4H8O2-D6	4-HYDROXYBUTYRALDEHYDE	X	X	X		
C4H8O2S	SULFOLANE	X	X	X	X	
C4H8O3	METHYL-LACTATE	X	X			
C4H8O3-D1	ALPHA-HYDROXYISOBUTYRIC-ACID	X				
C4H8OS	3-METHYLMERCAPTO-PROPANAL	X				
C4H8S	TETRAHYDROTHIOPHENE	X	X	X	X	
C4H9BR-D1	1-BROMOBUTANE	X	X	X	X	
C4H9BR-D2	2-BROMOBUTANE	X	X	X	X	
C4H9CL-1	1-CHLOROBUTANE	X	X	X	X	X
C4H9CL-2	2-CHLOROBUTANE	X	X	X	X	X
C4H9CL-3	TERT-BUTYL-CHLORIDE	X	X	X	X	X
C4H9CL-D1	ISOBUTYL-CHLORIDE	X	X	X		
C4H9I	N-BUTYL-IODIDE	X				
C4H9N	PYRROLIDINE	X	X	X	X	X
C4H9NO	MORPHOLINE	X	X	X	X	X
C4H9NO-D0	N,N-DIMETHYLACETAMIDE	X	X	X	X	
C4H9NO2	1-NITROBUTANE	X				

Pure Component Databanks: C5

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C5CL6	HEXACHLOROCYCLOPENTADIENE	X	X	X	X	
C5H10-1	CYCLOPENTANE	X	X	X	X	X
C5H10-2	1-PENTENE	X	X	X	X	X
C5H10-3	CIS-2-PENTENE	X	X	X	X	X
C5H10-4	TRANS-2-PENTENE	X	X	X	X	X

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C5H10-5	2-METHYL-1-BUTENE	X	X	X	X	X
C5H10-6	2-METHYL-2-BUTENE	X	X	X	X	X
C5H10-7	3-METHYL-1-BUTENE	X	X	X	X	X
C5H10CL2	1,5-DICHLOROPENTANE	X	X	X	X	
C5H10NNAS2	SODIUM-DIETHYLDITHIOCARBAMATE		X	X		
C5H10O-1	VALERALDEHYDE	X	X	X	X	X
C5H10O-2	METHYL-N-PROPYL-KETONE	X	X	X	X	X
C5H10O-3	METHYL-ISOPROPYL-KETONE	X	X	X	X	X
C5H10O-4	DIETHYL-KETONE	X	X	X	X	X
C5H10O2	NEOPENTANOIC-ACID	X	X	X		
C5H10O2-1	N-VALERIC-ACID	X	X	X	X	X
C5H10O2-2	ISOBUTYL-FORMATE	X	X	X	X	X
C5H10O2-3	N-PROPYL-ACETATE	X	X	X	X	X
C5H10O2-4	ETHYL-PROPIONATE	X	X	X	X	X
C5H10O2-5	METHYL-BUTYRATE	X	X	X	X	X
C5H10O2-6	METHYL-ISOBUTYRATE	X	X	X		X
C5H10O2-D1	N-BUTYL-FORMATE	X	X	X	X	
C5H10O2-D2	ISOPROPYL-ACETATE	X	X	X	X	
C5H10O2-D3	ISOVALERIC-ACID	X	X	X	X	
C5H10O2-D4	2-METHYLBUTYRIC-ACID	X	X	X	X	
C5H10O2-D5	TETRAHYDROFURFURYL-ALCOHOL	X	X	X	X	
C5H10O2-D6	SEC-BUTYL-FORMATE	X	X	X		
C5H10O2-D7	TERT-BUTYL-FORMATE	X	X	X		
C5H10O2S	3-METHYL-SULFOLANE	X	X	X	X	
C5H10O3-D1	DIETHYL-CARBONATE	X	X	X	X	
C5H10O3-D2	ETHYL-LACTATE	X	X	X	X	
C5H11CL	1-CHLOROPENTANE	X	X	X	X	
C5H11N	PIPERIDINE	X	X	X	X	X
C5H11N-D0	N-METHYLPYRROLIDINE	X	X	X	X	
C5H11N-D1	CYCLOPENTYLAMINE	X				
C5H11NO	TERT-BUTYLFORMAMIDE	X	X	X	X	
C5H12-1	N-PENTANE	X	X	X	X	X
C5H12-2	2-METHYL-BUTANE	X	X	X	X	X
C5H12-3	2,2-DIMETHYL-PROPANE	X	X	X	X	X
C5H12O	METHYL-SEC-BUTYL-ETHER	X	X	X	X	
C5H12O-1	1-PENTANOL	X	X	X	X	X
C5H12O-2	2-METHYL-1-BUTANOL	X	X	X	X	X
C5H12O-3	3-METHYL-1-BUTANOL	X	X	X	X	X
C5H12O-4	2-METHYL-2-BUTANOL	X	X	X	X	X
C5H12O-5	2,2-DIMETHYL-1-PROPANOL	X	X	X	X	X
C5H12O-6	ETHYL-PROPYL-ETHER	X	X	X	X	X
C5H12O-D1	3-METHYL-2-BUTANOL	X	X	X	X	
C5H12O-D2	METHYL-TERT-BUTYL-ETHER	X	X	X	X	
C5H12O-D3	2-PENTANOL	X	X	X	X	
C5H12O-D4	3-PENTANOL	X	X	X	X	

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C5H12O-D5	ETHYL-ISOPROPYL-ETHER	X	X	X		
C5H12O-E1	METHYL-ISOBUTYL-ETHER	X	X	X	X	
C5H12O-E2	METHYL-N-BUTYL-ETHER	X	X	X		
C5H12O2-D1	NEOPENTYL-GLYCOL	X	X	X	X	
C5H12O2-D2	1,5-PENTANEDIOL	X	X	X	X	
C5H12O2-D3	ETHYLENE-GLYCOL-MONOPROPYL-ETHER	X	X	X	X	
C5H12O2-D4	ETHYLAL	X	X	X		
C5H12O2-D5	2,4-PENTANEDIOL	X	X	X		
C5H12O3	2-2-METHOXYETHOXY-ETHANOL	X	X	X	X	
C5H12O4	PENTAERYTHRITOL	X	X	X	X	
C5H12S	1-PENTANETHIOL	X	X	X	X	
C5H12S-D1	METHYL-T-BUTYL-SULFIDE	X	X	X		
C5H12S-D2	METHYL-N-BUTYL-SULFIDE	X	X	X		
C5H13N	N-PENTYLAMINE	X	X	X	X	
C5H13NO2	METHYL-DIETHANOLAMINE	X	X	X	X	
C5H4O2	FURFURAL	X	X	X	X	
C5H4O3	METHYL-MALEIC-ANHYDRIDE	X	X			
C5H5N	PYRIDINE	X	X	X	X	X
C5H6	CYCLOPENTADIENE	X	X	X	X	
C5H6-E1	2-METHYL-1-BUTENE-3-YNE	X	X	X	X	
C5H6-E2	1-PENTENE-3-YNE	X	X	X	X	
C5H6-E3	1-PENTENE-4-YNE	X	X	X	X	
C5H6N2	GLUTARONITRILE	X	X	X	X	
C5H6O2	FURFURYL-ALCOHOL	X	X	X	X	
C5H6O3	GLUTARIC-ANHYDRIDE	X	X	X	X	
C5H6O4-E1	CITRACONIC-ACID	X	X	X	X	
C5H6O4-E2	ITACONIC-ACID	X	X	X	X	
C5H6S-E1	2-METHYLTHIOPHENE	X	X	X		
C5H6S-E2	3-METHYLTHIOPHENE	X	X	X		
C5H7N	N-METHYLPYRROLE	X	X	X	X	
C5H7NO2	ETHYL-CYANOACETATE	X	X	X	X	
C5H8	CIS-1,3-PENTADIENE	X	X	X	X	
C5H8-1	CYCLOPENTENE	X	X	X	X	X
C5H8-2	1,2-PENTADIENE	X	X	X	X	X
C5H8-3	1-TRANS-3-PENTADIENE	X	X	X	X	X
C5H8-4	1,4-PENTADIENE	X	X	X	X	X
C5H8-5	1-PENTYNE	X	X	X	X	X
C5H8-6	2-METHYL-1,3-BUTADIENE	X	X	X	X	X
C5H8-7	3-METHYL-1,2-BUTADIENE	X	X	X	X	X
C5H8-E2	3-METHYL-1-BUTYNE	X	X	X	X	
C5H8-E4	2,3-PENTADIENE	X	X	X	X	
C5H8-E5	2-PENTYNE	X	X	X		
C5H8N4O12	PENTAERYTHRITOL-TETRANITRATE	X	X	X	X	
C5H8O	CYCLOPENTANONE	X	X	X	X	X

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C5H8O-D1	METHYL-ISOPROPENYL-KETONE	X	X	X	X	
C5H8O2	ETHYL-ACRYLATE	X	X	X	X	X
C5H8O2-D1	ACETYLACETONE	X	X	X	X	
C5H8O2-D2	ALLYL-ACETATE	X	X	X	X	
C5H8O2-D3	METHYL-METHACRYLATE	X	X	X	X	
C5H8O2-D4	GAMMA-VALEROLACTONE	X	X	X		
C5H8O2-D5	VINYL-PROPIONATE	X	X	X	X	
C5H8O2-D6	GLUTARALDEHYDE	X	X	X		
C5H8O3	2-HYDROXYETHYL-ACRYLATE	X	X	X	X	
C5H8O3-D1	LEVULINIC-ACID	X	X	X	X	
C5H8O3-D2	METHYL-ACETOACETATE	X	X	X	X	
C5H8O4	GLUTARIC-ACID	X	X	X	X	
C5H9N	VALERONITRILE	X	X	X	X	
C5H9NO-D1	N-BUTYL-ISOCYANATE	X	X	X	X	
C5H9NO-D2	N-METHYL-2-PYRROLIDONE	X	X	X	X	
C5H9NO4	L-GLUTAMIC-ACID	X	X	X	X	
C5H9NS	N-METHYLTHIOPYRROLIDONE	X	X	X		

Pure Component Databanks: C6

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C6CL6	HEXACHLOROBENZENE	X	X	X	X	
C6F12	PERFLUOROCYCLOHEXANE	X	X	X		X
C6F14	PERFLUORO-N-HEXANE	X	X	X		X
C6F6	PERFLUOROBENZENE	X	X	X	X	X
C6H10-1	1,5-HEXADIENE	X	X	X	X	X
C6H10-2	CYCLOHEXENE	X	X	X	X	X
C6H10-D1	1-METHYLCYCLOPENTENE	X	X	X		
C6H10-D2	3-METHYLCYCLOPENTENE	X	X	X		
C6H10-D3	4-METHYLCYCLOPENTENE	X	X	X		
C6H10-D4	1,2-HEXADIENE	X	X	X		
C6H10-E2	1-HEXYNE	X	X	X	X	
C6H10-E3	2,3-DIMETHYL-1,3-BUTADIENE	X	X	X	X	
C6H10-E4	CIS,TRANS-2,4-HEXADIENE	X	X	X	X	
C6H10-E5	TRANS,TRANS-2,4-HEXADIENE	X	X	X	X	
C6H10-E6	2-HEXYNE	X	X	X	X	
C6H10-E7	3-HEXYNE	X	X	X	X	
C6H10-E8	1,4-HEXADIENE	X	X	X		
C6H10O	CYCLOHEXANONE	X	X	X	X	X
C6H10O-D0	MESITYL-OXIDE	X	X	X	X	
C6H10O-D1	2-METHYL-2-PENTENAL	X				
C6H10O2-D1	CAPROLACTONE	X	X	X	X	
C6H10O2-D2	ETHYL-METHACRYLATE	X	X	X	X	
C6H10O2-D3	N-PROPYL-ACRYLATE	X	X	X	X	
C6H10O2-D4	METHOXYDIHYDROPYRAN	X	X			
C6H10O2-D5	ISOPROPYL-ACRYLATE	X	X			

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C6H10O3	2-HYDROXYETHYL-METHACRYLATE	X	X			
C6H10O3-D1	ETHYLACETOACETATE	X	X	X	X	
C6H10O3-D2	PROPIONIC-ANHYDRIDE	X	X	X	X	
C6H10O4	ETHYLIDENE-DIACETATE	X	X	X	X	
C6H10O4-D1	ADIPIC-ACID	X	X	X	X	
C6H10O4-D2	DIETHYL-OXALATE	X	X	X	X	
C6H10O4-D3	ETHYLENE-GLYCOL-DIACETATE	X	X	X	X	
C6H10O5	DILACTIC-ACID	X	X			
C6H11N	HEXANENITRILE	X	X	X	X	
C6H11N-D1	DIALLYLAMINE	X	X	X		
C6H11NO	EPSILON-CAPROLACTAM	X	X	X	X	
C6H11NO-D1	CYCLOHEXANONE-OXIME	X	X	X	X	
C6H12-1	CYCLOHEXANE	X	X	X	X	X
C6H12-10	3-METHYL-TRANS-2-PENTENE	X	X	X		X
C6H12-11	4-METHYL-CIS-2-PENTENE	X	X	X	X	X
C6H12-12	4-METHYL-TRANS-2-PENTENE	X	X	X	X	X
C6H12-13	2,3-DIMETHYL-1-BUTENE	X	X	X	X	X
C6H12-14	2,3-DIMETHYL-2-BUTENE	X	X	X	X	X
C6H12-15	3,3-DIMETHYL-1-BUTENE	X	X	X	X	X
C6H12-2	METHYLCYCLOPENTANE	X	X	X	X	X
C6H12-3	1-HEXENE	X	X	X	X	X
C6H12-4	CIS-2-HEXENE	X	X	X	X	X
C6H12-5	TRANS-2-HEXENE	X	X	X	X	X
C6H12-6	CIS-3-HEXENE	X	X	X	X	X
C6H12-7	TRANS-3-HEXENE	X	X	X	X	X
C6H12-8	2-METHYL-2-PENTENE	X	X	X	X	X
C6H12-9	3-METHYL-CIS-2-PENTENE	X	X	X	X	X
C6H12-D1	2-ETHYL-1-BUTENE	X	X	X	X	
C6H12-D2	2-METHYL-1-PENTENE	X	X	X	X	
C6H12-D3	4-METHYL-1-PENTENE	X	X	X	X	
C6H12-E3	3-METHYL-1-PENTENE	X	X	X	X	
C6H12CL3PO3	BIS-2-CHLOROETHYL-2-CHLOROETHYL	X	X	X		
C6H12N2-E1	AMINOCAPRONITRILE	X	X	X		
C6H12N2-E2	TRIETHYLENEDIAMINE	X	X	X	X	
C6H12N4	HEXAMETHYLENETETRAMINE	X	X	X		
C6H12O	3-HEXANONE	X	X	X	X	
C6H12O-1	CYCLOHEXANOL	X	X	X	X	X
C6H12O-2	METHYL-ISOBUTYL-KETONE	X	X	X	X	X
C6H12O-D1	BUTYL-VINYL-ETHER	X	X	X	X	
C6H12O-D2	1-HEXANAL	X	X	X	X	
C6H12O-D3	2-HEXANONE	X	X	X	X	
C6H12O-E1	ETHYL-ISOPROPYL-KETONE	X	X	X	X	
C6H12O-E2	3-METHYL-2-PENTANONE	X	X	X		
C6H12O-E3	3,3-DIMETHYL-2-BUTANONE	X	X	X		
C6H12O2	TERT-BUTYL-ACETATE	X	X	X	X	

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C6H12O2-1	N-BUTYL-ACETATE	X	X	X	X	X
C6H12O2-2	ISOBUTYL-ACETATE	X	X	X	X	X
C6H12O2-3	ETHYL-BUTYRATE	X	X	X	X	X
C6H12O2-4	ETHYL-ISOBUTYRATE	X	X	X	X	X
C6H12O2-5	N-PROPYL-PROPIONATE	X	X	X	X	X
C6H12O2-D1	SEC-BUTYL-ACETATE	X	X	X	X	
C6H12O2-D2	CYCLOHEXYL-PEROXIDE	X	X	X	X	
C6H12O2-D3	DIACETONE-ALCOHOL	X	X	X	X	
C6H12O2-D4	2-ETHYL-BUTYRIC-ACID	X	X	X	X	
C6H12O2-D5	N-HEXANOIC-ACID	X	X	X	X	
C6H12O2-D6	NEOHEXANOIC-ACID	X	X	X		
C6H12O2-E1	N-PENTYL-FORMATE	X	X	X	X	
C6H12O3	6-HYDROXYHEXANOIC-ACID	X	X			
C6H12O3-D1	2-ETHOXYETHYL-ACETATE	X	X	X	X	
C6H12O3-D2	PARALDEHYDE	X	X	X	X	
C6H12O3-E1	HYDROXYCAPROIC-ACID	X	X	X	X	
C6H12O3-E2	PG-MONOMETHYL-ETHER-ACETATE	X	X	X		
C6H12O6	DEXTROSE	X	X	X	X	
C6H12O6-D1	INOSITOL	X	X	X		
C6H12S	CYCLOHEXYL-MERCAPTAN	X	X	X		
C6H13I	N-HEXYL-IODIDE	X				
C6H13N-D1	CYCLOHEXYLAMINE	X	X	X	X	
C6H13N-D2	HEXAMETHYLENEIMINE	X	X	X	X	
C6H13N-D3	N-ETHYL-2-METHYLALLYLAMINE	X				
C6H14-1	N-HEXANE	X	X	X	X	X
C6H14-2	2-METHYL-PENTANE	X	X	X	X	X
C6H14-3	3-METHYL-PENTANE	X	X	X	X	X
C6H14-4	2,2-DIMETHYL-BUTANE	X	X	X	X	X
C6H14-5	2,3-DIMETHYL-BUTANE	X	X	X	X	X
C6H14N2O	N-2-HYDROXYETHYL-PIPERAZINE	X	X			
C6H14N2O2	LYSINE	X	X	X	X	
C6H14O-1	1-HEXANOL	X	X	X	X	X
C6H14O-2	ETHYL-BUTYL-ETHER	X	X	X	X	X
C6H14O-3	DIISOPROPYL-ETHER	X	X	X	X	X
C6H14O-D1	DI-N-PROPYL-ETHER	X	X	X	X	
C6H14O-D2	2-ETHYL-1-BUTANOL	X	X	X	X	
C6H14O-D3	2-METHYL-1-PENTANOL	X	X	X	X	
C6H14O-D4	4-METHYL-2-PENTANOL	X	X	X	X	
C6H14O-D5	3-METHYL-1-PENTANOL	X				
C6H14O-D6	3-METHYL-3-PENTANOL	X				
C6H14O-E1	2-HEXANOL	X	X	X	X	
C6H14O-E2	METHYL-TERT-PENTYL-ETHER	X	X	X	X	
C6H14O-E3	TERT-BUTYL-ETHYL-ETHER	X	X	X		
C6H14O-E4	METHYL-N-PENTYL-ETHER	X	X	X		
C6H14O2-D1	ACETAL	X	X	X	X	

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C6H14O2-D2	2-BUTOXYETHANOL	X	X	X	X	
C6H14O2-D3	1,6-HEXANEDIOL	X	X	X	X	
C6H14O2-D4	HEXYLENE-GLYCOL	X	X	X	X	
C6H14O2-D5	1,2-DIETHOXYETHANE	X	X	X		
C6H14O2-D6	1-ISOPROPOXY-2-PROPANOL	X				
C6H14O2-D7	PROPYLENE-GLYCOL-N-PROPYL-ETHER	X				
C6H14O2S	DI-N-PROPYL-SULFONE	X	X	X	X	
C6H14O3-D1	DIETHYLENE-GLYCOL-DIMETHYL-ETHER	X	X	X	X	
C6H14O3-D2	DIPROPYLENE-GLYCOL	X	X	X	X	
C6H14O3-D3	2-2-ETHOXYETHOXY-ETHANOL	X	X	X	X	
C6H14O3-D4	TRIMETHYLOLPROPANE	X	X	X	X	
C6H14O4	TRIETHYLENE-GLYCOL	X	X	X	X	
C6H14O6	SORBITOL	X	X	X	X	
C6H14S	N-HEXYLMERCAPTAN	X	X	X	X	
C6H14S-D1	DI-N-PROPYL-SULFIDE	X	X	X		
C6H14S-D2	METHYL-T-PENTYL-SULFIDE	X	X	X		
C6H14S-D3	ETHYL-T-BUTYL-SULFIDE	X	X	X		
C6H14S2	DI-N-PROPYLDISULFIDE	X	X	X		
C6H15AL	TRIETHYL-ALUMINUM	X	X	X	X	
C6H15AL2CL3	ETHYL-ALUMINUM-SESQUICHLORIDE	X	X	X	X	
C6H15N-1	DIPROPYLAMINE	X	X	X	X	X
C6H15N-2	TRIETHYLAMINE	X	X	X	X	X
C6H15N-D1	DIISOPROPYLAMINE	X	X	X	X	
C6H15N-D2	N-HEXYLAMINE	X	X	X	X	
C6H15N-D3	N,N-DIMETHYL-N-BUTYLAMINE	X				
C6H15N3	N-AMINOETHYL-PIPERAZINE	X	X	X	X	
C6H15NO	6-AMINOHEXANOL	X	X	X	X	
C6H15NO-D1	DIETHYLETHANOLAMINE	X	X			
C6H15NO2	DIISOPROPANOLAMINE	X	X	X	X	X
C6H15NO3	TRIETHANOLAMINE	X	X	X	X	
C6H15O4P	TRIETHYL-PHOSPHATE	X	X	X	X	
C6H16N2	HEXAMETHYLENEDIAMINE	X	X	X	X	
C6H16N2-D1	TETRAMETHYLETHYLENEDIAMINE	X	X			
C6H18N3OP	HEXAMETHYL-PHOSPHORAMIDE	X	X	X	X	
C6H18N4	TRIETHYLENE-TETRAMINE	X	X	X	X	
C6H18O3SI3	HEXAMETHYLCYCLOTRISILOXANE	X	X	X	X	
C6H18OSI2	HEXAMETHYLDISILOXANE	X	X	X	X	
C6H19NSI2	HEXAMETHYLDISILAZANE	X	X	X	X	
C6H3CL2NO2	1,2-DICHLORO-4-NITROBENZENE	X	X	X	X	
C6H3CL3	1,2,4-TRICHLOROBENZENE	X	X	X	X	
C6H3CL3-D1	1,3,5-TRICHLOROBENZENE	X	X	X		
C6H3CL3-D2	1,2,3-TRICHLOROBENZENE	X				
C6H3CLN2O4	1-CHLORO-2,4-DINITROBENZENE	X	X	X	X	
C6H3N3O6	1,3,5-TRINITROBENZENE	X	X	X	X	
C6H4BR2	M-DIBROMOBENZENE	X	X	X	X	

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C6H4CL2-1	O-DICHLOROBENZENE	X	X	X	X	X
C6H4CL2-2	M-DICHLOROBENZENE	X	X	X	X	X
C6H4CL2-3	P-DICHLOROBENZENE	X	X	X	X	X
C6H4CLNO2-D1	M-CHLORONITROBENZENE	X	X	X	X	
C6H4CLNO2-D2	O-CHLORONITROBENZENE	X	X	X	X	
C6H4CLNO2-D3	P-CHLORONITROBENZENE	X	X	X	X	
C6H4N2	NICOTINONITRILE	X	X			
C6H4N2O4-E1	M-DINITROBENZENE	X	X	X	X	
C6H4N2O4-E2	O-DINITROBENZENE	X	X	X	X	
C6H4N2O4-E3	P-DINITROBENZENE	X	X	X	X	
C6H4O2	QUINONE	X	X	X		
C6H5BR	BROMOBENZENE	X	X	X	X	X
C6H5CL	CHLOROBENZENE	X	X	X	X	X
C6H5CL2N	3,4-DICHLOROANILINE	X	X	X	X	
C6H5CLO-E1	M-CHLOROPHENOL	X	X	X	X	
C6H5CLO-E2	O-CHLOROPHENOL	X	X	X	X	
C6H5CLO-E3	P-CHLOROPHENOL	X	X	X	X	
C6H5F	FLUOROBENZENE	X	X	X	X	X
C6H5I	IODOBENZENE	X	X	X	X	X
C6H5NO2	NITROBENZENE	X	X	X	X	
C6H5NO2-D1	NIACIN	X	X	X		
C6H5SICL3	PHENYLTRICHLOROSILANE	X	X			
C6H6	BENZENE	X	X	X	X	X
C6H6CLN-D1	M-CHLOROANILINE	X	X	X	X	
C6H6CLN-D2	O-CHLOROANILINE	X	X	X	X	
C6H6CLN-D3	P-CHLOROANILINE	X	X	X	X	
C6H6N2-E1	CIS-DICYANO-1-BUTENE	X	X	X	X	
C6H6N2-E2	TRANS-DICYANO-1-BUTENE	X	X	X	X	
C6H6N2-E3	1,4-DICYANO-2-BUTENE	X	X	X	X	
C6H6N2O2-D1	M-NITROANILINE	X	X	X	X	
C6H6N2O2-D2	O-NITROANILINE	X	X	X	X	
C6H6N2O2-D3	P-NITROANILINE	X	X	X	X	
C6H6N4	2,2,2-NITRILOTRIS-ACETONITRILE	X	X	X		
C6H6O	PHENOL	X	X	X	X	X
C6H6O2	P-HYDROQUINONE	X	X	X	X	
C6H6O2-E1	1,2-BENZENEDIOL	X	X	X	X	
C6H6O2-E2	1,3-BENZENEDIOL	X	X	X	X	
C6H6O3	1,2,3-BENZENETRIOL	X	X	X	X	
C6H6O3S	BENZENESULFONIC-ACID	X	X	X		
C6H6S	PHENYL-MERCAPTAN	X	X	X	X	
C6H7N-1	ANILINE	X	X	X	X	X
C6H7N-2	4-METHYLPYRIDINE	X	X	X	X	X
C6H7N-D1	2-METHYLPYRIDINE	X	X	X	X	
C6H7N-D2	3-METHYLPYRIDINE	X	X	X	X	
C6H7NO3S	SULFANILIC-ACID		X	X		

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C6H8-E1	1,3-CYCLOHEXADIENE	X	X	X	X	
C6H8-E2	METHYLCYCLOPENTADIENE	X	X	X	X	
C6H8-E3	1,4-CYCLOHEXADIENE	X	X	X		
C6H8N2	METHYLGLUTARONITRILE	X	X	X	X	
C6H8N2-D1	ADIPONITRILE	X	X	X	X	
C6H8N2-D2	M-PHENYLENEDIAMINE	X	X	X	X	
C6H8N2-D3	O-PHENYLENEDIAMINE	X	X	X	X	
C6H8N2-D4	P-PHENYLENEDIAMINE	X	X	X	X	
C6H8N2-D5	PHENYLHYDRAZINE	X	X	X	X	
C6H8N2O	BIS-CYANOETHYL-ETHER	X	X	X	X	
C6H8O4	DIMETHYL-MALEATE	X	X	X	X	
C6H8O6	ASCORBIC-ACID	X	X	X	X	
C6H8O7	CITRIC-ACID	X	X	X	X	

Pure Component Databanks: C7

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C7F14	PERFLUOROMETHYLCYCLOHEXANE	X	X	X		X
C7F16	PERFLUORO-N-HEPTANE		X	X		X
C7H10	2-NORBORNENE	X	X	X	X	
C7H10N2	TOLUENEDIAMINE	X	X	X	X	
C7H10N2-D1	2,6-DIAMINOTOLUENE	X				
C7H10O2	ALLYL-METHACRYLATE	X	X	X		
C7H11NO	CYCLOHEXYL-ISOCYANATE	X	X	X	X	
C7H12	CYCLOHEPTENE	X	X	X		
C7H12-D1	1-HEPTYNE	X	X	X		
C7H12O2	CYCLOPENTYLACETIC-ACID	X	X			
C7H12O2-D1	N-BUTYL-ACRYLATE	X	X	X	X	
C7H12O2-D2	ISOBUTYL-ACRYLATE	X	X	X	X	
C7H12O2-D3	N-PROPYL-METHACRYLATE	X	X	X	X	
C7H12O2-D4	CYCLOHEXYL-FORMATE	X	X	X		
C7H12O3	2-HYDROXYPROPYL-METHACRYLATE	X				
C7H12O4	DIETHYL-MALONATE	X	X	X	X	
C7H12O4-D1	PIMELIC-ACID	X	X	X		
C7H14-1	CYCLOHEPTANE	X	X	X	X	X
C7H14-2	1,1-DIMETHYLCYCLOPENTANE	X	X	X	X	X
C7H14-3	CIS-1,2-DIMETHYLCYCLOPENTANE	X	X	X	X	X
C7H14-4	TRANS-1,2-DIMETHYLCYCLOPENTANE	X	X	X	X	X
C7H14-5	ETHYLCYCLOPENTANE	X	X	X	X	X
C7H14-6	METHYLCYCLOHEXANE	X	X	X	X	X
C7H14-7	1-HEPTENE	X	X	X	X	X
C7H14-8	2,3,3-TRIMETHYL-1-BUTENE	X	X	X	X	X
C7H14-D1	CIS-2-HEPTENE	X	X	X	X	
C7H14-D2	CIS-3-HEPTENE	X	X	X	X	
C7H14-D3	5-METHYL-1-HEXENE	X				
C7H14-E10	3-METHYL-1-HEXENE	X	X	X	X	

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C7H14-E2	CIS-1,3-DIMETHYLCYCLOPENTANE	X	X	X	X	
C7H14-E3	TRANS-1,3-DIMETHYLCYCLOPENTANE	X	X	X	X	
C7H14-E4	TRANS-2-HEPTENE	X	X	X	X	
C7H14-E5	TRANS-3-HEPTENE	X	X	X	X	
C7H14-E6	4-METHYL-1-HEXENE	X	X	X	X	
C7H14-E7	2-ETHYL-1-PENTENE	X	X	X	X	
C7H14-E8	3-ETHYL-1-PENTENE	X	X	X	X	
C7H14-E9	2-METHYL-1-HEXENE	X	X	X	X	
C7H14O	DIISOPROPYL-KETONE	X	X	X	X	
C7H14O-D1	1-HEPTANAL	X	X	X	X	
C7H14O-D10	5-METHYL-2-HEXANONE	X	X	X	X	
C7H14O-D2	2-HEPTANONE	X	X	X	X	
C7H14O-D3	1-METHYLCYCLOHEXANOL	X	X	X	X	
C7H14O-D4	CIS-2-METHYLCYCLOHEXANOL	X	X	X	X	
C7H14O-D5	TRANS-2-METHYLCYCLOHEXANOL	X	X	X	X	
C7H14O-D6	CIS-3-METHYLCYCLOHEXANOL	X	X	X	X	
C7H14O-D7	TRANS-3-METHYLCYCLOHEXANOL	X	X	X	X	
C7H14O-D8	CIS-4-METHYLCYCLOHEXANOL	X	X	X	X	
C7H14O-D9	TRANS-4-METHYLCYCLOHEXANOL	X	X	X	X	
C7H14O-E1	3-HEPTANONE	X	X	X		
C7H14O-E2	4-HEPTANONE	X	X	X		
C7H14O-E3	2-METHYLHEXANAL	X	X	X		
C7H14O-E4	3-METHYLHEXANAL	X	X	X		
C7H14O2-D1	N-BUTYL-PROPIONATE	X	X	X	X	
C7H14O2-D2	ETHYL-ISOVALERATE	X	X	X	X	
C7H14O2-D3	N-HEPTANOIC-ACID	X	X	X	X	
C7H14O2-D4	ISOPENTYL-ACETATE	X	X	X	X	
C7H14O2-D5	N-PENTYL-ACETATE	X	X	X	X	
C7H14O2-D6	N-PROPYL-N-BUTYRATE	X	X	X	X	
C7H14O2-D7	N-PROPYL-ISOBUTYRATE	X	X	X		
C7H14O2-D8	N-HEXYL-FORMATE	X	X	X		
C7H14O2-D9	NEOHEPTANOIC-ACID	X	X	X		
C7H14O3	ETHYL-3-ETHOXYPROPIONATE	X	X	X	X	
C7H14O3-D1	PG-ETHYL-ETHER-ACETATE	X				
C7H15BR	1-BROMOHEPTANE	X	X	X	X	
C7H15N	N-METHYLCYCLOHEXYLAMINE	X	X	X	X	
C7H16-1	N-HEPTANE	X	X	X	X	X
C7H16-2	2-METHYLHEXANE	X	X	X	X	X
C7H16-3	3-METHYLHEXANE	X	X	X	X	X
C7H16-4	2,2-DIMETHYLPENTANE	X	X	X	X	X
C7H16-5	2,3-DIMETHYLPENTANE	X	X	X	X	X
C7H16-6	2,4-DIMETHYLPENTANE	X	X	X	X	X
C7H16-7	3,3-DIMETHYLPENTANE	X	X	X	X	X
C7H16-8	3-ETHYLPENTANE	X	X	X	X	X
C7H16-9	2,2,3-TRIMETHYLBUTANE	X	X	X	X	X

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C7H16O	1-HEPTANOL	X	X	X	X	X
C7H16O-D0	2-HEPTANOL	X	X	X	X	
C7H16O-D1	ISOPROPYL-BUTYL-ETHER	X	X	X		
C7H16O-D2	ISOPROPYL-ISOBUTYL-ETHER	X	X	X		
C7H16O-D3	2-METHYL-1-HEXANOL	X				
C7H16O-E1	ISOHEPTANOL	X	X	X	X	
C7H16O-E2	ETHYL-TERT-PENTYL-ETHER	X	X	X		
C7H16O2	PG-1-TERT-BUTYL-ETHER	X	X	X		
C7H16O2-D1	PG-2-TERT-BUTYL-ETHER	X	X	X		
C7H16O3	DPG-MONOMETHYL-ETHER	X	X	X		
C7H16O3-D1	DIETHYLENE-GLYCOL-PROPYL-ETHER	X	X	X		
C7H16O4	2-2-2-METHOXYETHOXY-ETHOXY-ETHAN	X				
C7H16S	N-HEPTYL-MERCAPTAN	X	X	X	X	
C7H17N	1-AMINOHEPTANE	X	X	X	X	
C7H3CL2F3	2,4-DICHLOROBENZOTRIFLUORIDE	X	X	X	X	
C7H3CL2NO	3,4-DICHLOROPHENYL-ISOCYANATE	X	X	X	X	
C7H3CLF3NO2	4-CHLORO-3-NITROBENZOTRIFLUORIDE	X	X	X	X	
C7H4CL2O	M-CHLOROBENZOYL-CHLORIDE	X	X	X	X	
C7H4CLF3	P-CHLOROBENZOTRIFLUORIDE	X	X	X	X	
C7H4F3NO2	3-NITROBENZOTRIFLUORIDE	X	X	X	X	
C7H5CL3	BENZOTRICHLORIDE	X	X	X	X	
C7H5CLO	BENZOYL-CHLORIDE	X	X	X	X	
C7H5CLO2	O-CHLOROBENZOIC-ACID	X	X	X	X	
C7H5F3	BENZOTRIFLUORIDE	X	X	X	X	
C7H5N	BENZONITRILE	X	X	X	X	X
C7H5N3O6	2,4,6-TRINITROTOLUENE	X	X	X	X	
C7H5N5O8	TETRYL	X	X	X		
C7H5NAO2	SODIUM-BENZOATE		X	X		
C7H5NO	PHENYL-ISOCYANATE	X	X	X	X	
C7H5NS2	2-MERCAPTOBENZOTHIAZOLE	X	X	X		
C7H6CL2	2,4-DICHLOROTOLUENE	X	X	X	X	
C7H6CL2-D1	BENZYL-DICHLORIDE	X	X	X	X	
C7H6N2O4-E1	2,4-DINITROTOLUENE	X	X	X	X	
C7H6N2O4-E2	2,5-DINITROTOLUENE	X	X	X	X	
C7H6N2O4-E3	2,6-DINITROTOLUENE	X	X	X	X	
C7H6N2O4-E4	3,4-DINITROTOLUENE	X	X	X	X	
C7H6N2O4-E5	3,5-DINITROTOLUENE	X	X	X	X	
C7H6O	BENZALDEHYDE	X	X	X	X	X
C7H6O2	BENZOIC-ACID	X	X	X	X	X
C7H6O2-D0	SALICYLALDEHYDE	X	X	X	X	
C7H6O2-E1	P-HYDROXY-BENZALDEHYDE	X	X	X	X	
C7H6O3	SALICYLIC-ACID	X	X	X	X	
C7H7BR	P-BROMOTOLUENE	X	X	X	X	
C7H7CL-D1	BENZYL-CHLORIDE	X	X	X	X	
C7H7CL-D2	O-CHLOROTOLUENE	X	X	X	X	

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C7H7CL-D3	P-CHLOROTOLUENE	X	X	X	X	
C7H7NO	FORMANILIDE	X	X	X	X	
C7H7NO2-D1	M-NITROTOLUENE	X	X	X	X	
C7H7NO2-D2	O-NITROTOLUENE	X	X	X	X	
C7H7NO2-D3	P-NITROTOLUENE	X	X	X	X	
C7H7NO3	O-NITROANISOLE	X	X	X	X	
C7H8	TOLUENE	X	X	X	X	X
C7H8O-1	METHYL-PHENYL-ETHER	X	X	X	X	X
C7H8O-2	BENZYL-ALCOHOL	X	X	X	X	X
C7H8O-3	O-CRESOL	X	X	X	X	X
C7H8O-4	M-CRESOL	X	X	X	X	X
C7H8O-5	P-CRESOL	X	X	X	X	X
C7H8O2	P-METHOXYPHENOL	X	X	X	X	
C7H8O2-E1	GUAIACOL	X	X	X	X	
C7H8O3S	P-TOLUENESULFONIC-ACID	X	X	X		
C7H8O3S-D1	O-TOLUENESULFONIC-ACID	X	X	X		
C7H8S	BENZYL-MERCAPTAN	X	X	X		
C7H8SICL2	PHENYLMETHYLDICHLOROSILANE	X	X			
C7H9N-1	2,3-DIMETHYLPYRIDINE	X	X	X		X
C7H9N-2	2,5-DIMETHYLPYRIDINE	X	X	X		X
C7H9N-3	3,4-DIMETHYLPYRIDINE	X	X	X		X
C7H9N-4	3,5-DIMETHYLPYRIDINE	X	X	X		X
C7H9N-5	METHYLPHENYLAMINE	X	X	X	X	X
C7H9N-6	O-TOLUIDINE	X	X	X	X	X
C7H9N-7	M-TOLUIDINE	X	X	X	X	X
C7H9N-8	P-TOLUIDINE	X	X	X	X	X
C7H9N-D1	BENZYLAMINE	X	X	X	X	
C7H9N-D2	2,6-DIMETHYLPYRIDINE	X	X	X	X	

Pure Component Databanks: C8

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C8H10-1	O-XYLENE	X	X	X	X	X
C8H10-2	M-XYLENE	X	X	X	X	X
C8H10-3	P-XYLENE	X	X	X	X	X
C8H10-4	ETHYLBENZENE	X	X	X	X	X
C8H10N4O2	CAFFEINE	X	X	X	X	
C8H10O	2-PHENYLETHANOL	X	X	X	X	
C8H10O-1	O-ETHYLPHENOL	X	X	X		X
C8H10O-10	3,5-XYLENOL	X	X	X	X	X
C8H10O-2	M-ETHYLPHENOL	X	X	X		X
C8H10O-3	P-ETHYLPHENOL	X	X	X	X	X
C8H10O-4	PHENETOLE	X	X	X	X	X
C8H10O-5	2,3-XYLENOL	X	X	X	X	X
C8H10O-6	2,4-XYLENOL	X	X	X	X	X
C8H10O-7	2,5-XYLENOL	X	X	X	X	X

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C8H10O-8	2,6-XYLENOL	X	X	X	X	X
C8H10O-9	3,4-XYLENOL	X	X	X	X	X
C8H10O-D1	ALPHA-METHYLBENZYL-ALCOHOL	X	X	X		
C8H10O-D2	P-TOLUALCOHOL	X	X			
C8H10O-D5	O-TOLUALCOHOL	X				
C8H10O-D6	M-TOLUALCOHOL	X				
C8H10O2	ETHYLBENZENE-HYDROPEROXIDE	X	X	X		
C8H10O4	ETHYLENE-GLYCOL-DIACRYLATE	X	X	X		
C8H11N	N,N-DIMETHYLANILINE	X	X	X	X	X
C8H11N-D0	O-ETHYLANILINE	X	X	X	X	
C8H11N-D1	2,4,6-TRIMETHYLPYRIDINE	X	X	X	X	
C8H11N-D2	N-ETHYLANILINE	X	X	X		
C8H11NO	P-PHENETIDINE	X	X	X	X	
C8H12	VINYLCYCLOHEXENE	X	X	X	X	
C8H12-D1	1,5-CYCLOOCTADIENE	X	X	X	X	
C8H12-D2	METHYLNORBORNENE	X	X			
C8H12O4-E1	1,4-CYCLOHEXANEDICARBOXYLIC-ACID	X	X	X	X	
C8H12O4-E2	DIETHYL-MALEATE	X	X	X	X	
C8H14	CYCLOOCTENE	X	X	X		
C8H14-D1	1-OCTYNE	X	X	X		
C8H14-D2	2,5-DIMETHYL-1,5-HEXADIENE	X	X	X		
C8H14-D3	2,5-DIMETHYL-2,4-HEXADIENE	X	X	X		
C8H14O	2-ETHYL-2-HEXENAL	X				
C8H14O2	N-BUTYL-METHACRYLATE	X	X	X	X	
C8H14O2-D1	ISOBUTYL-METHACRYLATE	X	X	X		
C8H14O2-D2	CYCLOHEXYL-ACETATE	X	X	X		
C8H14O3	BUTYRIC-ANHYDRIDE	X	X	X	X	
C8H14O4	DIETHYL-SUCCINATE	X	X	X	X	
C8H14O4-D1	SUBERIC-ACID	X	X	X		
C8H14O4-D2	6-ACETOXY-2,4-DIMETHYL-M-DIOXANE	X	X			
C8H16-1	1,1-DIMETHYLCYCLOHEXANE	X	X	X	X	X
C8H16-10	1,1,3-TRIMETHYLCYCLOPENTANE	X	X	X		X
C8H16-11	CIS,CIS,TRANS-1,2,4-TRIMETHYLCYC	X	X	X		X
C8H16-12	CIS,TRANS,CIS-1,2,4-TRIMETHYLCYC	X	X	X		X
C8H16-13	1-METHYL-1-ETHYLCYCLOPENTANE	X	X	X	X	X
C8H16-14	N-PROPYLCYCLOPENTANE	X	X	X	X	X
C8H16-15	ISOPROPYLCYCLOPENTANE	X	X	X		X
C8H16-16	1-OCTENE	X	X	X	X	X
C8H16-17	TRANS-2-OCTENE	X	X	X	X	X
C8H16-2	CIS-1,2-DIMETHYLCYCLOHEXANE	X	X	X	X	X
C8H16-3	TRANS-1,2-DIMETHYLCYCLOHEXANE	X	X	X	X	X
C8H16-4	CIS-1,3-DIMETHYLCYCLOHEXANE	X	X	X	X	X
C8H16-5	TRANS-1,3-DIMETHYLCYCLOHEXANE	X	X	X	X	X
C8H16-6	CIS-1,4-DIMETHYLCYCLOHEXANE	X	X	X	X	X
C8H16-7	TRANS-1,4-DIMETHYLCYCLOHEXANE	X	X	X	X	X

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C8H16-8	ETHYLCYCLOHEXANE	X	X	X	X	X
C8H16-9	1,1,2-TRIMETHYLCYCLOPENTANE	X	X	X		X
C8H16-D1	2-ETHYL-1-HEXENE	X	X	X	X	
C8H16-D10	6-METHYL-1-HEPTENE	X				
C8H16-D2	TRANS-3-OCTENE	X	X	X	X	
C8H16-D3	TRANS-4-OCTENE	X	X	X	X	
C8H16-D4	2,4,4-TRIMETHYL-1-PENTENE	X	X	X	X	
C8H16-D5	2,4,4-TRIMETHYL-2-PENTENE	X	X	X	X	
C8H16-D6	CYCLOOCTANE	X	X	X		
C8H16-D7	CIS-2-OCTENE	X	X	X		
C8H16-D8	CIS-4-OCTENE	X	X	X		
C8H16-D9	CIS-3-OCTENE	X	X	X		
C8H16-E1	2,3-DIMETHYL-1-HEXENE	X	X	X		
C8H16-E2	2-METHYL-1-HEPTENE	X	X	X		
C8H16O	2-ETHYLHEXANAL	X	X	X	X	
C8H16O-E1	1-OCTANAL	X	X	X	X	
C8H16O-E2	2-OCTANONE	X	X	X	X	
C8H16O2	1,4-CYCLOHEXANEDIMETHANOL	X	X			
C8H16O2-D1	N-BUTYL-N-BUTYRATE	X	X	X	X	
C8H16O2-D2	ISOBUTYL-ISOBUTYRATE	X	X	X	X	
C8H16O2-D3	N-OCTANOIC-ACID	X	X	X	X	
C8H16O2-D4	N-HEXYL-ACETATE	X	X	X	X	
C8H16O2-D5	N-HEPTYL-FORMATE	X	X	X		
C8H16O2-D6	2-ETHYL-HEXANOIC-ACID	X	X	X		
C8H16O3	EG-MONOBUTYL-ETHER-ACETATE	X	X			
C8H16O4	2-2-ETHOXYETHOXY-ETHYL-ACETATE	X	X	X	X	
C8H18	2,2,3,3-TETRAMETHYLBUTANE	X	X	X		
C8H18-1	N-OCTANE	X	X	X	X	X
C8H18-10	3,4-DIMETHYLHEXANE	X	X	X	X	X
C8H18-11	3-ETHYLHEXANE	X	X	X	X	X
C8H18-12	2,2,3-TRIMETHYLPENTANE	X	X	X	X	X
C8H18-13	2,2,4-TRIMETHYLPENTANE	X	X	X	X	X
C8H18-14	2,3,3-TRIMETHYLPENTANE	X	X	X	X	X
C8H18-15	2,3,4-TRIMETHYLPENTANE	X	X	X	X	X
C8H18-16	2-METHYL-3-ETHYLPENTANE	X	X	X	X	X
C8H18-17	3-METHYL-3-ETHYLPENTANE	X	X	X	X	X
C8H18-2	2-METHYLHEPTANE	X	X	X	X	X
C8H18-3	3-METHYLHEPTANE	X	X	X	X	X
C8H18-4	4-METHYLHEPTANE	X	X	X	X	X
C8H18-5	2,2-DIMETHYLHEXANE	X	X	X	X	X
C8H18-6	2,3-DIMETHYLHEXANE	X	X	X	X	X
C8H18-7	2,4-DIMETHYLHEXANE	X	X	X	X	X
C8H18-8	2,5-DIMETHYLHEXANE	X	X	X	X	X
C8H18-9	3,3-DIMETHYLHEXANE	X	X	X	X	X
C8H18O	DI-TERT-BUTYL-ETHER	X	X	X	X	

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C8H18O-1	1-OCTANOL	X	X	X	X	X
C8H18O-2	2-OCTANOL	X	X	X	X	X
C8H18O-3	2-ETHYLHEXANOL	X	X	X	X	X
C8H18O-4	BUTYL-ETHER	X	X	X	X	X
C8H18O-D1	DI-SEC-BUTYL-ETHER	X	X	X	X	
C8H18O-D2	DIISOBUTYL-ETHER	X	X	X		
C8H18O-D3	ETHYL-N-HEXYL-ETHER	X	X	X		
C8H18O2	DI-T-BUTYL-PEROXIDE	X	X	X	X	
C8H18O2-D1	2-HEXOXYETHANOL	X	X			
C8H18O2-E2	2,2,4-TRIMETHYL-1,3-PENTANEDIOL	X	X			
C8H18O2S	DI-N-BUTYL-SULFONE	X	X	X	X	
C8H18O3	DIETHYLENE-GLYCOL-MONOBUTYL-ETHE	X	X	X	X	
C8H18O3-D1	DIETHYLENE-GLYCOL-DIETHYL-ETHER	X	X	X	X	
C8H18O4	TRIETHYLENE-GLYCOL-DIMETHYL-ETHE	X	X	X	X	
C8H18O4-D1	TRIETHYLENE-GLYCOL-ETHYL-ETHER	X	X			
C8H18O5	TETRAETHYLENE-GLYCOL	X	X	X	X	
C8H18S	TERT-OCTYLMERCAPTAN	X	X	X	X	
C8H18S-D1	N-OCTYL-MERCAPTAN	X	X	X	X	
C8H18SO4	DI-N-BUTYL-SULFATE	X	X	X		
C8H19N	DIBUTYLAMINE	X	X	X	X	X
C8H19N-D0	N-OCTYLAMINE	X	X	X	X	
C8H19N-D1	DIISOBUTYLAMINE	X	X	X	X	
C8H20PB	TETRAETHYL-LEAD	X	X	X		
C8H20SI	TETRAETHYL-SILANE	X	X	X		
C8H23N5	TETRAETHYLENEPENTAMINE	X	X	X	X	
C8H24O4SI4	OCTAMETHYLCYCLOTETRASILOXANE	X	X	X	X	
C8H24SI3O2	OCTAMETHYLTRISILOXANE	X				
C8H4CL2O2	ISOPHTHALOYL-CHLORIDE	X	X	X	X	
C8H4O3	PHTHALIC-ANHYDRIDE	X	X	X	X	X
C8H6	ETHYNYLBENZENE	X	X	X		
C8H6O2	TEREPHTHALDEHYDE	X	X	X		
C8H6O3	4-CARBOXYBENZALDEHYDE	X	X	X		
C8H6O3-D1	2-FORMYL-BENZOIC-ACID	X	X			
C8H6O4-D1	ISOPHTHALIC-ACID	X	X	X	X	
C8H6O4-D2	PHTHALIC-ACID	X	X	X	X	
C8H6O4-D3	TEREPHTHALIC-ACID	X	X	X	X	
C8H6S	BENZOTHIOPHENE	X	X	X	X	
C8H7N	INDOLE	X	X	X	X	
C8H7N-D1	PHENYLACETONITRILE	X	X	X		
C8H8	STYRENE	X	X	X	X	X
C8H8O	METHYL-PHENYL-KETONE	X	X	X	X	X
C8H8O-D0	P-TOLUALDEHYDE	X	X	X	X	
C8H8O-D1	4-HYDROXYSTYRENE	X	X	X		
C8H8O-D2	O-TOLUALDEHYDE	X	X			

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C8H8O-D3	M-TOLUALDEHYDE	X				
C8H8O2	METHYL-BENZOATE	X	X	X	X	X
C8H8O2-D1	O-TOLUIC-ACID	X	X	X	X	
C8H8O2-D2	P-TOLUIC-ACID	X	X	X	X	
C8H8O2-D3	BENZYL-FORMATE	X	X	X		
C8H8O2-D4	2-HYDROXYACETOPHENONE	X	X	X		
C8H8O2-D5	4-HYDROXYACETOPHENONE	X	X	X		
C8H8O3	METHYL-SALICYLATE	X	X	X	X	
C8H8O3-D1	VANILLIN	X	X	X	X	
C8H9NO	ACETANILIDE	X	X	X	X	
C8H9NO2	ACETAMINOPHEN	X	X	X		

Pure Component Databanks: C9

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C9H10	ALPHA-METHYL-STYRENE	X	X	X	X	X
C9H10-E1	INDANE	X	X	X	X	
C9H10-E2	M-METHYL-STYRENE	X	X	X	X	
C9H10-E3	O-METHYL-STYRENE	X	X	X	X	
C9H10-E4	P-METHYL-STYRENE	X	X	X	X	
C9H10-E5	CIS-1-PROPENYLBENZENE	X	X	X		
C9H10-E6	TRANS-1-PROPENYLBENZENE	X	X	X		
C9H10O	2-PHENYLPROPIONALDEHYDE	X				
C9H10O2	ETHYL-BENZOATE	X	X	X	X	X
C9H10O2-D0	BENZYL-ACETATE	X	X	X	X	
C9H10O2-D1	ALPHA-METHYLBENZYL-FORMATE	X				
C9H10O3	ETHYL-VANILLIN	X	X	X	X	
C9H10O3-D1	ACETOVANILLONE	X	X	X		
C9H10O3-D2	4-METHOXYPHENYLACETIC-ACID	X				
C9H11NO	P-DIMETHYLAMINOBENZALDEHYDE	X	X	X	X	
C9H11NO2	L-PHENYLALANINE	X	X	X		
C9H12	5-ETHYLIDENE-2-NORBORNENE	X	X			
C9H12-1	N-PROPYLBENZENE	X	X	X	X	X
C9H12-2	ISOPROPYLBENZENE	X	X	X	X	X
C9H12-3	1-METHYL-2-ETHYLBENZENE	X	X	X	X	X
C9H12-4	1-METHYL-3-ETHYLBENZENE	X	X	X	X	X
C9H12-5	1-METHYL-4-ETHYLBENZENE	X	X	X	X	X
C9H12-6	1,2,3-TRIMETHYLBENZENE	X	X	X	X	X
C9H12-7	1,2,4-TRIMETHYLBENZENE	X	X	X	X	X
C9H12-8	1,3,5-TRIMETHYLBENZENE	X	X	X	X	X
C9H12-D1	VINYLNORBORNENE	X	X	X		
C9H12O	BENZYL-ETHYL-ETHER	X	X	X	X	
C9H12O-D1	1-PHENYL-1-PROPANOL	X	X	X		
C9H12O-D2	1-PHENYL-2-PROPANOL	X	X	X		
C9H12O-D3	2-PHENYL-1-PROPANOL	X	X			
C9H12O-D4	3-PHENYL-1-PROPANOL	X				

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C9H12O-E1	DIMETHYL-PHENYL-CARBINOL	X	X	X	X	
C9H12O2	CUMENE-HYDROPEROXIDE	X	X	X	X	
C9H14	PROPENYL-CYCLOHEXENE	X				
C9H14-D1	ETHYLNORBORNENE	X	X			
C9H14-D2	1-METHYL-4-VINYLCYCLOHEXENE	X	X			
C9H14O	ISOPHORONE	X	X	X	X	
C9H14O6	GLYCERYL-TRIACETATE	X	X	X	X	
C9H14O7	TRILACTIC-ACID	X				
C9H15N	TRIALLYLAMINE	X	X			
C9H16-D1	1-NONYNE	X				
C9H16O4	AZELAIC-ACID	X	X	X	X	
C9H18	1-TRANS-3,5-TRIMETHYLCYCLOHEXANE	X	X			
C9H18-1	N-PROPYLCYCLOHEXANE	X	X	X	X	X
C9H18-2	ISOPROPYLCYCLOHEXANE	X	X	X	X	X
C9H18-3	1-NONENE	X	X	X	X	X
C9H18-D1	N-BUTYLCYCLOPENTANE	X	X	X		
C9H18-D2	2-METHYL-1-OCTENE	X				
C9H18-D3	7-METHYL-1-OCTENE	X				
C9H18O	1-NONANAL	X	X	X	X	
C9H18O-D1	DIISOBUTYL-KETONE	X	X	X	X	
C9H18O-E1	2-NONANONE	X	X	X		
C9H18O-E2	5-NONANONE	X	X	X		
C9H18O2	N-NONANOIC-ACID	X	X	X	X	
C9H18O2-D1	N-BUTYL-VALERATE	X	X	X	X	
C9H18O2-D2	N-OCTYL-FORMATE	X	X	X	X	
C9H18O2-D3	N-HEPTYL-ACETATE	X	X	X		
C9H18O3	TRIACETONE-ALCOHOL	X	X			
C9H18O4	DPG-MONOMETHYL-ETHER-ACETATE	X	X	X		
C9H20-1	N-NONANE	X	X	X	X	X
C9H20-2	2,2,3-TRIMETHYLHEXANE	X	X	X		X
C9H20-3	2,2,4-TRIMETHYLHEXANE	X	X	X		X
C9H20-4	2,2,5-TRIMETHYLHEXANE	X	X	X	X	X
C9H20-5	3,3-DIETHYLPENTANE	X	X	X	X	X
C9H20-6	2,2,3,3-TETRAMETHYLPENTANE	X	X	X	X	X
C9H20-7	2,2,3,4-TETRAMETHYLPENTANE	X	X	X	X	X
C9H20-8	2,2,4,4-TETRAMETHYLPENTANE	X	X	X	X	X
C9H20-9	2,3,3,4-TETRAMETHYLPENTANE	X	X	X		X
C9H20-D1	2-METHYLOCTANE	X	X	X	X	
C9H20-D2	3-METHYLOCTANE	X	X	X	X	
C9H20-D3	4-METHYLOCTANE	X	X	X	X	
C9H20-D4	2,4,4-TRIMETHYLHEXANE	X	X	X		
C9H20-E1	2,2-DIMETHYLHEPTANE	X	X	X	X	
C9H20-E2	2,6-DIMETHYLHEPTANE	X	X	X	X	
C9H20-E3	2,2-DIMETHYL-3-ETHYLPENTANE	X	X	X	X	
C9H20-E4	2,4-DIMETHYL-3-ETHYLPENTANE	X	X	X	X	

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C9H20-E5	3-ETHYLHEPTANE	X	X	X	X	
C9H20O-D1	2,6-DIMETHYL-4-HEPTANOL	X	X	X	X	
C9H20O-D2	1-NONANOL	X	X	X	X	
C9H20O-E1	2-NONANOL	X	X	X	X	
C9H20O3	DPG-N-PROPYL-ETHER	X				
C9H20O4	TRIPROPYLENE-GLYCOL	X	X	X		
C9H20S	N-NONYL-MERCAPTAN	X	X	X	X	
C9H20S-D1	TERT-NONYL-MERCAPTAN	X	X			
C9H21N-D1	N-NONYLAMINE	X	X	X	X	
C9H21N-D2	TRIPROPYLAMINE	X	X	X	X	
C9H4O5	TRIMELLITIC-ANHYDRIDE	X	X	X	X	
C9H6N2O2	TOLUENE-DIISOCYANATE	X	X	X	X	
C9H6N2O2-D1	2,6-TOLUENE-DIISOCYANATE	X				
C9H6O6	TRIMELLITIC-ACID	X	X			
C9H7N-D1	ISOQUINOLINE	X	X	X	X	
C9H7N-D2	QUINOLINE	X	X	X	X	
C9H7NO	8-HYDROXYQUINOLINE	X	X	X	X	
C9H8	INDENE	X	X	X	X	
C9H8O	2-METHYLBENZOFURAN	X	X	X	X	
C9H8O2	CINNAMIC-ACID	X	X	X		
C9H8O4	ACETYLSALICYLIC-ACID	X	X	X		

Pure Component Databanks: C10

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C10H10-D1	M-DIVINYLBENZENE	X	X	X	X	
C10H10-D2	1-METHYLINDENE	X	X	X	X	
C10H10-D3	2-METHYLINDENE	X	X	X	X	
C10H10O4-D1	O-DIMETHYL-PHTHALATE	X	X	X	X	
C10H10O4-D2	DIMETHYL-TEREPHTHALATE	X	X	X	X	
C10H10O4-D3	DIMETHYL-ISOPHTHALATE	X	X	X		
C10H11NO2	ACETOACETANILIDE	X	X	X		
C10H12	1,2,3,4-TETRAHYDRONAPHTHALENE	X	X	X	X	X
C10H12-D0	DICYCLOPENTADIENE	X	X	X	X	
C10H12-E1	2-PHENYLBUTENE-1	X	X	X		
C10H12-E2	CIS-2-PHENYLBUTENE-2	X	X	X		
C10H12-E3	TRANS-2-PHENYLBUTENE-2	X	X	X		
C10H12O	ANETHOLE	X	X	X	X	
C10H12O2	N-PROPYL-BENZOATE	X	X	X		
C10H12O4	DIALLYL-MALEATE	X	X	X	X	
C10H14-1	N-BUTYLBENZENE	X	X	X	X	X
C10H14-2	ISOBUTYLBENZENE	X	X	X	X	X
C10H14-3	SEC-BUTYLBENZENE	X	X	X	X	X
C10H14-4	TERT-BUTYLBENZENE	X	X	X	X	X
C10H14-5	1-METHYL-2-ISOPROPYLBENZENE	X	X	X	X	X
C10H14-6	1-METHYL-3-ISOPROPYLBENZENE	X	X	X	X	X

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C10H14-7	1-METHYL-4-ISOPROPYLBENZENE	X	X	X	X	X
C10H14-8	1,4-DIETHYLBENZENE	X	X	X	X	X
C10H14-9	1,2,4,5-TETRAMETHYLBENZENE	X	X	X	X	X
C10H14-D1	M-DIETHYLBENZENE	X	X	X	X	
C10H14-D2	O-DIETHYLBENZENE	X	X	X	X	
C10H14-D3	1,2-DIMETHYL-3-ETHYLBENZENE	X	X	X	X	
C10H14-E1	2-ETHYL-M-XYLENE	X	X	X	X	
C10H14-E10	1-METHYL-4-N-PROPYLBENZENE	X	X	X		
C10H14-E2	2-ETHYL-P-XYLENE	X	X	X	X	
C10H14-E3	4-ETHYL-M-XYLENE	X	X	X	X	
C10H14-E4	4-ETHYL-O-XYLENE	X	X	X	X	
C10H14-E5	5-ETHYL-M-XYLENE	X	X	X	X	
C10H14-E6	1,2,3,5-TETRAMETHYL-BENZENE	X	X	X	X	
C10H14-E7	1,2,3,4-TETRAMETHYL-BENZENE	X	X	X		
C10H14-E8	1-METHYL-2-N-PROPYLBENZENE	X	X	X		
C10H14-E9	1-METHYL-3-N-PROPYLBENZENE	X	X	X		
C10H14O	P-TERT-BUTYLPHENOL	X	X	X	X	
C10H14O2	P-TERT-BUTYLCATECHOL	X	X	X	X	
C10H14O5	2-ACETOACETOXY-ETHYL-METHACRYLAT	X	X			
C10H15N	N-BUTYLANILINE	X	X	X		X
C10H15N-E1	N,N-DIETHYLANILINE	X	X	X	X	
C10H15N-E2	2,6-DIETHYLANILINE	X	X	X	X	
C10H16-D1	D-LIMONENE	X	X	X	X	
C10H16-D2	ALPHA-PINENE	X	X	X	X	
C10H16-D3	BETA-PINENE	X	X	X	X	
C10H16-D4	TERPINOLENE	X	X	X	X	
C10H16-D5	ADAMANTANE	X	X	X		
C10H16-E1	CAMPHENE	X	X	X	X	
C10H16-E2	ALPHA-PHELLANDRENE	X	X	X	X	
C10H16-E3	BETA-PHELLANDRENE	X	X	X	X	
C10H16-E4	ALPHA-TERPINENE	X	X	X	X	
C10H16-E5	GAMMA-TERPINENE	X	X	X	X	
C10H16N2O8	ETHYLENEDIAMINETETRAACETIC-ACID	X	X	X		
C10H16O	CAMPHOR	X	X	X	X	
C10H16O4	DIPROPYL-MALEATE	X	X	X		
C10H16O4-D1	DIMETHYL-1,4-CYCLOHEXANEDICARBOX	X	X			
C10H18-1	CIS-DECALIN	X	X	X	X	X
C10H18-2	TRANS-DECALIN	X	X	X	X	X
C10H18-D1	1-DECYNE	X				
C10H18O4	SEBACIC-ACID	X	X	X	X	
C10H19N	CAPRYLONITRILE	X	X	X		X
C10H19O6PS2	MALATHION	X	X	X		
C10H20-1	N-BUTYLCYCLOHEXANE	X	X	X	X	X
C10H20-2	ISOBUTYLCYCLOHEXANE	X	X	X		X

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C10H20-3	SEC-BUTYLCYCLOHEXANE	X	X	X		X
C10H20-4	TERT-BUTYLCYCLOHEXANE	X	X	X		X
C10H20-5	1-DECENE	X	X	X	X	X
C10H20-D1	CIS-2-DECENE	X	X			
C10H20-D2	TRANS-2-DECENE	X	X			
C10H20-D3	1,1-DIETHYLCYCLOHEXANE	X	X			
C10H20-D4	1,2,3,4-TETRAMETHYLCYCLOHEXANE	X	X			
C10H20-D5	2-METHYL-1-NONENE	X				
C10H20-D6	8-METHYL-1-NONENE	X				
C10H20O	1-DECANAL	X	X	X	X	
C10H20O-D1	L-MENTHOL	X	X	X		
C10H20O2	P-MENTHANE-HYDROPEROXIDE	X	X	X		
C10H20O2-D1	N-DECANOIC-ACID	X	X	X	X	
C10H20O2-D2	2-ETHYLHEXYL-ACETATE	X	X	X	X	
C10H20O2-D3	ISOPENTYL-ISOVALERATE	X	X	X	X	
C10H20O2-D4	N-OCTYL-ACETATE	X	X	X		
C10H20O2-D5	N-NONYL-FORMATE	X	X	X		
C10H20O4	DIGLYCOL-MONOBUTYL-ETHER-ACETATE	X	X	X		
C10H22-1	N-DECANE	X	X	X	X	X
C10H22-2	3,3,5-TRIMETHYLHEPTANE	X	X	X		X
C10H22-3	2,2,3,3-TETRAMETHYLHEXANE	X	X	X		X
C10H22-4	2,2,5,5-TETRAMETHYLHEXANE	X	X	X		X
C10H22-D1	2,3-DIMETHYLOCTANE	X	X	X		
C10H22-D2	2,4-DIMETHYLOCTANE	X	X	X		
C10H22-D3	2,5-DIMETHYLOCTANE	X	X	X		
C10H22-D4	2,6-DIMETHYLOCTANE	X	X	X		
C10H22-D5	2,7-DIMETHYLOCTANE	X	X	X		
C10H22-E1	2,2-DIMETHYL-OCTANE	X	X	X	X	
C10H22-E2	2-METHYLNONANE	X	X	X	X	
C10H22-E3	3-METHYLNONANE	X	X	X	X	
C10H22-E4	4-METHYLNONANE	X	X	X	X	
C10H22-E5	5-METHYLNONANE	X	X	X	X	
C10H22O	1-DECANOL	X	X	X	X	X
C10H22O-D0	ISODECANOL	X	X	X	X	
C10H22O-D1	DI-N-PENTYL-ETHER	X	X	X	X	
C10H22O2	ETHYLENE-GLYCOL-2-ETHYLHEXYL-ETH	X	X			
C10H22O3-D1	2-2-HEXOXYETHOXY-ETHANOL	X	X			
C10H22O3-E1	DIPROPYLENE-GLYCOL-T-BUTYL-ETHER	X	X			
C10H22O4	TRIPROPYLENE-GLYCOL-MONOMETHYL-E	X	X	X		
C10H22O4-D1	TRIETHYLENE-GLYCOL-BUTYL-ETHER	X	X			
C10H22O5	TETRAETHYLENE-GLYCOL-DIMETHYL-ET	X	X	X	X	
C10H22S	N-DECYL-MERCAPTAN	X	X	X	X	
C10H22S-D1	ETHYL-N-OCTYL-SULFIDE	X				

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C10H23N	N-DECYLAMINE	X	X	X	X	
C10H23N-D1	DIAMYLAMINE	X	X	X		
C10H24N2	N,N-DI-TERT-BUTYLETHYLENEDIAMINE	X	X			
C10H28N6	PENTAETHYLENE-HEXAMINE	X				
C10H30SI4O3	DECAMETHYLTETRASILOXANE	X	X	X		
C10H30SI5O5	DECAMETHYLCYCLOPENTASILOXANE	X	X	X		
C10H6O8	PYROMELLITIC-ACID	X	X	X	X	
C10H7BR	1-BROMONAPHTHALENE	X	X	X	X	
C10H7CL	1-CHLORONAPHTHALENE	X	X	X	X	
C10H8	NAPHTHALENE	X	X	X	X	X
C10H9N	QUINALDINE	X	X	X	X	

Pure Component Databanks: C11

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C11H10-1	1-METHYLNAPHTHALENE	X	X	X	X	X
C11H10-2	2-METHYLNAPHTHALENE	X	X	X	X	X
C11H12	P-ISOPROPENYLSTYRENE	X	X	X		
C11H14O2	BUTYL-BENZOATE	X	X	X	X	X
C11H16	N-PENTYLBENZENE	X	X	X	X	
C11H16-D1	1-ETHYL-2-ISOPROPYLBENZENE	X	X			
C11H16-D2	PENTAMETHYLBENZENE	X	X			
C11H16O	P-TERT-AMYLPHENOL	X	X	X	X	
C11H20O2	2-ETHYLHEXYL-ACRYLATE	X	X	X	X	
C11H22-1	N-HEXYLCYCLOPENTANE	X	X	X		X
C11H22-2	1-UNDECENE	X	X	X	X	X
C11H22O	1-UNDECANAL	X	X	X	X	
C11H22O2	N-NONYL-ACETATE	X	X	X		
C11H22O2-D1	N-DECYL-FORMATE	X	X	X		
C11H22O2-D2	METHYL-DECANOATE	X	X	X		
C11H22O2-D3	N-UNDECANOIC-ACID	X	X	X		
C11H24	N-UNDECANE	X	X	X	X	X
C11H24O	1-UNDECANOL	X	X	X	X	
C11H24S	UNDECYL-MERCAPTAN	X	X	X	X	
C11H25N	UNDECYLAMINE	X	X	X		

Pure Component Databanks: C12

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C12H10	DIPHENYL	X	X	X	X	X
C12H10-D0	ACENAPHTHENE	X	X	X	X	
C12H10N2O2-A	O-NITRODIPHENYLAMINE	X	X	X		
C12H10N2O2-B	P-NITRODIPHENYLAMINE	X	X	X		
C12H10O	DIPHENYL-ETHER	X	X	X	X	X
C12H11N	DIPHENYLAMINE	X	X	X	X	
C12H11N-D1	P-AMINODIPHENYL	X	X	X	X	
C12H11N3-E1	P-AMINOAZOBENZENE	X	X	X	X	

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C12H11N3-E2	1,3-DIPHENYLTRIAZENE	X	X	X	X	
C12H12-E1	2,6-DIMETHYLNAPHTHALENE	X	X	X	X	
C12H12-E2	2,7-DIMETHYLNAPHTHALENE	X	X	X	X	
C12H12-E3	1-ETHYLNAPHTHALENE	X	X	X	X	
C12H12-E4	2-ETHYLNAPHTHALENE	X	X	X		
C12H12N2-D1	P-AMINODIPHENYLAMINE	X	X	X	X	
C12H12N2-D2	HYDRAZOBENZENE	X	X	X	X	
C12H12N2-D3	BENZIDINE	X	X	X		
C12H14	1,2,3-TRIMETHYLINDENE	X	X	X	X	
C12H14O4	DIETHYL-PHTHALATE	X	X	X	X	
C12H14O6	BIS-2-HYDROXYETHYL-TEREPHTHALATE	X	X	X		
C12H16	CYCLOHEXYLBENZENE	X	X	X	X	
C12H16-D1	P-TERT-BUTYLSTYRENE	X	X	X		
C12H16-D2	4-ISOBUTYLSTYRENE	X	X	X		
C12H18	1,3,5-TRIETHYLBENZENE	X				
C12H18-D1	M-DIISOPROPYLBENZENE	X	X	X	X	
C12H18-D2	P-DIISOPROPYLBENZENE	X	X	X	X	
C12H18-D3	N-HEXYLBENZENE	X	X	X	X	
C12H18-D4	P-TERT-BUTYL-ETHYLBENZENE	X	X	X		
C12H18-D5	1,5,9-CYCLODODECATRIENE	X	X			
C12H18-D6	1,2,4-TRIETHYLBENZENE	X	X			
C12H18-D7	HEXAMETHYLBENZENE	X	X			
C12H18-D8	1,2,3-TRIETHYLBENZENE	X	X			
C12H18O2	M-DIISOPROPYL-BENZENE-HYDROPEROX	X	X	X		
C12H18O2-D1	P-DIISOPROPYLBENZ-HYDROPEROXIDE	X	X	X		
C12H20O	2-CYCLOHEXYL-CYCLOHEXANONE	X	X	X		
C12H20O4	DIBUTYL-MALEATE	X	X	X	X	
C12H22	BICYCLOHEXYL	X	X	X	X	
C12H22O11	SUCROSE	X	X	X		
C12H23N	DICYCLOHEXYLAMINE	X	X	X	X	
C12H24-1	N-HEPTYLCYCLOPENTANE	X	X	X		X
C12H24-2	1-DODECENE	X	X	X	X	X
C12H24-D1	CIS-2-DODECENE	X				
C12H24-D2	TRANS-2-DODECENE	X				
C12H24O	1-DODECANAL	X	X	X	X	
C12H24O2	N-DODECANOIC-ACID	X	X	X	X	
C12H24O2-E1	N-DECYL-ACETATE	X	X	X		
C12H24O3	2,2,4-TM-1,3-PD-MONOISOBUTYNATE	X				
C12H26	N-DODECANE	X	X	X	X	X
C12H26-D1	3-METHYLUNDECANE	X				
C12H26O-1	DIHEXYLETHER	X	X	X	X	X
C12H26O-2	DODECANOL	X	X	X	X	X
C12H26O3	DIETHYLENE-GLYCOL-DI-N-BUTYL-ETH	X	X	X	X	
C12H26S	N-DODECYL-MERCAPTAN	X	X	X	X	
C12H26S-E1	TERT-DODECYL-MERCAPTAN	X	X	X		

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C12H27BO3	TRI-N-BUTYL-BORATE	X	X	X	X	
C12H27N	TRIBUTYLAMINE	X	X	X	X	X
C12H27N-D0	DODECYLAMINE	X	X	X	X	
C12H36SI5O4	DODECAMETHYLPENTASILOXANE	X				
C12H36SI6O6	DODECAMETHYLCYCLOHEXASILOXANE	X	X	X		
C12H6N2O2	1,5-NAPHTHALENE-DIISOCYANATE	X	X	X		
C12H8	ACENAPHTHALENE	X	X	X		
C12H8O	DIBENZOFURAN	X	X	X	X	
C12H8O4	2,6-NAPHTHALENEDICARBOXYLIC-ACID	X				
C12H8S	DIBENZOTHIOPHENE	X	X	X		
C12H9N	DIBENZOPYRROLE	X	X	X	X	
C12H9N3O4	4,4-DINITRODIPHENYLAMINE	X	X	X		

Pure Component Databanks: C13

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C13H10	FLUORENE	X	X	X	X	
C13H10O	BENZOPHENONE	X	X	X	X	
C13H12	DIPHENYLMETHANE	X	X	X	X	X
C13H14	1-N-PROPYLNAPHTHALENE	X	X	X		
C13H18O2	IBUPROFEN	X	X	X		
C13H20	N-HEPTYLBENZENE	X	X	X	X	
C13H26-1	N-OCTYLCYCLOPENTANE	X	X	X		X
C13H26-2	1-TRIDECENE	X	X	X	X	X
C13H26O	1-TRIDECANAL	X	X	X	X	
C13H26O2	METHYL-DODECANOATE	X	X	X	X	
C13H26O2-D1	N-BUTYL-NONANOATE	X	X	X	X	
C13H26O2-D2	N-TRIDECANOIC-ACID	X	X	X		
C13H28	N-TRIDECANE	X	X	X	X	X
C13H28O	1-TRIDECANOL	X	X	X	X	
C13H9N	ACRIDINE	X	X	X		

Pure Component Databanks: C14

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C14H10	DIPHENYLACETYLENE	X	X	X	X	
C14H10-1	ANTHRACENE	X	X	X	X	X
C14H10-2	PHENANTHRENE	X	X	X	X	X
C14H10O4	BENZOYL-PEROXIDE	X	X	X		
C14H12-D1	CIS-STILBENE	X	X	X	X	
C14H12-D2	TRANS-STILBENE	X	X	X	X	
C14H12O2	BENZYL-BENZOATE	X	X	X	X	
C14H12O4	DIMETHYL-2,6-NAPHTHALENEDICARBOX	X				
C14H14-D1	1,1-DIPHENYLETHANE	X	X	X	X	
C14H14-D2	1,2-DIPHENYLETHANE	X	X	X	X	
C14H14O	DIBENZYL-ETHER	X	X	X	X	
C14H16	1-N-BUTYLNAPHTHALENE	X	X	X	X	

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C14H16-D1	2,6-DIETHYLNAPHTHALENE	X	X	X		
C14H18O4	DIPROPYL-PHTHALATE	X	X	X		
C14H20	DIAMANTANE	X	X	X		
C14H22	N-OCTYLBENZENE	X	X	X	X	
C14H22-D1	1,2,3,5-TETRAETHYLBENZENE	X	X			
C14H22-D2	1,4-DI-TERT-BUTYLBENZENE	X				
C14H22O	P-TERT-OCTYLPHENOL	X	X	X	X	
C14H28-1	N-NONYLCYCLOPENTANE	X	X	X		X
C14H28-2	1-TETRADECENE	X	X	X	X	X
C14H28O2	N-TETRADECANOIC-ACID	X	X	X	X	
C14H30	N-TETRADECANE	X	X	X	X	X
C14H30O	1-TETRADECANOL	X	X	X	X	
C14H31N	TETRADECYLAMINE	X	X	X	X	
C14H42SI6O5	TETRADECAMETHYLHEXASILOXANE	X	X	X		
C14H8O2	ANTHRAQUINONE	X	X	X	X	

Pure Component Databanks: C15

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C15H10N2O2	DIPHENYLMETHANE-4,4-DIISOCYANATE	X	X	X	X	
C15H12	1-PHENYLINDENE	X	X	X		
C15H16O	P-CUMYLPHENOL	X	X	X	X	
C15H16O2	BISPHENOL-A	X	X	X	X	
C15H18	1-N-PENTYLNAPHTHALENE	X	X	X		
C15H24	N-NONYLBENZENE	X	X	X	X	
C15H24O-D1	2,6-DI-TERT-BUTYL-P-CRESOL	X	X	X	X	
C15H24O-D2	NONYLPHENOL	X	X	X	X	
C15H30-1	N-DECYLCYCLOPENTANE	X	X	X		X
C15H30-2	1-PENTADECENE	X	X	X	X	X
C15H30O2	PENTADECANOIC-ACID	X	X	X	X	
C15H32	N-PENTADECANE	X	X	X	X	X
C15H32O	1-PENTADECANOL	X	X	X		
C15H33N	TRIAMYLAMINE	X	X	X		

Pure Component Databanks: C16

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C16H10-D1	FLUORANTHENE	X	X	X	X	
C16H10-D2	PYRENE	X	X	X	X	
C16H12	1-PHENYLNAPHTHALENE	X	X	X	X	
C16H18	1-4-ETHYLPHENYL-2-PHENYLETHANE	X	X			
C16H20	1-N-HEXYLNAPHTHALENE	X	X	X	X	
C16H22O4	DIBUTYL-O-PHTHALATE	X	X	X	X	X
C16H22O4-D1	DIISOBUTYL-PHTHALATE	X	X	X		
C16H24	1-N-HEXYL-1,2,3,4-TETRAHYDRONAPH	X	X	X		
C16H26	N-DECYLBENZENE	X	X	X	X	
C16H26-D1	PENTAETHYLBENZENE	X				

			Available in Databank				
	Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
	C16H32-1	N-DECYLCYCLOHEXANE	X	X	X	X	X
	C16H32-2	1-HEXADECENE	X	X	X	X	X
	C16H32O2	N-HEXADECANOIC-ACID	X	X	X	X	
	C16H34	N-HEXADECANE	X	X	X	X	X
	C16H34-D1	2,2,4,4,6,8,8-HEPTAMETHYLNONANE	X	X			
	C16H34O	1-HEXADECANOL	X	X	X	X	
	C16H34O-D1	DI-N-OCTYL-ETHER	X	X	X	X	
	C16H34S	DI-N-OCTYL-SULFIDE	X				
	C16H48SI7O6	HEXADECAMETHYLHEPTASILOXANE	X				

Pure Component Databanks: C17

			Available in Databank				
	Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
	C17H28	N-UNDECYLBENZENE	X	X	X	X	
	C17H34	N-DODECYLCYCLOPENTANE	X	X	X		X
	C17H34-D1	1-HEPTADECENE	X	X	X	X	
	C17H34O2	N-HEPTADECANOIC-ACID	X	X	X		
	C17H34O2-D1	ISOPROPYL-MYRISTATE	X	X	X		
	C17H36	N-HEPTADECANE	X	X	X	X	X
	C17H36O	HEPTADECANOL	X	X	X	X	X

Pure Component Databanks: C18

			Available in Databank				
	Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
	C18H12	CHRYSENE	X	X	X	X	
	C18H12-D1	BENZANTHRACENE	X				
	C18H12-D2	NAPHTHACENE	X				
	C18H13N3O4	4,4-DINITROTRIPHENYLAMINE	X	X	X		
	C18H14-1	O-TERPHENYL	X	X	X	X	X
	C18H14-2	M-TERPHENYL	X	X	X	X	X
	C18H14-3	P-TERPHENYL	X	X	X	X	X
	C18H15O4P	TRIPHENYL-PHOSPHATE	X	X	X	X	
	C18H15P	TRIPHENYLPHOSPHINE	X	X	X	X	
	C18H15PO	TRIPHENYLPHOSPHINE-OXIDE	X	X	X		
	C18H16N2	N-N-DIPHENYL-P-PHENYLENEDIAMINE	X	X	X	X	
	C18H20	2,4-DIPHENYL-4-METHYLPENTENE-1	X	X	X		
	C18H22	2,3-DIMETHYL-2,3-DIPHENYLBUTANE	X	X	X	X	
	C18H22O2	DICUMYLPEROXIDE	X	X	X	X	
	C18H30	N-DODECYLBENZENE	X	X	X	X	
	C18H30-D1	HEXAETHYLBENZENE	X				
	C18H30O2	LINOLENIC-ACID	X	X	X		
	C18H32O2	LINOLEIC-ACID	X	X	X	X	
	C18H34O2	OLEIC-ACID	X	X	X	X	
	C18H34O4-D1	DIBUTYL-SEBACATE	X	X	X	X	
	C18H34O4-D2	DIHEXYL-ADIPATE	X	X	X	X	
	C18H36-1	1-OCTADECENE	X	X	X	X	X
	C18H36-2	N-TRIDECYLCYCLOPENTANE	X	X	X		X

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C18H36O2	STEARIC-ACID	X	X	X	X	
C18H38	N-OCTADECANE	X	X	X	X	X
C18H38O	1-OCTADECANOL	X	X	X	X	X
C18H38O-D0	DINONYL-ETHER	X	X	X	X	
C18H54SI8O7	OCTADECAMETHYLOCTA SILOXANE					

Pure Component Databanks: C19

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C19H16	TRIPHENYLMETHANE	X	X	X		
C19H26	1-N-NONYLNAPHTHALENE	X	X	X	X	
C19H32	N-TRIDECYLBENZENE	X	X	X	X	
C19H36O2	METHYL-OLEATE	X	X	X	X	
C19H38	N-TETRADECYLCYCLOPENTANE	X	X	X		X
C19H38-D1	1-NONADECENE	X	X	X	X	
C19H38O2	NONADECANOIC-ACID	X	X	X	X	
C19H40	N-NONADECANE	X	X	X	X	X
C19H40O	1-NONADECANOL	X	X	X		

Pure Component Databanks: C20

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
C20H16	TRIPHENYLETHYLENE	X	X	X	X	
C20H18	1,1,2-TRIPHENYLETHANE	X	X	X		
C20H28	1-N-DECYLNAPHTHALENE	X	X	X	X	
C20H28O2	DEHYDROABIETIC-ACID	X				
C20H30O2	ABIETIC-ACID	X	X	X	X	
C20H30O2-D1	NEOABIETIC-ACID	X				
C20H30O4	DI-N-HEXYL-PHTHALATE	X				
C20H31N	DEHYDROABIETYLAMINE	X	X	X	X	
C20H34	N-TETRADECYLBENZENE	X	X	X		
C20H37NAO7S	DIOCTYLSODIUM-SULFOSUCCINATE		X	X		
C20H38O2	CETYL-METHACRYLATE	X	X	X		
C20H40	N-PENTADECYLCYCLOPENTANE	X	X	X		X
C20H40-D1	1-EICOSENE	X	X	X	X	
C20H40O2	N-EICOSANIC-ACID	X	X	X		
C20H42	N-EICOSANE	X	X	X	X	X
C20H42O	1-EICOSANOL	X	X	X	X	X

Alias	Name	Available in Databank P11	P10	P93	P856	PCD
C21H21O4P	TRI-O-CRESYL-PHOSPHATE	X	X	X	X	
C21H36	N-PENTADECYLBENZENE	X	X	X		
C21H40O4	MONOOLEIN	X				
C21H42	N-HEXADECYLCYCLOPENTANE	X	X	X		X
C21H44	N-HENEICOSANE	X	X	X		
C22H34O4	DIHEPTYL-PHTHALATE	X	X			
C22H38	N-HEXADECYLBENZENE	X	X	X		
C22H42O4	DI-2-ETHYLHEXYL-ADIPATE	X	X	X		
C22H42O4-D1	DIOCTYLADIPATE	X				
C22H44O2	N-BUTYL-STEARATE	X	X	X	X	
C22H46	N-DOCOSANE	X	X	X		
C23H40	N-HEPTADECYLBENZENE	X	X	X		
C23H48	N-TRICOSANE	X	X	X		
C24H38O4	DIOCTYL-PHTHALATE	X	X	X	X	
C24H38O4-D1	DIISOOCTYL-PHTHALATE	X	X	X	X	
C24H38O4-D2	DIOCTYL-TEREPHTHALATE	X	X	X		
C24H42	N-OCTADECYLBENZENE	X	X	X		
C24H42O	DINONYLPHENOL	X	X	X	X	
C24H50	N-TETRACOSANE	X	X	X		
C24H51N	TRI-N-OCTYLAMINE	X				
C25H20	TETRAPHENYLMETHANE	X	X	X		
C25H52	N-PENTACOSANE	X	X	X		
C26H20	TETRAPHENYLETHYLENE	X	X	X	X	
C26H22	1,1,2,2-TETRAPHENYLETHANE	X	X	X		
C26H42O4	DI-N-NONYL-PHTHALATE	X	X			
C26H42O4-D1	DIISONONYL-PHTHALATE	X				
C26H54	N-HEXACOSANE	X	X	X		
C27H46O	BETA-CHOLESTEROL	X	X			
C27H56	N-HEPTACOSANE	X	X	X		
C28H46O4	DIISODECYL-PHTHALATE	X	X	X	X	
C28H46O4-D1	DI-N-DECYL-PHTHALATE	X				
C28H58	N-OCTACOSANE	X	X	X		
C29H50O	SITOSTEROL	X				
C29H60	N-NONACOSANE	X	X	X		
C30H48O6	TRI-N-HEPTYL-TRIMELLITATE	X				
C30H50O4	DI-N-UNDECYL-PHTHALATE	X				
C30H62	N-TRIACONTANE	X	X	X		
C30H62-D1	SQUALANE	X	X	X		
C32H66	N-DOTRIACONTANE	X	X	X		
C36H74	N-HEXATRIACONTANE	X	X	X		
C39H72O5	DIOLEIN	X				
C57H104O6	TRIOLEIN	X				

Pure Component Databanks: Ca

Alias	Name	Available in Databank P11	P10	P93	P856	PCD
CA	CALCIUM	X	X	X		
CA(OH)2	CALCIUM-HYDROXIDE	X	X	X	X	
CACL2	CALCIUM-CHLORIDE	X	X	X	X	
CACL2O2	CALCIUM-HYPOCHLORITE		X	X		
CACO3	CALCIUM-CARBONATE-CALCITE	X	X	X	X	
CAF2	CALCIUM-FLUORIDE	X	X	X	X	
CAO	CALCIUM-OXIDE	X	X	X	X	
CASO4	CALCIUM-SULFATE	X	X	X	X	

Pure Component Databanks: Cl

Alias	Name	Available in Databank P11	P10	P93	P856	PCD
CL2	CHLORINE	X	X	X	X	X
CLH4NO	HYDROXYLAMINE-HYDROCHLORIDE	X	X	X		
CLHO3S	CHLOROSULFONIC-ACID	X	X	X	X	
CLO2	CHLORINE-DIOXIDE	X	X	X	X	
CLO3F	PERCHLORYL-FLUORIDE	X	X	X	X	

Pure Component Databanks: Fe

Alias	Name	Available in Databank P11	P10	P93	P856	PCD
FE	IRON	X	X	X	X	
FE2O3	HEMATITE	X	X	X	X	
FECL2	FERROUS-CHLORIDE	X	X	X		
FECL3	FERRIC-CHLORIDE	X	X	X		
FEO	FERROUS-OXIDE	X	X	X	X	
FESO4	FERROUS-SULFATE	X	X	X	X	

Pure Component Databanks: H

Alias	Name	Available in Databank P11	P10	P93	P856	PCD
H2	HYDROGEN	X	X	X	X	X
H2-PARA	HYDROGEN-PARA	X	X	X		
H2O	WATER	X	X	X	X	X
H2O2	HYDROGEN-PEROXIDE	X	X	X	X	
H2S	HYDROGEN-SULFIDE	X	X	X	X	X
H2SE	HYDROGEN-SELENIDE	X	X	X		
H2SO4	SULFURIC-ACID	X	X	X	X	
H3BO3	HYDROGEN-ORTHOBORATE	X	X	X	X	
H3N	AMMONIA	X	X	X	X	X
H3NO	HYDROXYLAMINE	X	X	X	X	
H3NO3S	SULFAMIC-ACID	X	X	X	X	
H3PO2	HYPOPHOSPHOROUS-ACID	X	X	X	X	
H3PO3	PHOSPHOROUS-ACID	X	X	X	X	
H3PO4	ORTHOPHOSPHORIC-ACID	X	X	X	X	
H4N2	HYDRAZINE	X	X	X	X	X
HBR	HYDROGEN-BROMIDE	X	X	X	X	X
HCL	HYDROGEN-CHLORIDE	X	X	X	X	X

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
HCLO	HYPOCHLOROUS-ACID	X	X	X		
HCLO4	PERCHLORIC-ACID	X	X	X	X	
HF	HYDROGEN-FLUORIDE	X	X	X	X	X
HI	HYDROGEN-IODIDE	X	X	X	X	X
HNO2	NITROUS-ACID	X	X	X		
HNO3	NITRIC-ACID	X	X	X	X	
HNO5S	NITROSYLSULFURIC-ACID		X	X		

Pure Component Databanks: K

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
K	POTASSIUM	X	X	X	X	
K2CO3	POTASSIUM-CARBONATE	X	X	X	X	
K2HPO4	DIPOTASSIUM-PHOSPHATE		X	X		
KBR	POTASSIUM-BROMIDE	X	X	X		
KC2H3O2	POTASSIUM-ACETATE	X	X	X		
KCL	POTASSIUM-CHLORIDE	X	X	X	X	
KCLO3	POTASSIUM-CHLORATE	X	X	X	X	
KI	POTASSIUM-IODIDE	X	X	X		
KOH	POTASSIUM-HYDROXIDE	X	X	X	X	

Pure Component Databanks: N

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
N2	NITROGEN	X	X	X	X	X
N2F4	TETRAFLUOROHYDRAZINE	X	X	X	X	
N2O	NITROUS-OXIDE	X	X	X	X	X
N2O3	NITROGEN-TRIOXIDE	X	X	X	X	
N2O4	NITROGEN-TETROXIDE	X	X	X	X	
N2O5	NITROGEN-PENTOXIDE	X	X	X	X	
NCL3	NITROGEN-TRICHLORIDE	X	X	X	X	
NF3	NITROGEN-TRIFLUORIDE	X	X	X	X	X
NH4CL	AMMONIUM-CHLORIDE	X	X	X	X	
NH4CLO4	AMMONIUM-PERCHLORATE	X	X	X		
NH4HSO4	AMMONIUM-BISULFATE	X	X	X		
NH4NO3	AMMONIUM-NITRATE	X	X	X	X	
NH4OH	AMMONIUM-HYDROXIDE	X	X	X	X	
(NH4)2HPO4	DIAMMONIUM-PHOSPHATE	X	X	X		
(NH4)2SO3	AMMONIUM-SULFITE	X	X	X	X	
(NH4)2SO4	AMMONIUM-SULFATE	X	X	X	X	
NH5SO3	AMMONIUM-BISULFITE	X	X	X	X	
NH6PO4	AMMONIUM-PHOSPHATE	X	X	X		
NO	NITRIC-OXIDE	X	X	X	X	X
NO2	NITROGEN-DIOXIDE	X	X	X	X	X
NOCL	NITROSYL-CHLORIDE	X	X	X	X	X

Pure Component Databanks: Na

Alias	Name	Available in Databank P11	P10	P93	P856	PCD
NA	SODIUM	X	X	X	X	
NA2CO3	SODIUM-CARBONATE	X	X	X	X	
NA2CR2O7	SODIUM-DICHROMATE	X	X	X	X	
NA2HPO4	DISODIUM-PHOSPHATE	X	X	X		
NA2O2	SODIUM-PEROXIDE	X	X	X	X	
NA2S	SODIUM-SULFIDE	X	X	X	X	
NA2S2O3	SODIUM-THIOSULFATE	X	X	X	X	
NA2S2O4	SODIUM-HYDROSULFITE	X	X	X	X	
NA2SIO3	SODIUM-SILICATE	X	X	X	X	
NA2SO4	SODIUM-SULFATE	X	X	X	X	
NA3PO4	TRISODIUM-PHOSPHATE	X	X	X	X	
NA4P2O7	TETRASODIUM-PYROPHOSPHATE	X	X	X	X	
NA5P3O10	SODIUM-TRIPOLYPHOSPHATE	X	X	X		
NA6P6O18	SODIUM-HEXAMETAPHOSPHATE	X	X	X	X	
NABO3	SODIUM-PERBORATE		X	X		
NABR	SODIUM-BROMIDE	X	X	X	X	
NAC5H8NO4	MONOSODIUM-GLUTAMATE		X	X		
NACHO2	SODIUM-FORMATE	X	X	X	X	
NACL	SODIUM-CHLORIDE	X	X	X	X	
NACLO	SODIUM-HYPOCHLORITE		X	X		
NACLO3	SODIUM-CHLORATE	X	X	X	X	
NACN	SODIUM-CYANIDE	X	X	X	X	
NAF	SODIUM-FLUORIDE	X	X	X	X	
NAH2PO4	MONOSODIUM-PHOSPHATE		X	X		
NAHCO3	SODIUM-BICARBONATE	X	X	X	X	
NAHSO3	SODIUM-BISULFITE		X	X		
NAHSO4	SODIUM-BISULFATE	X	X	X	X	
NAI	SODIUM-IODIDE	X	X	X		
NANH2	SODIUM-AMIDE	X	X	X	X	
NANO2	SODIUM-NITRITE	X	X	X	X	
NANO3	SODIUM-NITRATE	X	X	X	X	
NAOH	SODIUM-HYDROXIDE	X	X	X	X	

Pure Component Databanks: O

Alias	Name	Available in Databank P11	P10	P93	P856	PCD
O2	OXYGEN	X	X	X	X	X
O2S	SULFUR-DIOXIDE	X	X	X	X	X
O3	OZONE	X	X	X	X	X
O3S	SULFUR-TRIOXIDE	X	X	X	X	X

Pure Component Databanks: P

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
P-R	PHOSPHORUS-RED	X				
P-W	PHOSPHORUS-WHITE	X	X	X	X	
P4O10	TETRAPHOSPHORUS-DECAOXIDE	X	X	X	X	
P4S10	PHOSPHORUS-PENTASULFIDE	X	X	X	X	
PCL3	PHOSPHORUS-TRICHLORIDE	X	X	X	X	X
PCL5	PHOSPHORUS-PENTACHLORIDE	X	X	X	X	
PH3	PHOSPHINE	X	X	X	X	
POCL3	PHOSPHORUS-OXYCHLORIDE	X	X	X	X	
PSCL3	PHOSPHORUS-THIOCHLORIDE	X	X	X	X	

Pure Component Databanks: S

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
S	SULFUR	X	X	X	X	
SCL2	SULFUR-DICHLORIDE	X	X	X		
SF6	SULFUR-HEXAFLUORIDE	X	X	X	X	X
SO2CL2	SULFURYL-CHLORIDE	X	X	X	X	
SOCL2	THIONYL-CHLORIDE	X	X	X	X	

Pure Component Databanks: Si

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
SI	SILICON	X	X	X	X	
SI2H6	DISILANE	X	X	X	X	
SIC	SILICON-CARBIDE	X	X	X	X	
SICL4	SILICON-TETRACHLORIDE	X	X	X	X	X
SIF4	SILICON-TETRAFLUORIDE	X	X	X	X	X
SIH2CL2	DICHLOROSILANE	X	X	X	X	
SIH4	SILANE	X	X	X	X	
SIHCL3	TRICHLOROSILANE	X	X	X	X	
SIO2	SILICON-DIOXIDE	X	X	X	X	

Pure Component Databanks: Other Elements

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
AG	SILVER	X	X	X	X	
AIR	AIR	X	X	X	X	
AR	ARGON	X	X	X	X	X
AS	ARSENIC	X	X	X		
AS2O3	ARSENIC-TRIOXIDE	X	X	X		
ASH3	ARSINE	X	X	X	X	
BACO3	BARIUM-CARBONATE	X	X	X	X	
BE	BERYLLIUM	X	X	X		
BI	BISMUTH	X	X	X		
BR2	BROMINE	X	X	X	X	X
CRO3	CHROMIUM-TRIOXIDE	X	X	X	X	
CUCL	CUPROUS-CHLORIDE	X	X	X	X	
CUCL2	COPPER-DICHLORIDE	X	X	X	X	

		Available in Databank				
Alias	**Name**	**P11**	**P10**	**P93**	**P856**	**PCD**
CUSO4	COPPER-SULFATE	X	X	X	X	
D2	DEUTERIUM	X	X	X	X	X
D2O	DEUTERIUM-OXIDE	X	X	X	X	X
F2	FLUORINE	X	X	X	X	X
FHO3S	FLUOROSULFONIC-ACID	X	X	X		
GACL3	GALLIUM-TRICHLORIDE	X	X	X	X	
GE	GERMANIUM	X	X	X		
GEH4	GERMANIUM-TETRAHYDRIDE	X	X	X	X	
HE-3	HELIUM-3	X	X	X	X	
HE-4	HELIUM-4	X	X	X	X	X
HG	MERCURY	X	X	X	X	
I2	IODINE	X	X	X	X	X
KR	KRYPTON	X	X	X	X	X
LI	LITHIUM	X	X	X	X	
LIH2PO4	MONOLITHIUM-PHOSPHATE	X				
LII	LITHIUM-IODIDE	X				
MG(NO3)2	MAGNESIUM-NITRATE	X	X	X		
MGO	MAGNESIUM-OXIDE	X	X	X	X	
MGSO4	MAGNESIUM-SULFATE	X	X	X	X	
NE	NEON	X	X	X	X	X
SBCL3	ANTIMONY-TRICHLORIDE	X	X	X	X	
SELEXOL	SELEXOL					X
TICL3	TITANIUM-TRICHLORIDE	X	X	X	X	
TICL4	TITANIUM-TETRACHLORIDE	X	X	X	X	
TIO2	TITANIUM-DIOXIDE-RUTILE	X	X	X	X	
V	VANADIUM	X	X	X		
VCL3O	VANADIUM-OXYTRICHLORIDE	X	X	X	X	
VCL4	VANADIUM-TETRACHLORIDE	X	X	X	X	
XE	XENON	X	X	X	X	X
ZN	ZINC	X	X	X	X	
ZNO	ZINC-OXIDE	X	X	X	X	
ZNSO4	ZINC-SULFATE	X	X	X	X	

Pure Component Databanks: Heating Fluids

		Available in Databank	
Alias	**Name**	**P11**	**P10**
CACL2-15	CALCIUM-CHLORIDE-15-WT-%	X	X
CACL2-25	CALCIUM-CHLORIDE-25-WT%	X	X
CALFLO-AF	CALFLO-AF	X	X
CALFLO-HTF	CALFLO-HTF	X	X
CHEM550	CHEMTHERM-550	X	X
DEGLY-20	DIETHLENE-GLYCOL-20-WT-%	X	X
DEGLY-40	DIETHYLENE-GLYCOL-40-WT-%	X	X
DEGLY-60	DIETHYLENE-GLYCOL-60-WT-%	X	X
DEGLY-80	DIETHLENE-GLYCOL-80-WT-%	X	X
DEPG	DIMETHYL-ETHER-POLYETHYLENE-	X	

		Available in Databank	
Alias	**Name**	**P11**	**P10**
	GLYC		
DOWA	DOWTHERM-A	X	X
DOWG	DOWTHERM-G	X	X
DOWJ	DOWTHERM-J	X	X
EGLY-20	ETHYLENE-GLYCOL-20-WT-%	X	X
EGLY-40	ETHYLENE-GLYCOL-40-WT-%	X	X
EGLY-60	ETHYLENE-GLYCOL-60-WT-%	X	X
MARLO-S	MARLOTHERM-S	X	X
MBL603	MOBILTHERM-603	X	X
MBL605	MOBILTHERM-605	X	X
MBLLIGHT	MOBILTHERM-LIGHT	X	X
PGLY-20	PROPYLENE-GLYCOL-20-WT-%	X	X
PGLY-60	PROPYLENE-GLYCOL-60-WT-%	X	X
R123	REFRIGERANT-123	X	X
R502	REFRIGERANT-502	X	X
R503	REFRIGERANT-503	X	X
SHELL15	SHELL15	X	X
SHELL33	SHELL33	X	X
SYL-XLT	SYLTHERM-XLT	X	X
SYL800	SYLTHERM-800	X	X
SYN350	SYNTREL-350	X	X
TEGLY-40	TRIETHYLENE-GLYCOL-40-WT-%	X	X
TEGLY-80	TRIETHYLENE-GLYCOL-80-WT-%	X	X
TEGLY-L	TEGLY-L	X	X
THERM44	THERMINOL-44	X	X
THERM55	THERMINOL-55	X	X
THERM550	THERMALANE-550-(FG-1)	X	X
THERM60	THERMINOL-60	X	X
THERM600	THERMALANE-600	X	X
THERM66	THERMINOL-66	X	X
THERM77	THERMINOL-77	X	X
THERM800	THERMALANE-800	X	X
THERMFG1	THERMFG1	X	X
THERMFR0	THERMINOL-FR-0	X	X
THERMFR1	THERMINOL-FR-1	X	X
THERMFR2	THERMINOL-FR-2	X	X
THERMFR3	THERMINOL-FR-3	X	X
THERMVP1	THERMINOL-VP-1	X	X

Aqueous Component Databanks

The tables below list the components present in the aqueous component databanks AQUEOUS and AQU92.

Components beginning with:

C1	C2	C3	C4	C5	C6	C7	C8	C9	C10
C11+	Ag	Al	Au	B	Ba	Br	Ca	Cd	Ce
Cl	Co	Cr	Cs	Cu	Dy	Er	Eu	Fe	Ga
Gd	Ge	H	Hg	Ho	I	In	K	La	Li
Lu	Mg	Mn	N	Na	Nd	Ni	O	P	Pb
Pd	Pr	Pt	Rb	S	Sc	Sm	Sn	Sr	Tb
Th	Tl	Tm	U	V	Y	Yb	Zn	Zr	Other

Aqueous Component Databank Parameters

The AQUEOUS and AQU92 databanks have data for the following parameters:

Parameter Name	Description
ATOMNO	Vector containing the atom types (atomic numbers) for a given molecule (e.g., H=1, C=6, O=8). Must use the vector NOATOM to define the number of occurrences of each atom.
CHARGE	Ionic charge
CPAQ0	Aqueous phase heat capacity at infinite dilution
CPIG	Ideal gas heat capacity coefficients
DGAQFM	Aqueous free energy of formation at infinite dilution
DGFORM	Standard free energy of formation
DHAQFM	Aqueous heat of formation at infinite dilution
DHFORM	Standard heat of formation
GMBPB	Bromley-Pitzer model ion-specific B parameter
GMBPD	Bromley-Pitzer model ion-specific delta parameter
IONTYP	Criss-Cobble ion type
MW	Molecular weight
NOATOM	Vector containing the number of occurrences of each atom defined in ATOMNO for a given molecule. ATOMNO and NOATOM define the chemical formula of the molecule.
PLXANT	Antoine liquid vapor pressure coefficients
PRADII	Pauling ion radius

Parameter Name	Description
S025C	Criss-Cobble absolute entropy at 25°C
VLBROC	Partial molal volume at infinite dilution

AQ = AQUEOUS Databank

AQ9 = AQ92 Databank

Aqueous Component Databanks: Ag

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
AG(C2H4NO2)	AG(NH2CH2COO)	X	X
AG(C2H6NH)2+	AG(C2H6NH)2+	X	X
AG(CH3CO2)2-	AG(CH3COO)2-	X	X
AG(CH3NH2)2+	AG(CH3NH2)2+	X	X
AG(CN)2-	AG(CN)2-	X	X
AG(CN)OH-	AG(CN)OH-	X	X
AG(CO3)-	AG(CO3)-	X	
AG(CO3)2-3	AG(CO3)2---	X	
AG(NH3)+	AG(NH3)+	X	X
AG(NH3)2+	AG(NH3)2+	X	X
AG(NH3)2BR	AG(NH3)2BR	X	X
AG(NH3)2CL	AG(NH3)2CL	X	X
AG(NO2)2-	AG(NO2)2-	X	X
AG(OH)2-	AG(OH)2-	X	X
AG(S2O3)2-3	AG(S2O3)2---	X	X
AG(SCN)2-	AG(CNS)2-	X	X
AG(SCN)3-2	AG(CNS)3--	X	X
AG(SCN)4-3	AG(CNS)4---	X	X
AG+	AG+	X	X
AG+2	AG++	X	X
AG2(CH3CO2)+	AG2(CH3COO)+	X	X
AG2SO3	AG2SO3	X	X
AGBR	SILVER-BROMIDE	X	X
AGBR2-	AGBR2-	X	X
AGBR3-2	AGBR3--	X	X
AGC2H4+	AGC2H4+	X	X
AGCH3CO2	SILVER-ACETATE	X	X
AGCL	SILVER-CHLORIDE	X	X
AGCL2-	AGCL2-	X	X
AGCL3-2	AGCL3--	X	
AGCL3BR-3	AGBRCL3---	X	X
AGCL4-3	AGCL4---	X	
AGCLBR3-3	AGBR3CL---	X	X
AGF	SILVER-FLUORIDE	X	X
AGI	SILVER-IODIDE	X	X
AGI2-	AGI2-	X	X
AGI3-2	AGI3--	X	X
AGI4-3	AGI4---	X	X

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	AGNO3	SILVER-NITRATE	X	X
	AGOH	SILVER-HYDROXIDE	X	X
	AGSCN	SILVER-THIOCYANATE	X	X
	AGSO3-	AGSO3-	X	X
	AGSO4-	AGSO4-	X	X

Aqueous Component Databanks: Al

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	AL(AC)+2	ALCH3COO+2	X	
	AL(AC)2+	AL(CH3COO)2+	X	
	AL(OH)2+	AL(OH)2+	X	
	AL(OH)4-	AL(OH)4-	X	X
	AL(SO4)2-	AL(SO4)2-	X	X
	AL+3	AL+++	X	X
	ALF+2	ALF++	X	X
	ALF2+	ALF2+	X	X
	ALF3	ALUMINIUM-FLUORIDE	X	X
	ALF4-	ALF4-	X	X
	ALF5-2	ALF5--	X	X
	ALF6-3	ALF6---	X	X
	ALO2-	ALO2-	X	X
	ALOH+2	ALOH++	X	X
	ALSO4+	ALSO4+	X	X

Aqueous Component Databanks: Au

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	AU(AC)	AUCH3COO	X	
	AU(AC)2-	AU(CH3COO)2-	X	
	AU(CN)2-	AU(CN)2-	X	X
	AU(OH)3	GOLD-HYDROXIDE	X	X
	AU(SCN)2-	AU(CNS)2-	X	X
	AU(SCN)4-	AU(CNS)4-	X	X
	AU(SCN)5-2	AU(CNS)5-2	X	X
	AU(SCN)6-3	AU(CNS)6-3	X	X
	AU+	AU+	X	X
	AU+3	AU+++	X	
	AUBR2-	AUBR2-	X	X
	AUBR4-	AUBR4-	X	X
	AUCL2-	AUCL2-	X	X
	AUCL4-	AUCL4-	X	X
	AUO3-3	AUO3---	X	X

Aqueous Component Databanks: B

Alias	Name	Available in Databank AQ	AQ9
B(OH)4-	B(OH)4-	X	X
B4O7-2	B4O7--	X	X
BF2(OH)2-	BF2(OH)2-	X	X
BF3OH-	BF3OH-	X	X
BF4-	BF4-	X	X
BH4-	BH4-	X	X
BO2-	BO2-	X	X

Aqueous Component Databanks: Ba

Alias	Name	Available in Databank AQ	AQ9
BA(AC)+	BACH3COO+	X	
BA(AC)2	BA(CH3COO)2	X	
BA(ALA)+	BA(C3H6NO2)+	X	
BA(ALA)2	BA(C3H6NO2)2	X	
BA(BUT)+	BACH3(CH2)2CO2+	X	
BA(BUT)2	BA(CH3CH2CH2CO2)2	X	
BA(FOR)+	BACHO2+	X	
BA(FOR)2	BA(CHO2)2	X	
BA(GLY)+	BA(C2H4NO2)+	X	
BA(GLY)2	BA(C2H4NO2)2	X	
BA(GLYC)+	BACH3OCO2+	X	
BA(GLYC)2	BA(CH3OCO2)2	X	
BA(LAC)+	BACH3CH2OCO2+	X	
BA(LAC)2	BA(CH3CH2OCO2)2	X	
BA(PENT)+	BACH3(CH2)3CO2+	X	
BA(PENT)2	BA(CH3CH2CH2CH2CO2)2	X	
BA(PROP)+	BACH3CH2CO2+	X	
BA(PROP)2	BA(CH3CH2CO2)2	X	
BA+2	BA++	X	X
BACL+	BACL+	X	
BACO3	BARIUM-CARBONATE	X	
BAF+	BAF+	X	
BANO3+	BANO3+	X	X
BAOH+	BA(OH)+	X	X

Aqueous Component Databanks: Br

Alias	Name	Available in Databank AQ	AQ9
BR-	BR-	X	X
BR2	BROMINE	X	X
BR2CL-	BR2CL-	X	X
BR3-	BR3-	X	X
BR5-	BR5-	X	X
BRI2-	BRI2-	X	X
BRO-	BRO-	X	X
BRO3-	BRO3-	X	X

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	BRO4-	BRO4-	X	X

Aqueous Component Databanks: C1

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
CH2O	FORMALDEHYDE	X	
CH2O2	FORMIC-ACID	X	X
(CH3)2NH2+	(CH3)2NH2+	X	X
(CH3)3NH+	(CH3)3NH+	X	X
CH3CL	METHYL-CHLORIDE	X	X
CH3COO-	CH3COO-	X	X
CH3NH3+	CH3NH3+	X	X
CH3NH3OH	CH3NH3OH	X	X
CH4	METHANE	X	X
CH4N2O	UREA	X	
CH4O	METHANOL	X	X
CH5N	METHYL-AMINE	X	X
CH5N3O	NH2CONHNH2	X	X
CHN	HYDROGEN-CYANIDE	X	X
CHO2-	HCOO-	X	X
CN-	CN-	X	X
SCN-	CNS-	X	X
CO	CARBON-MONOXIDE	X	X
CO2	CARBON-DIOXIDE	X	X
CO3-2	CO3--	X	X

Aqueous Component Databanks: C2

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
C2H2	ACETYLENE	X	
C2H2O4	OXALIC-ACID	X	X
C2H3O3-	GLYCOLATE	X	
C2H4	ETHYLENE	X	X
C2H4O-1	ACETALDEHYDE	X	
C2H4O2-1	ACETIC-ACID	X	X
C2H4O3-D1	GLYCOLIC-ACID	X	
C2H5COO-	PROPANOATE	X	
C2H5NO-D1	ACETAMIDE	X	
C2H5NO2-D1	GLYCINE	X	
C2H5O-	CH3CH2O-	X	X
C2H6	ETHANE	X	X
C2H6NSO3-	NH2(CH2)2SO3-	X	X
C2H6O-2	ETHANOL	X	X
C2H7N-1	ETHYL-AMINE	X	
C2H7N-2	DIMETHYLAMINE	X	X
C2H7NSO3	NH2(CH2)2SO3H	X	X
C2H8NO+	MEA+	X	X

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	C2H9NO	(CH3)2NH2OH	X	X
	C2O4-2	C2O4--	X	X

Aqueous Component Databanks: C3

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
C3H11NO	(CH3)3NHOH	X	X
C3H2O4-2	MALONATE	X	
C3H3O4-	H-MALONATE	X	
C3H4-2	METHYL-ACETYLENE	X	
C3H4O4	MALONIC-ACID	X	
C3H5O3-	LACTATE	X	
C3H6-2	PROPYLENE	X	
C3H6NO3-	MEACOO-	X	X
C3H6O-1	ACETONE	X	
C3H6O-3	N-PROPIONALDEHYDE	X	
C3H6O2-1	PROPIONIC-ACID	X	
C3H6O3-D1	LACTIC-ACID	X	
C3H7COO-	BUTANOATE	X	
C3H7NO2	ALANINE	X	
C3H7NO3	SERINE	X	
C3H8	PROPANE	X	
C3H8O-1	1-PROPANOL	X	
C3H9N-1	N-PROPYL-AMINE	X	
C3H9N-3	TRIMETHYL-AMINE	X	X

Aqueous Component Databanks: C4

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
C4H10-1	N-BUTANE	X	
C4H10O-1	N-BUTANOL	X	
C4H11N-1	N-BUTYL-AMINE	X	
C4H11NO-1	2-AMINO-2-METHYL-1-PROPANOL	X	X
C4H12NO+	AMP+	X	X
C4H12NO2+	DEA+	X	X
C4H12NOO+	DGA+	X	X
C4H4O4-2	SUCCINATE	X	
C4H5O4-	H-SUCCINATE	X	
C4H6-1	1-BUTYNE	X	
C4H6N2O2	DIKETOPIPERAZINE	X	
C4H6O4-2	SUCCINIC-ACID	X	
C4H7NO4	ASPARTIC-ACID	X	
C4H7O3-	2-HYDROXYBUTANOATE	X	
C4H8-1	1-BUTENE	X	
C4H8N2O3-A	ASPARAGINE	X	
C4H8N2O3-D	DIGLYCINE	X	
C4H8O-1	N-BUTYRALDEHYDE	X	

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
C4H8O-2	ISOBUTYRALDEHYDE	X	
C4H8O2-1	N-BUTYRIC-ACID	X	
C4H8O2-3	ETHYL-ACETATE	X	
C4H8O3-1	2-HYDROXYBUTANOIC-ACID	X	
C4H9COO-	PENTANOATE	X	
C4H9NO2	A-AMINOBUTYRIC	X	
C4H9NO3	THREONINE	X	

Aqueous Component Databanks: C5

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
C5H10-2	1-PENTENE	X	
C5H10N2O3-A	ALANYLGLYCINE	X	
C5H10N2O3-G	GLUTAMINE	X	
C5H10NO4-	DEACOO-	X	X
C5H10NOO3-	DGACOO-	X	X
C5H10O-1	VALERALDEHYDE	X	
C5H10O-2	METHYL-N-PROPYL-KETONE	X	
C5H10O2	NEOPENTANOIC-ACID	X	
C5H10O3	2-HYDROXYPENTANOIC-ACID	X	
C5H11COO-	HEXANOATE	X	
C5H11NO2	VALINE	X	
C5H11NO2S	METHIONINE	X	
C5H12-1	N-PENTANE	X	
C5H12O-1	1-PENTANOL	X	
C5H13N	N-PENTYLAMINE	X	
C5H14NO2+	MDEA+	X	X
C5H6O4-2	GLUTARATE	X	
C5H7O4-	H-GLUTARATE	X	
C5H8-5	1-PENTYNE	X	
C5H8O4	GLUTARIC-ACID	X	
C5H9NO4	L-GLUTAMIC-ACID	X	
C5H9O3-	2-HYDROXYPENTANOATE	X	

Aqueous Component Databanks: C6

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
C6H10-E2	1-HEXYNE	X	
C6H10O4-D1	ADIPIC-ACID	X	
C6H11O3-	2-HYDROXYHEXANOATE	X	
C6H12-3	1-HEXENE	X	
C6H12O-D2	1-HEXANAL	X	
C6H12O-D3	2-HEXANONE	X	
C6H12O2-D5	N-HEXANOIC-ACID	X	
C6H12O3-E1	HYDROXYCAPROIC-ACID	X	
C6H13COO-	HEPTANOATE	X	
C6H13NO2	LEUCINE	X	

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	C6H13NO2-I	ISOLEUCINE	X	
	C6H14-1	N-HEXANE	X	
	C6H14O-1	1-HEXANOL	X	
	C6H15N-D2	N-HEXYLAMINE	X	
	C6H6	BENZENE	X	
	C6H6O	PHENOL	X	
	C6H8O4-2	ADIPATE	X	
	C6H9O4-	H-ADIPATE	X	

Aqueous Component Databanks: C7

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	C7H10O4-2	PIMELATE	X	
	C7H11O4-	H-PIMELATE	X	
	C7H12-D1	1-HEPTYNE	X	
	C7H12O4-D1	PIMELIC-ACID	X	
	C7H13O3-	2-HYDROXYHEPTANOATE	X	
	C7H14-7	1-HEPTENE	X	
	C7H14O-D1	1-HEPTANAL	X	
	C7H14O-D2	2-HEPTANONE	X	
	C7H14O2-D3	N-HEPTANOIC-ACID	X	
	C7H14O3-1	2-HYDROXYHEPTANOIC-ACID	X	
	C7H15COO-	OCTANOATE	X	
	C7H16-1	N-HEPTANE	X	
	C7H16O	1-HEPTANOL	X	
	C7H17N	1-AMINOHEPTANE	X	
	C7H5O2-	BENZOATE	X	
	C7H6O2	BENZOIC-ACID	X	
	C7H8	TOLUENE	X	

Aqueous Component Databanks: C8

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	C8H10-4	ETHYLBENZENE	X	
	C8H12O4-2	SUBERATE	X	
	C8H13O4-	H-SUBERATE	X	
	C8H14-D1	1-OCTYNE	X	
	C8H14O4-D1	SUBERIC-ACID	X	
	C8H15O3-	2-HYDROXYOCTANOATE	X	
	C8H16-16	1-OCTENE	X	
	C8H16N2O3	LEUCYLGLYCINE	X	
	C8H16O-E1	1-OCTANAL	X	
	C8H16O-E2	2-OCTANONE	X	
	C8H16O2-D3	N-OCTANOIC-ACID	X	
	C8H16O3-1	2-HYDROXYOCTANOIC-ACID	X	
	C8H18-1	N-OCTANE	X	
	C8H18O-1	1-OCTANOL	X	

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	C8H19N-D0	N-OCTYLAMINE	X	
	M-C8H7O2-	M-TOLUATE	X	
	O-C8H7O2-	O-TOLUATE	X	
	P-C8H7O2-	P-TOLUATE	X	
	C8H8O2-D1	O-TOLUIC-ACID	X	
	C8H8O2-D2	P-TOLUIC-ACID	X	
	C8H8O2-M	M-TOLUIC-ACID	X	

Aqueous Component Databanks: C9

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
C9H11NO2	L-PHENYLALANINE	X	
C9H11NO3	TYROSINE	X	
C9H12-1	N-PROPYLBENZENE	X	
C9H14O4-2	AZELATE	X	
C9H15O4-	H-AZELATE	X	
C9H16O4	AZELAIC-ACID	X	
C9H17O2-	NONANOATE	X	
C9H17O3-	2-HYDROXYNONANOATE	X	
C9H18O	1-NONANAL	X	
C9H18O2	N-NONANOIC-ACID	X	
C9H18O3-1	2-HYDROXYNONANOIC-ACID	X	

Aqueous Component Databanks: C10

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
C10H14-1	N-BUTYLBENZENE	X	
C10H16O4-2	SEBACATE	X	
C10H17O4-	H-SEBACATE	X	
C10H18O4	SEBACIC-ACID	X	
C10H19O2-	DECANOATE	X	
C10H19O3-	2-HYDROXYDECANOATE	X	
C10H20O	1-DECANAL	X	
C10H20O2-D1	N-DECANOIC-ACID	X	
C10H20O3	2-HYDROXYDECANOIC-ACID	X	

Aqueous Component Databanks: C11+

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
C11H12N2O2	TRYPTOPHAN	X	
C11H16	N-PENTYLBENZENE	X	
C11H21O2-	UNDECANOATE	X	
C11H22O2-D3	N-UNDECANOIC-ACID	X	
C12H18-D3	N-HEXYLBENZENE	X	
C12H23O2-	DODECANOATE	X	
C12H24O2	N-DODECANOIC-ACID	X	
C13H20	N-HEPTYLBENZENE	X	
C14H22	N-OCTYLBENZENE	X	

Aqueous Component Databanks: Ca

Alias	Name	Available in Databank AQ	AQ9
CA(AC)2	CA(CH3COO)2	X	
CA(ALA)+	CA(C3H6NO2)+	X	
CA(ALA)2	CA(C3H6NO2)2	X	
CA(BUT)+	CACH3(CH2)2CO2+	X	
CA(BUT)2	CA(CH3CH2CH2CO2)2	X	
CA(FOR)+	CACHO2+	X	
CA(FOR)2	CA(CHO2)2	X	
CA(GLY)+	CA(C2H4NO2)+	X	
CA(GLY)2	CA(C2H4NO2)2	X	
CA(GLYC)+	CACH3OCO2+	X	
CA(GLYC)2	CA(CH3OCO2)2	X	
CA(HCO3)+	CA(HCO3)+	X	
CA(LAC)+	CACH3CH2OCO2+	X	
CA(LAC)2	CA(CH3CH2OCO2)2	X	
CA(PENT)+	CACH3(CH2)3CO2+	X	
CA(PENT)2	CA(CH3CH2CH2CH2CO2)2	X	
CA(PROP)+	CACH3CH2CO2+	X	
CA(PROP)2	CA(CH3CH2CO2)2	X	
CA+2	CA++	X	X
CACH3CO2+	CACH3CO2+	X	X
CACL+	CACL+	X	
CACL2	CALCIUM-CHLORIDE	X	
CACO3	CALCIUM-CARBONATE-CALCITE	X	X
CAF+	CAF+	X	
CAOH+	CAOH+	X	X
CASO4	CALCIUM-SULFATE	X	X

Aqueous Component Databanks: Cd

Alias	Name	Available in Databank AQ	AQ9
CD(AC)+	CDCH3COO+	X	
CD(AC)2	CD(CH3COO)2	X	
CD(AC)3-	CD(CH3COO)3-	X	
CD(ALA)+	CD(C3H6NO2)+	X	
CD(ALA)2	CD(C3H6NO2)2	X	
CD(BUT)+	CDCH3(CH2)2CO2+	X	
CD(BUT)2	CD(CH3CH2CH2CO2)2	X	
CD(CH5N)2+2	CD(NH2CH3)2++	X	X
CD(CH5N)4+2	CD(NH2CH3)4++	X	X
CD(CN)4-2	CD(CN)4--	X	X
CD(FOR)+	CDCHO2+	X	
CD(FOR)2	CD(CHO2)2	X	
CD(GLY)+	CD(C2H4NO2)+	X	
CD(GLY)2	CD(C2H4NO2)2	X	
CD(GLYC)+	CDCH3OCO2+	X	
CD(GLYC)2	CD(CH3OCO2)2	X	

Alias	Name	Available in Databank AQ	AQ9
CD(LAC)+	CDCH3CH2OCO2+	X	
CD(LAC)2	CD(CH3CH2OCO2)2	X	
CD(NH3)2+2	CD(NH3)2++	X	X
CD(NH3)4+2	CD(NH3)4++	X	X
CD(PENT)+	CDCH3(CH2)3CO2+	X	
CD(PENT)2	CD(CH3CH2CH2CH2CO2)2	X	
CD(PROP)+	CDCH3CH2CO2+	X	
CD(PROP)2	CD(CH3CH2CO2)2	X	
CD+2	CD++	X	X
CDBR+	CDBR+	X	X
CDCL+	CDCL+	X	X
CDCL2	CADMIUM-CHLORIDE	X	X
CDCL3-	CDCL3-	X	X
CDI+	CDI+	X	X
CDI3-	CDI3-	X	X
CDI4-2	CDI4--	X	X

Aqueous Component Databanks: Ce

Alias	Name	Available in Databank AQ	AQ9
CE(CH3CO2)2+	CE(CH3CO2)2+	X	X
CE(CH3CO2)3	CERIUM-TRIACETATE	X	X
CE(SO4)2-	CE(SO4)2-	X	X
CE+3	CE+++	X	X
CE+4	CE++++	X	X
CEBR+2	CEBR+2	X	
CECH3CO2+2	CECH3CO2++	X	X
CECL+2	CECL++	X	X
CECL2+	CECL2+	X	
CECL3-AQ	CERIUM-CHLORIDE,AQ	X	
CECL4-	CECL4-	X	
CECLO4+2	CECLO4++	X	X
CECO3+	CECO3+	X	
CEF+2	CEF+2	X	
CEF2+	CEF2+	X	
CEF3-AQ	CERIUM-FLUORIDE,AQ	X	
CEF4-	CEF4-	X	
CEH2PO4+2	CEH2PO4+2	X	
CEHCO3+2	CEHCO3+2	X	
CEIO3+2	CEIO3+2	X	
CENO3+2	CENO3+2	X	
CEO+	CEO+	X	
CEO2-	CEO2-	X	
CEO2H	CEO2H,AQ	X	
CEOH+2	CEOH+2	X	
CEOH+3	CEOH+++	X	X

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	CESO4+	CESO4+	X	X

Aqueous Component Databanks: Cl

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
CL-	CL-	X	X
CL2	CHLORINE	X	X
CL2O	DICHLORINE-MONOXIDE	X	X
CL3-	CL3-	X	X
CLO-	CLO-	X	X
CLO2	CHLORINE-DIOXIDE	X	X
CLO2-	CLO2-	X	X
CLO3-	CLO3-	X	X
CLO4-	CLO4-	X	X

Aqueous Component Databanks: Co

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
COC2O4	COBALT-OXALATE	X	X
CO(AC)+	COCH3COO+	X	
CO(AC)2	CO(CH3COO)2	X	
CO(AC)3-	CO(CH3COO)3-	X	
CO(ALA)+	CO(C3H6NO2)+	X	
CO(ALA)2	CO(C3H6NO2)2	X	
CO(BUT)+	COCH3(CH2)2CO2+	X	
CO(BUT)2	CO(CH3CH2CH2CO2)2	X	
CO(C2H4NO2)2	CO(NH2CH2COO)2	X	X
CO(C2O4)2-2	CO(C2O4)2--	X	X
CO(FOR)+	COCHO2+	X	
CO(FOR)2	CO(CHO2)2	X	
CO(GLYC)+	COCH3OCO2+	X	
CO(GLYC)2	CO(CH3OCO2)2	X	
CO(LAC)+	COCH3CH2OCO2+	X	
CO(LAC)2	CO(CH3CH2OCO2)2	X	
CO(NH3)+2	CO(NH3)++	X	X
CO(NH3)5CL+2	CO(NH3)5CL++	X	X
CO(NH3)5NO2	CO(NH3)5NO2++	X	X
CO(NH3)6+3	CO(NH3)6+3	X	X
CO(NH3)6BR+2	CO(NH3)6BR++	X	X
CO(NH3)6CL+2	CO(NH3)6CL++	X	X
CO(NH3)6I+2	CO(NH3)6I++	X	X
CO(NH3)6N3+2	CO(NH3)6N3++	X	X
CO(NH3)6SO4+	CO(NH3)6SO4+	X	X
CO(PENT)+	COCH3(CH2)3CO2+	X	
CO(PENT)2	CO(CH3CH2CH2CH2CO2)2	X	
CO(PROP)+	COCH3CH2CO2+	X	
CO(PROP)2	CO(CH3CH2CO2)2	X	

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	CO+2	CO++	X	X
	CO+3	CO+++	X	X
	COC2H4NO2+	CONH2CH2COO+	X	X
	COCL+	COCL+	X	X

Aqueous Component Databanks: Cr

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	CR+2	CR++	X	
	CR+3	CR+++	X	X
	CR2O7-2	CR2O7--	X	X
	CRCL2+	CRCL2+	X	X
	CRO4-2	CRO4--	X	X
	CROH+2	CROH++	X	X

Aqueous Component Databanks: Cs

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	CS(AC)	CSCH3COO	X	
	CS(AC)2-	CS(CH3COO)2-	X	
	CS+	CS+	X	X
	CSBR	CESIUM-BROMIDE	X	
	CSCL	CESIUM-CHLORIDE	X	
	CSI	CESIUM-IODIDE	X	

Aqueous Component Databanks: Cu

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	CU(AC)	CUCH3COO	X	
	CU(AC)2-	CU(CH3COO)2-	X	
	CU(AC)3-	CU(CH3COO)3-	X	
	CU(ALA)+	CU(C3H6NO2)+	X	
	CU(ALA)2	CU(C3H6NO2)2	X	
	CU(BUT)+	CUCH3(CH2)2CO2+	X	
	CU(BUT)2	CU(CH3CH2CH2CO2)2	X	
	CU(C2H4NO2)+	CU(NH2CH2COO)+	X	X
	CU(C2H4NO2)2	CU(NH2CH2COO)2	X	X
	CU(C2O4)2-2	CU(C2O4)2--	X	X
	CU(CH3CO2)2	COPPER-DIACETATE	X	X
	CU(CN)2-	CU(CN)2-	X	X
	CU(CN)3-2	CU(CN)3--	X	X
	CU(CN)4-3	CU(CN)4---	X	X
	CU(GLYC)+	CUCH3OCO2+	X	
	CU(GLYC)2	CU(CH3OCO2)2	X	
	CU(LAC)+	CUCH3CH2OCO2+	X	
	CU(LAC)2	CU(CH3CH2OCO2)2	X	
	CU(NH3)+2	CU(NH3)++	X	X
	CU(NH3)2+2	CU(NH3)2++	X	X

Alias	Name	Available in Databank AQ	AQ9
CU(NH3)3+2	CU(NH3)3++	X	X
CU(NH3)4+2	CU(NH3)4++	X	X
CU(NH3)5+2	CU(NH3)5++	X	X
CU(P2O7)2-6	CU(P2O7)2-6	X	X
CU(PENT)+	CUCH3(CH2)3CO2+	X	
CU(PENT)2	CU(CH3CH2CH2CH2CO2)2	X	
CU(PROP)+	CUCH3CH2CO2+	X	
CU(PROP)2	CU(CH3CH2CO2)2	X	
CU(SCN)2	COPPER-THIOCYANATE	X	X
CU(SCN)4-3	CU(CNS)4-3	X	X
CU(SO3)2-3	CU(SO3)2---	X	X
CU(SO3)3-5	CU(SO3)3-5	X	X
CU+	CU+	X	X
CU+2	CU++	X	X
CUBR+	CUBR+	X	X
CUC2H2O4	CU(CHO2)2	X	
CUC2O4	COPPER-OXALATE	X	X
CUCH3CO2+	CUCH3COO+	X	X
CUCHO2+	CUHCOO+	X	X
CUCL+	CUCL+	X	X
CUCL2	COPPER-DICHLORIDE	X	X
CUCL2-	CUCL2-	X	X
CUCL3-2	CUCL3--	X	X
CUF+	CUF+	X	X
CUN2H6P2O7-2	CU(NH3)2P2O7-2	X	X
CUO2-2	CUO2--	X	X
CUP2O7-2	CUP2O7--	X	X
CUSCN+	CUCNS+	X	X
CUSO3-	CUSO3-	X	X
CUSO4	COPPER-SULFATE	X	X

Aqueous Component Databanks: Dy

Alias	Name	Available in Databank AQ	AQ9
DY(CH3CO2)2+	DY(CH3CO2)2+	X	X
DY(CH3CO2)3	DYSPROSIUM-TRIACETATE	X	X
DY(SO4)2-	DY(SO4)2-	X	X
DY+3	DY+3	X	X
DYCH3CO2+2	DYCH3CO2++	X	X
DYCL+2	DYCL+2	X	
DYCL2+	DYCL2+	X	
DYCL3-AQ	DYSPROSIUM-CHLORIDE,AQ	X	
DYCL4-	DYCL4-	X	
DYCO3+	DYCO3+	X	
DYF+2	DYF+2	X	
DYF2+	DYF2+	X	

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	DYF3-AQ	DYSPROSIUM-FLUORIDE,AQ	X	
	DYF4-	DYF4-	X	
	DYH2PO4+2	DYH2PO4+2	X	
	DYHCO3+2	DYHCO3+2	X	
	DYNO3+2	DYNO3+2	X	
	DYO+	DYO+	X	
	DYO2-	DYO2-	X	
	DYO2H	DYO2H,AQ	X	
	DYOH+2	DYOH+2	X	
	DYSO4+	DYSO4+	X	X

Aqueous Component Databanks: Er

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	ER(CH3CO2)2+	ER(CH3CO2)2+	X	X
	ER(CH3CO2)3	ERBIUM-TRIACETATE	X	X
	ER(SO4)2-	ER(SO4)2-	X	X
	ER+3	ER+3	X	X
	ERCH3CO2+2	ERCH3CO2++	X	X
	ERCL+2	ERCL+2	X	
	ERCL2+	ERCL2+	X	
	ERCL3-AQ	ERBIUM-CHLORIDE,AQ	X	
	ERCL4-	ERCL4-	X	
	ERCO3+	ERCO3+	X	
	ERF+2	ERF+2	X	
	ERF2+	ERF2+	X	
	ERF3-AQ	ERBIUM-FLUORIDE,AQ	X	
	ERF4-	ERF4-	X	
	ERH2PO4+2	ERH2PO4+2	X	
	ERHCO3+2	ERHCO3+2	X	
	ERNO3+2	ERNO3+2	X	
	ERO+	ERO+	X	
	ERO2-	ERO2-	X	
	ERO2H	ERO2H,AQ	X	
	EROH+2	EROH+2	X	
	ERSO4+	ERSO4+	X	X

Aqueous Component Databanks: Eu

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	EU(AC)+2	EUCH3COO+2	X	
	EU(AC)2+	EU(CH3COO)2+	X	
	EU(AC)3	EU(CH3COO)3	X	
	EU(ALA)+	EU(C3H6NO2)+	X	
	EU(ALA)2	EU(C3H6NO2)2	X	
	EU(BUT)+	EUCH3(CH2)2CO2+	X	
	EU(BUT)+2	EUCH3(CH2)2CO2+2	X	

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
EU(BUT)2	EU(CH3CH2CH2CO2)2	X	
EU(BUT)2+	EU(CH3CH2CH2CO2)2+	X	
EU(FOR)+	EUCHO2+	X	
EU(FOR)+2	EUCHO2+2	X	
EU(FOR)2	EU(CHO2)2	X	
EU(FOR)2+	EU(CHO2)2+	X	
EU(GLY)+	EU(C2H4NO2)+	X	
EU(GLY)2	EU(C2H4NO2)2	X	
EU(GLYC)+	EUCH3OCO2+	X	
EU(GLYC)2	EU(CH3OCO2)2	X	
EU(LAC)+	EU(CH3CH2OCO2)+	X	
EU(LAC)2	EU(CH3CH2OCO2)2	X	
EU(PENT)+	EUCH3(CH2)3CO2+	X	
EU(PENT)+2	EUCH3(CH2)3CO2+2	X	
EU(PENT)2+	EU(CH3CH2CH2CH2CO2)2+	X	
EU(PROP)+	EUCH3CH2CO2+	X	
EU(PROP)+2	EUCH3CH2CO2+2	X	
EU(PROP)2	EU(CH3CH2CO2)2	X	
EU(PROP)2+	EU(CH3CH2CO2)2+	X	
EU(SO4)2-	EU(SO4)2-	X	X
EU+2	EU+2	X	X
EU+3	EU+3	X	X
EUCL+	EUCL+	X	
EUCL+2	EUCL++	X	X
EUCL2+	EUCL2+	X	
EUCL2-AQ	EUCL2,AQ	X	
EUCL3-	EUCL3-	X	
EUCL3-AQ	EUROPIUM-CHLORIDE,AQ	X	
EUCL4-	EUCL4-	X	
EUCL4-2	EUCL4-2	X	
EUCO3+	EUCO3+	X	
EUF+	EUF+	X	
EUF+2	EUF+2	X	
EUF2	EUF2,AQ	X	
EUF2+	EUF2+	X	
EUF3-	EUF3-	X	
EUF3-AQ	EUROPIUM-FLUORIDE,AQ	X	
EUF4-	EUF4-	X	
EUF4-2	EUF4-2	X	
EUH2PO4+2	EUH2PO4+2	X	
EUHCO3+2	EUHCO3+2	X	
EUNO3+2	EUNO3+2	X	
EUO+	EUO+	X	
EUO2-	EUO2-	X	
EUO2H	EUO2H,AQ	X	

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	EUOH+2	EUOH+2	X	
	EUSO4+	EUSO4+	X	X

Aqueous Component Databanks: Fe

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	FE(ALA)+	FE(C3H6NO2)+	X	
	FE(ALA)2	FE(C3H6NO2)2	X	
	FE(BUT)+	FECH3(CH2)2CO2+	X	
	FE(BUT)2	FE(CH3CH2CH2CO2)2	X	
	FE(CH3COO)+	FE(CH3COO)+	X	
	FE(CH3COO)2	FE(CH3COO)2	X	
	FE(CN)6-3	FE(CN)6-3	X	X
	FE(CN)6-4	FE(CN)6-4	X	X
	FE(FOR)+	FECHO2+	X	
	FE(FOR)2	FE(CHO2)2	X	
	FE(GLY)+	FE(C2H4NO2)+	X	
	FE(GLY)2	FE(C2H4NO2)2	X	
	FE(GLYC)+	FECH3OCO2+	X	
	FE(GLYC)2	FE(CH3OCO2)2	X	
	FE(LAC)+	FECH3CH2OCO2+	X	
	FE(LAC)2	FE(CH3CH2OCO2)2	X	
	FE(OH)2+	FE(OH)2+	X	X
	FE(OH)3	IRON-TRIHYDROXIDE	X	X
	FE(OH)3-	FE(OH)3-	X	X
	FE(OH)4-2	FE(OH)4--	X	X
	FE(PENT)+	FECH3(CH2)3CO2+	X	
	FE(PENT)2	FE(CH3CH2CH2CH2CO2)2	X	
	FE(PROP)+	FECH3CH2CO2+	X	
	FE(PROP)2	FE(CH3CH2CO2)2	X	
	FE(SO4)2-	FE(SO4)2-	X	X
	FE+2	FE++	X	X
	FE+3	FE+++	X	X
	FE2(OH)2+4	FE2(OH)2+4	X	X
	FEBR+2	FEBR++	X	X
	FECL+	FECL+	X	
	FECL+2	FECL++	X	X
	FECL2	FERROUS-CHLORIDE	X	X
	FECL2+	FECL2+	X	
	FECL3	FERRIC-CHLORIDE	X	X
	FECLO4+2	FECLO4++	X	X
	FEF+2	FEF++	X	X
	FEF2+	FEF2+	X	X
	FEHPO4+	FEHPO4+	X	X
	FEI+2	FEI++	X	X
	FEN3+2	FEN3++	X	X

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	FENO+2	FENO++	X	X
	FENO3+2	FENO3++	X	X
	FEO2-2	FEO2--	X	X
	FEOH+	FEOH+	X	X
	FEOH+2	FEOH++	X	X
	FESCN+2	FESCN++	X	X
	FESO4+	FESO4+	X	X

Aqueous Component Databanks: Ga

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	GA+3	GA+3	X	X
	GABR4-	GABR4-	X	X
	GAF+2	GAF++	X	X
	GAF2+	GAF2+	X	X

Aqueous Component Databanks: Gd

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	GD(BUT)+2	GDCH3(CH2)2CO2+2	X	
	GD(BUT)2+	GD(CH3CH2CH2CO2)2+	X	
	GD(CH3CO2)2+	GD(CH3CO2)2+	X	X
	GD(CH3CO2)3	GADOLINIUM-TRIACETATE	X	X
	GD(FOR)+2	GDCHO2+2	X	
	GD(FOR)2+	GD(CHO2)2+	X	
	GD(PENT)+2	GDCH3(CH2)3CO2+2	X	
	GD(PENT)2+	GD(CH3CH2CH2CH2CO2)2+	X	
	GD(PROP)+2	GDCH3CH2CO2+2	X	
	GD(PROP)2+	GD(CH3CH2CO2)2+	X	
	GD(SO4)2-	GD(SO4)2-	X	X
	GD+3	GD+3	X	X
	GDCH3CO2+2	GDCH3CO2++	X	X
	GDCL+2	GDCL+2	X	
	GDCL2+	GDCL2+	X	
	GDCL3-AQ	GADOLINIUM-CHLORIDE,AQ	X	
	GDCL4-	GDCL4-	X	
	GDCO3+	GDCO3+	X	
	GDF+2	GDF+2	X	
	GDF2+	GDF2+	X	
	GDF3-AQ	GADOLINIUM-FLUORIDE,AQ	X	
	GDF4-	GDF4-	X	
	GDH2PO4+2	GDH2PO4+2	X	
	GDHCO3+2	GDHCO3+2	X	
	GDNO3+2	GDNO3+2	X	
	GDO+	GDO+	X	
	GDO2-	GDO2-	X	
	GDO2H	GDO2H,AQ	X	

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
GDOH+2	GDOH+2	X	
GDSO4+	GDSO4+	X	X

Aqueous Component Databanks: Ge

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
GE(OH)2+2	GE(OH)2++	X	X
GE(OH)3+	GE(OH)3+	X	X
GE(OH)4	GERMANIUM-TETRAHYDROXIDE	X	X
GE(OH)5-	GE(OH)5-	X	X
GE(OH)6-2	GE(OH)6--	X	X
GE+2	GE++	X	X
GE+4	GE+4	X	X
GEF4OH-	GEF4OH-	X	X
GEF5-	GEF5-	X	X
GEF6-2	GEF6--	X	X
GEOH+3	GE(OH)+++	X	X

Aqueous Component Databanks: H

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
H+	H+	X	X
H2	HYDROGEN	X	X
H2+	H2+	X	X
H2ASO3-	H2ASO3-	X	X
H2ASO4-	H2ASO4-	X	X
H2AUO3-	H2AUO3-	X	X
H2B4O7	HYDROGEN-TETRABORATE	X	X
H2CO3	CARBONIC-ACID	X	X
H2FE(CN)6-2	H2FE(CN)6--	X	X
H2O2	HYDROGEN-PEROXIDE	X	X
H2OI+	H2OI+	X	X
H2P2O7-2	H2P2O7--	X	X
H2PBO2	H2PBO2	X	X
H2PO3F	H2PO3F	X	X
H2PO4-	H2PO4-	X	X
H2S	HYDROGEN-SULFIDE	X	X
H2S2O4	H2S2O4	X	X
H2S2O8	HYDROGEN-PEROXODISULFIDE	X	X
H2SE	HYDROGEN-SELENIDE	X	X
H2SEO3	SELENIOUS-ACID	X	X
H2SIO3	METASILICIC-ACID	X	X
H2SIO4-2	H2SIO4--	X	X
H2SO3	SULFUROUS-ACID	X	X
H2SO4	SULFURIC-ACID	X	X
H2TEO3	TELLURIC-ACID	X	X
H2VO4-	H2VO4-	X	X

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
H2WO4	TUNGSTIC-ACID	X	X
H3ASO3	H3ASO3	X	X
H3ASO4	ARSENIC-ACID	X	X
H3BO3	HYDROGEN-ORTHOBORATE	X	X
H3N	AMMONIA	X	X
H3O+	H3O+	X	X
H3P2O7-	H3P2O7-	X	X
H3PO4	ORTHOPHOSPHORIC-ACID	X	X
H3SIO4-	H3SIO4-	X	X
H4BO5-	H2BO3.H2O2-	X	X
H4N2	HYDRAZINE	X	X
H4P2O7	PYROPHOSPHORIC-ACID	X	X
H4SIO4	H4SIO4	X	X
H7(WO4)6-5	H7(WO4)6-5	X	X
H7SIO6-	HSI(OH)6-	X	X
H8SIO6	H2(SI(OH)6)	X	X
H9B2O10-	H2BO3.H3BO3.(H2O2)2-	X	X
HALO2	HALO2	X	
HASO2	ARSENOUS-ACID	X	X
HASO3F-	HASO3F-	X	X
HASO4-2	HASO4--	X	X
HAUO3-2	HAUO3--	X	X
HB4O7-	HB4O7-	X	X
HBR	HYDROGEN-BROMIDE	X	X
HBRI2	HBRI2	X	X
HBRO	HYDROGEN-HYPOBROMITE	X	X
HBRO3	HYDROGEN-BROMATE	X	X
HC2O4-	HC2O4-	X	X
HCL	HYDROGEN-CHLORIDE	X	X
HCLO	HYPOCHLOROUS-ACID	X	X
HCLO2	CHLOROUS-ACID	X	X
HCLO3	CHLORIC-ACID	X	X
HCLO4	PERCHLORIC-ACID	X	X
HCO3-	HCO3-	X	X
HCOONH4	AMMONIUM-FORMATE	X	X
HCRO4-	HCRO4-	X	X
HCUO2-	HCUO2-	X	X
HF	HYDROGEN-FLUORIDE	X	X
HF2-	HF2-	X	X
HFE(CN)6-3	HFE(CN)6-3	X	X
HFEO2-	HFEO2-	X	X
HHGO2-	HHGO2-	X	X
HI	HYDROGEN-IODIDE	X	X
HIO	HIO	X	X
HIO3	IODIC-ACID	X	X

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
HN3	HYDROGEN-AZIDE	X	X
HNBO3	HNBO3	X	X
HNO2	NITROUS-ACID	X	X
HNO2-1	NITROUS-ACID(CIS)	X	X
HNO2-2	NITROUS-ACID(TRANS)	X	X
HNO3	NITRIC-ACID	X	X
HOCN	HYDROGEN-CYANATE	X	X
HP2O7-3	HP2O7---	X	X
HPBO2-	HPBO2-	X	X
HPO3F-	HPO3F-	X	X
HPO4-2	HPO4--	X	X
HS-	HS-	X	X
HS2O4-	HS2O4-	X	X
HSBO2	HSBO2	X	X
HSCN	HYDROGEN-THIOCYANATE	X	X
HSE-	HSE-	X	X
HSEO3-	HSEO3-	X	X
HSEO4-	HSEO4-	X	X
HSIO3-	HSIO3-	X	
HSO3-	HSO3-	X	X
HSO4-	HSO4-	X	X
HSO5-	HSO5-	X	
HTAO3	HTAO3	X	X
HVO4-2	HVO4--	X	X
HWO4-	HWO4-	X	X
HZNO2-	HZNO2-	X	X

Aqueous Component Databanks: Hg

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
HG	MERCURY	X	X
HG(AC)3-	HG(CH3COO)3-	X	
HG(C2H4NO2)2	HG(NH2CH2COO)2	X	X
HG(C2O4)2-2	HG(C2O4)2--	X	X
HG(CH5N)2+2	HG(CH3NH2)2++	X	X
HG(CN)2	MERCURY-DICYANIDE	X	X
HG(CN)2CL-	HG(CN)2CL-	X	X
HG(CN)3-	HG(CN)3-	X	X
HG(CN)3BR-2	HG(CN)3BR--	X	X
HG(CN)3CL-2	HG(CN)3CL--	X	X
HG(CN)4-2	HG(CN)4--	X	X
HG(HS)2	HG(HS)2	X	X
HG(NH3)2+2	HG(NH3)2++	X	X
HG(NH3)3+2	HG(NH3)3++	X	X
HG(NH3)4+2	HG(NH3)4++	X	X
HG(OH)2	MERCURY-DIHYDROXIDE	X	X

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
HG(SCN)2	MERCURY-THIOCYANATE	X	X
HG(SCN)3-	HG(CNS)3-	X	X
HG(SCN)4-2	HG(CNS)4-2	X	X
HG(SCN)BR	HG(CNS)BR	X	X
HG(SCN)CL	HG(CNS)CL	X	X
HG+2	HG++	X	X
HG2+2	HG2++	X	X
HG2HC2O5-	HG2(OH)C2O4-	X	X
HG2HP2O8-2	HG2(OH)P2O7--		X
HG2HP2O8-3	HG2(OH)P2O7---	X	
HG2P2O7-2	HG2P2O7--	X	X
HGBR+	HGBR+	X	X
HGBR2	MERCURY-DIBROMIDE	X	X
HGBR3-	HGBR3-	X	X
HGBR4-2	HGBR4--	X	X
HGBRCL	HGCLBR	X	X
HGC2H4NO2+	HG(NH2CH2COO)+	X	X
HGC4H6O4	HG(CH3COO)2	X	
HGCH3COO+	HGCH3COO+	X	X
HGCH5N+2	HG(CH3NH2)++	X	X
HGCL+	HGCL+	X	X
HGCL2	MERCURY-DICHLORIDE	X	X
HGCL3-	HGCL3-	X	X
HGCL4-2	HGCL4--	X	X
HGCLC2H4NO2	HGCL(NH2CH2COO)	X	X
HGCN+	HGCN+	X	X
HGF+	HGF+	X	X
HGI+	HGI+	X	X
HGI2	MERCURY-DIIODIDE	X	X
HGI2BR2-2	HGBR2I2--	X	X
HGI3-	HGI3-	X	X
HGI3BR-2	HGBRI3--	X	X
HGI4-2	HGI4--	X	X
HGIBR	HGBRI	X	X
HGIBR3-2	HGIBR3--	X	X
HGICL	HGCLI	X	X
HGOH+	HGOH+	X	X
HGS2-2	HGS2--	X	X
HGSC4N4-2	HG(CNS)(CN)3--	X	X
HGSO4	MERCURY-SULFATE	X	X

Aqueous Component Databanks: Ho

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
HO(CH3CO2)2+	HO(CH3CO2)2+	X	X
HO(CH3CO2)3	HOLMIUM-TRIACETATE	X	X

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
HO(SO4)2-	HO(SO4)2-	X	X
HO+3	HO+3	X	X
HOCH3CO2+2	HOCH3CO2++	X	X
HOCL+2	HOCL+2	X	
HOCL2+	HOCL2+	X	
HOCL3-AQ	HOLMIUM-CHLORIDE,AQ	X	
HOCL4-	HOCL4-	X	
HOCO3+	HOCO3+	X	
HOF+2	HOF+2	X	
HOF2+	HOF2+	X	
HOF3-AQ	HOLMIUM-FLUORIDE,AQ	X	
HOF4-	HOF4-	X	
HOH2PO4+2	HOH2PO4+2	X	
HOHCO3+2	HOHCO3+2	X	
HONO3+2	HONO3+2	X	
HOO+	HOO+	X	
HOO2-	HOO2-	X	
HOO2H	HOO2H,AQ	X	
HOOH+2	HOOH+2	X	
HOSO4+	HOSO4+	X	X

Aqueous Component Databanks: I

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
I(CN)2-	I(CN)2-	X	X
I-	I-	X	X
I2	IODINE	X	X
I2CL-	I2CL-	X	X
I2CN-	I2CN-	X	X
I2O-2	I2O--	X	X
I2OH-	I2OH-	X	X
I3-	I3-	X	X
IBR	IODINE-BROMIDE	X	X
IBR2-	IBR2-	X	X
IBRCL-	IBRCL-	X	X
ICL	IODINE-CHLORIDE	X	X
ICL2-	ICL2-	X	X
IO-	IO-	X	X
IO3-	IO3-	X	X
IO4-	IO4-	X	X

Aqueous Component Databanks: In

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
IN(C2O4)2-	IN(C2O4)2-	X	X
IN(OH)2+	IN(OH)2+	X	X
IN(SCN)2+	IN(CNS)2+	X	X

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	IN(SCN)3	INDIUM-THIOCYANATE	X	X
	IN+	IN+	X	X
	IN+2	IN++	X	X
	IN+3	IN+++	X	X
	INC2O4+	INC2O4+	X	X
	INOH+2	INOH++	X	X
	INSCN+2	INSCN++	X	X
	INSO4+	INSO4+	X	X

Aqueous Component Databanks: K

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	K(AC)	KCH3COO	X	
	K(AC)2-	K(CH3COO)2-	X	
	K(BUT)	KCH3(CH2)2CO2	X	
	K(BUT)2-	K(CH3CH2CH2CO2)2-	X	
	K(FOR)	KCHO2	X	
	K(FOR)2-	K(CHO2)2-	X	
	K(GLYC)	KCH3OCO2	X	
	K(GLYC)2-	K(CH3OCO2)2-	X	
	K(LAC)	KCH3CH2OCO2	X	
	K(LAC)2-	K(CH3CH2OCO2)2-	X	
	K(PENT)	KCH3(CH2)3CO2	X	
	K(PENT)2-	K(CH3CH2CH2CH2CO2)2-	X	
	K(PROP)	KCH3CH2CO2	X	
	K(PROP)2-	K(CH3CH2CO2)2-	X	
	K+	K+	X	X
	KBR	POTASSIUM-BROMIDE	X	
	KCL	POTASSIUM-CHLORIDE	X	
	KHSO4	KHSO4	X	
	KI	POTASSIUM-IODIDE	X	
	KOH	POTASSIUM-HYDROXIDE	X	
	KP2O7-3	KP2O7-3	X	X
	KS2O8-	KS2O8-	X	X
	KSO4-	KSO4-	X	X

Aqueous Component Databanks: La

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	LA(BUT)+2	LACH3(CH2)2CO2+2	X	
	LA(BUT)2+	LA(CH3CH2CH2CO2)2+	X	
	LA(CH3CO2)2+	LA(CH3CO2)2+	X	X
	LA(CH3CO2)3	LANTHANUM-TRIACETATE	X	X
	LA(FOR)+2	LACHO2+2	X	
	LA(FOR)2+	LA(CHO2)2+	X	
	LA(PENT)+2	LACH3(CH2)3CO2+2	X	
	LA(PENT)2+	LA(CH3CH2CH2CH2CO2)2+	X	

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
LA(PROP)+2	LACH3CH2CO2+2	X	
LA(PROP)2+	LA(CH3CH2CO2)2+	X	
LA(SO4)2-	LA(SO4)2-	X	X
LA+3	LA+3	X	X
LACH3CO2+2	LACH3CO2++	X	X
LACL+2	LACL+2	X	
LACL2+	LACL2+	X	
LACL3-AQ	LANTHANUM-CHLORIDE,AQ	X	
LACL4-	LACL4-	X	
LACO3+	LACO3+	X	
LAF+2	LAF+2	X	
LAF2+	LAF2+	X	
LAF3-AQ	LANTHANUM-FLUORIDE,AQ	X	
LAF4-	LAF4-	X	
LAH2PO4+2	LAH2PO4+2	X	
LAHCO3+2	LAHCO3+2	X	
LANO3+2	LANO3+2	X	
LAO+	LAO+	X	
LAO2-	LAO2-	X	
LAO2H	LAO2H,AQ	X	
LAOH+2	LAOH+2	X	
LASO4+	LASO4+	X	X

Aqueous Component Databanks: Li

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
LI(AC)	LICH3COO	X	
LI(AC)2-	LI(CH3COO)2-	X	
LI+	LI+	X	X
LICL	LITHIUM-CHLORIDE	X	
LIHP2O7-2	LIHP2O7--	X	X
LIHPO4-	LIHPO4-	X	X
LINO3	LITHIUM-NITRATE	X	X
LIOH	LITHIUM-HYDROXIDE	X	X
LIP2O7-3	LIP2O7---	X	X
LISO4-	LISO4-	X	X

Aqueous Component Databanks: Lu

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
LU(AC)+2	LUCH3COO+2	X	
LU(AC)2+	LU(CH3COO)2+	X	
LU(AC)3	LU(CH3COO)3	X	
LU(SO4)2-	LU(SO4)2-	X	X
LU+3	LU+3	X	X
LUCL+2	LUCL+2	X	
LUCL2+	LUCL2+	X	

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
LUCL3-AQ	LUCL3,AQ	X	
LUCL4-	LUCL4-	X	
LUCO3+	LUCO3+	X	
LUF+2	LUF+2	X	
LUF2+	LUF2+	X	
LUF3	LUF3,AQ	X	
LUF4-	LUF4-	X	
LUH2PO4+2	LUH2PO4+2	X	
LUHCO3+2	LUHCO3+2	X	
LUNO3+2	LUNO3+2	X	
LUO+	LUO+	X	
LUO2-	LUO2-	X	
LUO2H	LUO2H,AQ	X	
LUOH+2	LUOH+2	X	
LUSO4+	LUSO4+	X	X

Aqueous Component Databanks: Mg

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
MG(AC)2	MG(CH3COO)2	X	
MG(ALA)+	MG(C3H6NO2)+	X	
MG(ALA)2	MG(C3H6NO2)2	X	
MG(BUT)+	MGCH3(CH2)2CO2+	X	
MG(BUT)2	MG(CH3CH2CH2CO2)2	X	
MG(C2O4)2-2	MG(C2O4)2--	X	X
MG(FOR)+	MGCHO2+	X	
MG(FOR)2	MG(CHO2)2	X	
MG(GLY)+	MG(C2H4NO2)+	X	
MG(GLY)2	MG(C2H4NO2)2	X	
MG(GLYC)+	MGCH3OCO2+	X	
MG(GLYC)2	MG(CH3OCO2)2	X	
MG(LAC)+	MGCH3CH2OCO2+	X	
MG(LAC)2	MG(CH3CH2OCO2)2	X	
MG(PENT)+	MGCH3(CH2)3CO2+1	X	
MG(PENT)2	MG(CH3CH2CH2CH2CO2)2	X	
MG(PROP)+	MGCH3CH2CO2+	X	
MG(PROP)2	MG(CH3CH2CO2)2	X	
MG+2	MG++	X	X
MGCH3CO2+	MGCH3CO2+	X	X
MGCL+	MGCL+	X	
MGCO3	MAGNESIUM-CARBONATE	X	X
MGF+	MGF+	X	X
MGHCO3+	MGHCO3+	X	X
MGIO3+	MGIO3+	X	X
MGOH+	MGOH+	X	X
MGP2O7-2	MGP2O7--	X	X

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	MGSO4	MAGNESIUM-SULFATE	X	X

Aqueous Component Databanks: Mn

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
MN(AC)2	MN(CH3COO)2	X	
MN(AC)3-	MN(CH3COO)3-	X	
MN(ALA)+	MN(C3H6NO2)+	X	
MN(ALA)2	MN(C3H6NO2)2	X	
MN(BUT)+	MNCH3(CH2)2CO2+	X	
MN(BUT)2	MN(CH3CH2CH2CO2)2	X	
MN(C2O4)2-2	MN(C2O4)2--	X	X
MN(FOR)+	MNCHO2+	X	
MN(GLY)+	MN(C2H4NO2)+	X	
MN(GLY)2	MN(C2H4NO2)2	X	
MN(GLYC)+	MNCH3OCO2+	X	
MN(GLYC)2	MN(CH3OCO2)2	X	
MN(LAC)+	MNCH3CH2OCO2+	X	
MN(LAC)2	MN(CH3CH2OCO2)2	X	
MN(OH)3-	MN(OH)3-	X	X
MN(PENT)+	MNCH3(CH2)3CO2+	X	
MN(PENT)2	MN(CH3CH2CH2CH2CO2)2	X	
MN(PROP)+	MNCH3CH2CO2+	X	
MN(PROP)2	MN(CH3CH2CO2)2	X	
MN(SCN)2	MANGANESE-THIOCYANATE	X	X
MN+2	MN++	X	X
MN+3	MN+++	X	X
MNC2H2O4	MN(CHO2)2	X	
MNC2O4	MANGANESE-OXALATE	X	X
MNCH3CO2+	MNCH3COO+	X	X
MNCL+	MNCL+	X	
MNCL2	MANGANESE-DICHLORIDE	X	X
MNCL3-	MNCL3-	X	X
MNHCO3+	MNHCO3+	X	X
MNO4-	MNO4-	X	X
MNO4-2	MNO4--	X	X
MNOH+	MNOH+	X	X
MNSCN+	MNCNS+	X	X
MNSO4	MANGANESE-SULFATE	X	X

Aqueous Component Databanks: N

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
N2	NITROGEN	X	X
N2H5+	N2H5+	X	X
N2H5BR	N2H5BR	X	X
N2H5CL	N2H5CL	X	X

Alias	Name	Available in Databank AQ	AQ9
N2H5NO3	N2H5NO3	X	X
N2H5OH	N2H5OH	X	X
N3-	N3-	X	X
NH2CH2COO-	NH2CH2COO-	X	X
NH2CH2COOH	NH2CH2COOH	X	X
NH2COO-	CARBAMATE	X	X
NH3CH2COOH+	NH3CH2COOH+	X	X
NH4(AC)	NH4CH3COO	X	
NH4(AC)2-	NH4(CH3COO)2-	X	
NH4+	NH4+	X	X
NH4BR	AMMONIUM-BROMIDE	X	X
NH4CL	AMMONIUM-CHLORIDE	X	X
NH4CL3	AMMONIUM-TRICHLORIDE	X	X
NH4CN	AMMONIUM-CYANIDE	X	X
NH4CNO	AMMONIUM-CYANATE	X	X
NH4F	AMMONIUM-FLUORIDE	X	X
NH4HF2	AMMONIUM-HYDROGEN-FLUORIDE	X	X
NH4HO2	NH4HO2	X	X
NH4HS	AMMONIUM-HYDROGEN-SULFIDE	X	X
NH4I	AMMONIUM-IODIDE	X	X
NH4N3	AMMONIUM-AZIDE	X	X
NH4NO2	AMMONIUM-NITRITE	X	X
NH4NO3	AMMONIUM-NITRATE	X	X
NH4OH	AMMONIUM-HYDROXIDE	X	X
NO2-	NO2-	X	X
NO3-	NO3-	X	X
NOCL	NITROSYL-CHLORIDE	X	X

Aqueous Component Databanks: Na

Alias	Name	Available in Databank AQ	AQ9
NA(AC)	NACH3COO	X	
NA(AC)2-	NA(CH3COO)2-	X	
NA(BUT)	NACH3(CH2)2CO2	X	
NA(BUT)2-	NA(CH3CH2CH2CO2)2-	X	
NA(FOR)2-	NA(CH02)2-	X	
NA(GLYC)	NA(CH3OCO2)	X	
NA(GLYC)2-	NA(CH3OCO2)2-	X	
NA(LAC)	NACH3CH2OCO2	X	
NA(LAC)2-	NA(CH3CH2OCO2)2-	X	
NA(PENT)	NACH3(CH2)3CO2	X	
NA(PENT)2-	NA(CH3CH2CH2CH2CO2)2-	X	
NA(PROP)	NACH3CH2CO2	X	
NA(PROP)2-	NA(CH3CH2CO2)2-	X	
NA+	NA+	X	X
NA2P2O7-2	NA2P2O7--	X	X

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	NAALO2	SODIUM-ALUMINATE	X	
	NABR	SODIUM-BROMIDE	X	
	NACHO2	SODIUM-FORMATE	X	
	NACL	SODIUM-CHLORIDE	X	
	NACLO	SODIUM-HYPOCHLORITE	X	X
	NACO3-	NACO3-	X	X
	NAF	SODIUM-FLUORIDE	X	
	NAHCO3	SODIUM-BICARBONATE	X	X
	NAHP2O7-2	NAHP2O7--	X	X
	NAHSIO3	NAHSIO3	X	
	NAI	SODIUM-IODIDE	X	
	NAOH	SODIUM-HYDROXIDE	X	
	NAS2O3-	NAS2O3-	X	X
	NASO4-	NASO4-	X	X

Aqueous Component Databanks: Nd

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	ND(CH3CO2)2+	ND(CH3CO2)2+	X	X
	ND(CH3CO2)3	NEODYMIUM-TRIACETATE	X	X
	ND(SO4)2-	ND(SO4)2-	X	X
	ND+3	ND+3	X	X
	NDCH3CO2+2	NDCH3CO2++	X	X
	NDCL+2	NDCL+2	X	
	NDCL2+	NDCL2+	X	
	NDCL3-AQ	NEODYMIUM-CHLORIDE,AQ	X	
	NDCL4-	NDCL4-	X	
	NDCO3+	NDCO3+	X	
	NDF+2	NDF+2	X	
	NDF2+	NDF2+	X	
	NDF3-AQ	NEODYMIUM-FLUORIDE,AQ	X	
	NDF4-	NDF4-	X	
	NDH2PO4+2	NDH2PO4+2	X	
	NDHCO3+2	NDHCO3+2	X	
	NDNO3+2	NDNO3+2	X	
	NDO+	NDO+	X	
	NDO2-	NDO2-	X	
	NDO2H	NDO2H,AQ	X	
	NDOH+2	NDOH+2	X	
	NDSO4+	NDSO4+	X	X

Aqueous Component Databanks: Ni

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	NI(AC)+	NICH3COO+	X	
	NI(AC)2	NI(CH3COO)2	X	
	NI(AC)3-	NI(CH3COO)3-	X	

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
NI(ALA)+	NI(C3H6NO2)+	X	
NI(ALA)2	NI(C3H6NO2)2	X	
NI(BUT)+	NICH3(CH2)2CO2+	X	
NI(BUT)2	NI(CH3CH2CH2CO2)2	X	
NI(CH5N)6+2	NI(CH3NH2)6++	X	X
NI(CN)4-2	NI(CN)4--	X	X
NI(FOR)+	NICHO2+	X	
NI(FOR)2	NI(CHO2)2	X	
NI(GLY)+	NI(C2H4NO2)+	X	
NI(GLY)2	NI(C2H4NO2)2	X	
NI(GLYC)+	NICH3OCO2+	X	
NI(GLYC)2	NI(CH3OCO2)2	X	
NI(LAC)+	NICH3CH2OCO2+	X	
NI(LAC)2	NI(CH3CH2OCO2)2	X	
NI(NH3)2+2	NI(NH3)2++	X	X
NI(NH3)4+2	NI(NH3)4++	X	
NI(NH3)6+2	NI(NH3)6++	X	X
NI(PENT)+	NICH3(CH2)3CO2+	X	
NI(PENT)2	NI(CH3CH2CH2CH2CO2)2	X	
NI(PROP)+	NICH3CH2CO2+	X	
NI(PROP)2	NI(CH3CH2CO2)2	X	
NI+2	NI++	X	X
NIC2O4	NICKEL-OXALATE	X	X
NICL+	NICL+	X	
NIOH+	NIOH+	X	X
NIP2O7-2	NIP2O7--	X	X
NISCN+	NICNS+	X	X
NISO4	NICKEL-SULFATE	X	X

Aqueous Component Databanks: O

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
O2	OXYGEN	X	X
O2H-	HO2-	X	X
O2S	SULFUR-DIOXIDE	X	X
O3	OZONE	X	X
OCN-	CNO-	X	X
OH-	OH-	X	X

Aqueous Component Databanks: P

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
P2O7-4	P2O7----	X	X
PH3	PHOSPHINE	X	X
PH4+	PH4+	X	X
PH4OH	PH3.H2O	X	X
PO3F-2	PO3F--	X	X

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	PO4-3	PO4---	X	X

Aqueous Component Databanks: Pb

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
PB(AC)3-	PB(CH3COO)3-	X	
PB(ALA)+	PB(C3H6NO2)+	X	
PB(ALA)2	PB(C3H6NO2)2	X	
PB(BUT)+	PBCH3(CH2)2CO2+	X	
PB(BUT)2	PB(CH3CH2CH2CO2)2	X	
PB(CH3CO2)+	PB(CH3CO2)+	X	X
PB(CH3CO2)2	LEAD-DIACETATE	X	X
PB(CLO3)2	PB(CLO3)2	X	X
PB(GLY)+	PB(C2H4NO2)+	X	
PB(GLY)2	PB(C2H4NO2)2	X	
PB(GLYC)+	PBCH3OCO2+	X	
PB(GLYC)2	PB(CH3OCO2)2	X	
PB(LAC)+	PBCH3CH2OCO2+	X	
PB(LAC)2	PB(CH3CH2OCO2)2	X	
PB(OH)3-	PB(OH)3-	X	X
PB(PENT)+	PBCH3(CH2)3CO2+	X	
PB(PENT)2	PB(CH3CH2CH2CH2CO2)2	X	
PB(PROP)+	PBCH3CH2CO2+	X	
PB(PROP)2	PB(CH3CH2CO2)2	X	
PB(SCN)2	LEAD-THIOCYANATE	X	X
PB+2	PB++	X	X
PB3(OH)4+2	PB3(OH)4++	X	X
PB4(OH)4+4	PB4(OH)4+4	X	X
PB6(OH)8+4	PB6(OH)8+4	X	X
PBBR+	PBBR+	X	X
PBBR2	LEAD-DIBROMIDE	X	X
PBBR3-	PBBR3-	X	X
PBBRO3+	PBBRO3+	X	X
PBC2H2O4	PB(HCO2)2	X	X
PBCL+	PBCL+	X	X
PBCL2	LEAD-DICHLORIDE	X	X
PBCL3-	PBCL3-	X	X
PBCL4-2	PBCL4--	X	
PBCLO3+	PBCLO3+	X	X
PBF+	PBF+	X	X
PBF2	LEAD-DIFLUORIDE	X	X
PBHCO2+	PBHCO2+	X	X
PBI+	PBI+	X	X
PBI2	LEAD-DIIODIDE	X	X
PBI3-	PBI3-	X	X
PBI4-2	PBI4--	X	X

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	PBNO3+	PBNO3+	X	X
	PBOH+	PBOH+	X	X
	PBP2O7-2	PBP2O7--	X	X
	PBSCN+	PBCNS+	X	X

Aqueous Component Databanks: Pd

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	PD+2	PD++	X	X
	PDBR4-2	PDBR4--	X	X
	PDCL+	PDCL+	X	X
	PDCL3(C2H4)-	PDCL3(C2H4)-	X	X

Aqueous Component Databanks: Pr

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	PR(CH3CO2)2+	PR(CH3CO2)2+	X	X
	PR(CH3CO2)3	PRASEODYMIUM-TRIACETATE	X	X
	PR(OH)2+	PR(OH)2+	X	X
	PR(SO4)2-	PR(SO4)2-	X	X
	PR+3	PR+3	X	X
	PRCH3CO2+2	PRCH3CO2++	X	X
	PRCL+2	PRCL++	X	X
	PRCL2+	PRCL2+	X	
	PRCL3-AQ	PRASEODYMIUM-CHLORIDE,AQ	X	
	PRCL4-	PRCL4-	X	
	PRCO3+	PRCO3+	X	
	PRF+2	PRF+2	X	
	PRF2+	PRF2+	X	
	PRF3-AQ	PRASEODYMIUM-FLUORIDE,AQ	X	
	PRF4-	PRF4-	X	
	PRH2PO4+2	PRH2PO4+2	X	
	PRHCO3+2	PRHCO3+2	X	
	PRMOO4+	PRMOO4+	X	X
	PRNO3+2	PRNO3+2	X	X
	PRO+	PRO+	X	
	PRO2-	PRO2-	X	
	PRO2H	PRO2H,AQ	X	
	PROH+2	PROH+2	X	X
	PRSO4+	PRSO4+	X	X

Aqueous Component Databanks: Pt

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	PT(NH3)3CL+	PT(NH3)3CL+	X	X
	PT(NH3)4+2	PT(NH3)4++	X	X
	PT(NH3)CL3-	PT(NH3)CL3-	X	X
	PT+2	PT++	X	X

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	PTBR4-2	PTBR4--	X	X
	PTBR6-2	PTBR6--	X	X
	PTCL4-2	PTCL4--	X	X
	PTCL6-2	PTCL6--	X	X
	PTI6-2	PTI6--	X	X

Aqueous Component Databanks: Rb

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	RB(AC)	RBCH3COO	X	
	RB(AC)2-	RB(CH3COO)2-	X	
	RB+	RB+	X	X
	RBBR	RUBIDIUM-BROMIDE	X	
	RBCL	RUBIDIUM-CHLORIDE	X	
	RBF	RUBIDIUM-FLUORIDE	X	
	RBI	RUBIDIUM-IODIDE	X	

Aqueous Component Databanks: S

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	S-2	S--	X	X
	S2-2	S2--	X	X
	S2O3-2	S2O3--	X	X
	S2O4-2	S2O4--	X	X
	S2O5-2	S2O5--	X	
	S2O6-2	S2O6--	X	
	S2O8-2	S2O8--	X	X
	S3-2	S3--	X	X
	S3O6-2	S3O6--	X	
	S4-2	S4--	X	X
	S4O6-2	S4O6--	X	X
	S5-2	S5--	X	X
	S5O6-2	S5O6--	X	
	SF6	SULFUR-HEXAFLUORIDE	X	X
	SO3-2	SO3--	X	X
	SO4-2	SO4--	X	X

Aqueous Component Databanks: Sc

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	SC(AC)+2	SCCH3COO+2	X	
	SC(AC)2+	SC(CH3COO)2+	X	
	SC(AC)3	SC(CH3COO)3	X	
	SC(SEO4)2-	SC(SEO4)2-	X	X
	SC+3	SC+3	X	X
	SCBR+2	SCBR++	X	X
	SCBR2+	SCBR2+	X	X
	SCCL+2	SCCL++	X	X

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	SCCL2+	SCCL2+	X	X
	SCOH+2	SCOH++	X	X
	SCSEO4+	SCSEO4+	X	X

Aqueous Component Databanks: Sm

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	SM(CH3CO2)2+	SM(CH3CO2)2+	X	X
	SM(CH3CO2)3	SAMARIUM-TRIACETATE	X	X
	SM(SO4)2-	SM(SO4)2-	X	X
	SM+2	SM++	X	
	SM+3	SM+3	X	X
	SMCH3CO2+2	SMCH3CO2++	X	X
	SMCL+2	SMCL+2	X	
	SMCL2+	SMCL2+	X	
	SMCL3-AQ	SAMARIUM-TRICHLORIDE,AQ	X	
	SMCL4-	SMCL4-	X	
	SMCO3+	SMCO3+	X	
	SMF+2	SMF+2	X	
	SMF2+	SMF2+	X	
	SMF3-AQ	SMF3,AQ	X	
	SMF4-	SMF4-	X	
	SMH2PO4+2	SMH2PO4+2	X	
	SMHCO3+2	SMHCO3+2	X	
	SMNO3+2	SMNO3+2	X	
	SMO+	SMO+	X	
	SMO2-	SMO2-	X	
	SMO2H	SMO2H,AQ	X	
	SMOH+2	SMOH+2	X	
	SMSO4+	SMSO4+	X	X

Aqueous Component Databanks: Sn

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	SN(SO4)2	TIN-DISULFATE	X	X
	SN+2	SN++	X	X
	SNF+	SNF+	X	X
	SNOH+	SNOH+	X	X
	SNOHBR	SNOHBR	X	X
	SNOHCL	SNOHCL	X	X
	SNOOH+	SNOOH+	X	X
	SNOOHF	SNO(OH)F	X	X
	SNSO4+2	SNSO4++	X	X

Aqueous Component Databanks: Sr

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	SR(AC)+	SRCH3COO+	X	

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
SR(AC)2	SR(CH3COO)2	X	
SR(ALA)+	SR(C3H6NO2)+	X	
SR(ALA)2	SR(C3H6NO2)2	X	
SR(BUT)+	SRCH3(CH2)2CO2+	X	
SR(BUT)2	SR(CH3CH2CH2CO2)2	X	
SR(FOR)+	SRCHO2+	X	
SR(FOR)2	SR(CHO2)2	X	
SR(GLY)+	SR(C2H4NO2)+	X	
SR(GLY)2	SR(C2H4NO2)2	X	
SR(GLYC)+	SRCH3OCO2+	X	
SR(GLYC)2	SR(CH3OCO2)2	X	
SR(LAC)+	SRCH3CH2OCO2+	X	
SR(LAC)2	SR(CH3CH2OCO2)2	X	
SR(PENT)+	SRCH3(CH2)3CO2+	X	
SR(PENT)2	SR(CH3CH2CH2CH2CO2)2	X	
SR(PROP)+	SRCH3CH2CO2+	X	
SR(PROP)2	SR(CH3CH2CO2)2	X	
SR+2	SR++	X	X
SRCL+	SRCL+	X	
SRCO3	STRONTIUM-CARBONATE	X	
SRF+	SRF+	X	
SROH+	SR(OH)+	X	X

Aqueous Component Databanks: Tb

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
TB(AC)+2	TBCH3COO+2	X	
TB(AC)2+	TB(CH3COO)2+	X	
TB(AC)3	TB(CH3COO)3	X	
TB(SO4)2-	TB(SO4)2-	X	X
TB+3	TB+3	X	X
TBCL+2	TBCL+2	X	
TBCL2+	TBCL2+	X	
TBCL3-AQ	TERBIUM-TRICHLORIDE,AQ	X	
TBCL4-	TBCL4-	X	
TBCO3+	TBCO3+	X	
TBF+2	TBF+2	X	
TBF2+	TBF2+	X	
TBF3	TBF3,AQ	X	
TBF4-	TBF4-	X	
TBH2PO4+2	TBH2PO4+2	X	
TBHCO3+2	TBHCO3+2	X	
TBNO3+2	TBNO3+2	X	
TBO+	TBO+	X	
TBO2-	TBO2-	X	
TBO2H	TBO2H,AQ	X	

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
TBOH+2	TBOH+2	X	
TBSO4+	TBSO4+	X	X

Aqueous Component Databanks: Th

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
TH(BRO3)2+2	TH(BRO3)2++	X	X
TH(C2O4)3-2	TH(C2O4)3-2	X	X
TH(H2PO4)2+2	TH(H2PO4)2+2	X	X
TH(IO3)2+2	TH(IO3)2++	X	X
TH(IO3)3+	TH(IO3)3+	X	X
TH(NO3)2+2	TH(NO3)2+2	X	X
TH(OH)2+2	TH(OH)2++	X	X
TH(SCN)2+2	TH(SCN)2++	X	X
TH(SCN)3+	TH(SCN)3+	X	X
TH(SCN)4	TH(SCN)4	X	X
TH(SO4)3-2	TH(SO4)3--	X	X
TH(SO4)4-4	TH(SO4)4-4	X	X
TH+4	TH+4	X	X
TH2(OH)2+6	TH2(OH)2+6	X	X
THBRO3+3	THBRO3+3	X	X
THC2O4+2	THC2O4++	X	X
THCH3COO+3	THCH3COO+3	X	X
THCL+3	THCL+3	X	X
THCL2+2	THCL2++	X	X
THCL3+	THCL3+	X	X
THCLO3+	THCLO3+	X	X
THF+3	THF+3	X	X
THF2+2	THF2++	X	X
THF3+	THF3+	X	X
THF4	THORIUM-TETRAFLUORIDE	X	X
THH2PO4+3	THH2PO4+3	X	X
THIO3+3	THIO3+3	X	X
THNO3+3	THNO3+3	X	X
THOH+3	THOH+3	X	X
THSCN+3	THSCN+3	X	X
THSO4+2	THSO4++	X	X

Aqueous Component Databanks: Tl

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
TL(AC)	TLCH3COO	X	
TL(AC)2-	TL(CH3COO)2-	X	
TL(CN)4-	TL(CN)4-	X	X
TL(OH)2+	TL(OH)2+	X	X
TL+	TL+	X	X
TL+3	TL+++	X	X

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
TLBR+	TLBR+	X	X
TLBR+2	TLBR++	X	X
TLBR2+	TLBR2+	X	X
TLBR2-	TLBR2-	X	X
TLBR3	THALLIUM-TRIBROMIDE	X	X
TLBR4-	TLBR4-	X	X
TLBRCL-	TLBRCL-	X	X
TLCL	THALLIUM-CHLORIDE	X	X
TLCL+2	TLCL++	X	X
TLCL2+	TLCL2+	X	X
TLCL2-	TLCL2-	X	X
TLCL3	THALLIUM-TRICHLORIDE	X	X
TLCL4-	TLCL4-	X	X
TLCLO3	THALLIUM-CHLORATE	X	X
TLCNS	THALLIUM-THIOCYANATE	X	X
TLF	THALLIUM-FLUORIDE	X	X
TLI	THALLIUM-IODIDE	X	X
TLI2-	TLI2-	X	X
TLI4-	TLI4-	X	X
TLIBR-	TLIBR-	X	X
TLNH3+	TLNH3+	X	X
TLNO3	THALLIUM-NITRATE	X	X
TLNO3+2	TLNO3++	X	X
TLOH	THALLIUM-HYDROXIDE	X	X
TLOH+2	TLOH++	X	X
TLSO4-	TLSO4-	X	X

Aqueous Component Databanks: Tm

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
TM(AC)+2	TMCH3COO+2	X	
TM(AC)2+	TM(CH3COO)2+	X	
TM(AC)3	TM(CH3COO)3	X	
TM(SO4)2-	TM(SO4)2-	X	X
TM+3	TM+3	X	X
TMCL+2	TMCL+2	X	
TMCL2+	TMCL2+	X	
TMCL3-AQ	THULIUM-TRICHLORIDE,AQ	X	
TMCL4-	TMCL4-	X	
TMCO3+	TMCO3+	X	
TMF+2	TMF+2	X	
TMF2+	TMF2+	X	
TMF3-AQ	THULIUM-TRIFLUORIDE,AQ	X	
TMF4-	TMF4-	X	
TMH2PO4+2	TMH2PO4+2	X	
TMHCO3+2	TMHCO3+2	X	

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	TMNO3+2	TMNO3+2	X	
	TMO+	TMO+	X	
	TMO2-	TMO2-	X	
	TMO2H	TMO2H,AQ	X	
	TMOH+2	TMOH+2	X	
	TMSO4+	TMSO4+	X	X

Aqueous Component Databanks: U

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	U(AC)+2	UCH3COO+2	X	
	U(AC)2+	U(CH3COO)2+	X	
	U(AC)3	U(CH3COO)3	X	
	U(BUT)+2	UCH3(CH2)2CO2+2	X	
	U(BUT)2+	U(CH3CH2CH2CO2)2+	X	
	U(CO3)4-4	U(CO3)4-4	X	X
	U(CO3)5-6	U(CO3)5-6	X	X
	U(FOR)+2	UCHO2+2	X	
	U(FOR)2+	U(CHO2)2+	X	
	U(NO3)2+2	U(NO3)2++	X	X
	U(OH)4	U(OH)4	X	X
	U(OH)5-	U(OH)5-	X	X
	U(PENT)+2	UCH3(CH2)3CO2+2	X	
	U(PROP)+2	UCH3CH2CO2+2	X	
	U(PROP)2+	U(CH3CH2CO2)2+	X	
	U(SCN)2+2	U(SCN)2++	X	X
	U(SO4)2	URANIUM-DISULFATE	X	X
	U+3	U+3	X	X
	U+4	U+4	X	X
	U2CO7(OH)3-	U2CO7(OH)3-	X	X
	U3O10H4+2	U3O10H4++	X	X
	U3O11H5+	U3O11H5+	X	X
	U3O13H7-	U3O13H7-	X	X
	U3O6(CO3)6-6	U3O6(CO3)6-6	X	X
	U4O15H7+	U4O15H7+	X	X
	UBR+3	UBR+3	X	X
	UCL+3	UCL+3	X	X
	UF+3	UF+3	X	X
	UF2+2	UF2++	X	X
	UF3+	UF3+	X	X
	UF4	URANIUM-TETRAFLUORIDE	X	X
	UF5-	UF5-	X	X
	UF6-2	UF6--	X	X
	UI+3	UI+3	X	X
	UNO3+3	UNO3+3	X	X
	(UO2)2OH+3	(UO2)2OH+3	X	X

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
(UO2OH)2+2	(UO2OH)2++	X	X
UO2(AC)+	UO2CH3COO+	X	
UO2(AC)2	UO2(CH3COO)2	X	
UO2(AC)3-	UO2(CH3COO)3-	X	
UO2(CO3)2-2	UO2(CO3)2--	X	X
UO2(CO3)3-4	UO2(CO3)3-4	X	X
UO2(CO3)3-5	UO2(CO3)3-5	X	X
UO2(H2PO4)2	UO2(H2PO4)2	X	X
UO2(IO3)2	UO2(IO3)2	X	X
UO2(N3)2	UO2(N3)2	X	X
UO2(N3)3-	UO2(N3)3-	X	X
UO2(N3)4-2	UO2(N3)4--	X	X
UO2(OH)2	UO2(OH)2	X	X
UO2(OH)3-	UO2(OH)3-	X	X
UO2(OH)4-2	UO2(OH)4--	X	X
UO2(SCN)2	UO2(SCN)2	X	X
UO2(SCN)3-	UO2(SCN)3-	X	X
UO2(SO4)2-2	UO2(SO4)2--	X	X
UO2+	UO2+	X	X
UO2+2	UO2++	X	X
UO2BR+	UO2BR+	X	X
UO2BRO3+	UO2BRO3+	X	X
UO2CL+	UO2CL+	X	X
UO2CL2	URANIUM-DICHLORIDE-DIOXIDE	X	X
UO2CLO3+	UO2CLO3+	X	X
UO2CO3	UO2CO3	X	X
UO2F+	UO2F+	X	X
UO2F2	URANIUM-DIFLUORIDE-DIOXIDE	X	X
UO2F3-	UO2F3-	X	X
UO2F4-2	UO2F4--	X	X
UO2H2PO4+	UO2H2PO4+	X	X
UO2H3PO4+2	UO2H3PO4++	X	X
UO2H5P2O8+	UO2H5P2O8+	X	X
UO2HPO4	UO2HPO4	X	X
UO2IO3+	UO2IO3+	X	X
UO2N3+	UO2N3+	X	X
UO2NO3+	UO2NO3+	X	X
UO2OH+	UO2OH+	X	X
UO2PO4-	UO2PO4-	X	X
UO2S2O3	UO2S2O3	X	X
UO2SCN+	UO2SCN+	X	X
UO2SO3	UO2SO3	X	X
UO2SO4	URANIUM-SULFATE-DIOXIDE	X	X
UOH+3	UOH+3	X	X
USCN+3	USCN+3	X	X

			Available in Databank	
	Alias	**Name**	**AQ**	**AQ9**
	USO4+2	USO4++	X	X

Aqueous Component Databanks: V

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
V+2	V++	X	X
V+3	V+++	X	X
VO+2	VO++	X	X
VO2+	VO2+	X	X
VO3-	VO3-	X	X
VOSCN+	VOSCN+	X	X

Aqueous Component Databanks: Y

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
Y(AC)+2	YCH3COO+2	X	
Y(AC)2+	Y(CH3COO)2+	X	
Y(AC)3	Y(CH3COO)3	X	
Y(C2O4)2-	Y(C2O4)2-	X	X
Y(C2O4)3-3	Y(C2O4)3-3	X	X
Y(SO4)2-	Y(SO4)2-	X	X
Y+3	Y+3	X	X
Y2(OH)2+4	Y2(OH)2+4	X	X
YBR+2	YBR++	X	X
YC2O4+	YC2O4+	X	X
YCL+2	YCL++	X	X
YNO3+2	YNO3++	X	X
YOH+2	YOH++	X	X
YSCN+2	YCNS++	X	X
YSO4+	YSO4+	X	X

Aqueous Component Databanks: Yb

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
YB(BUT)+2	YBCH3(CH2)2CO2+2	X	
YB(BUT)2+	YB(CH3CH2CH2CO2)2+	X	
YB(CH3CO2)2+	YB(CH3CO2)2+	X	X
YB(CH3CO2)3	YTTERBIUM-TRIACETATE	X	X
YB(FOR)+2	YBCHO2+2	X	
YB(FOR)2+	YB(CHO2)2+	X	
YB(PENT)+2	YBCH3(CH2)3CO2+2	X	
YB(PENT)2+	YB(CH3CH2CH2CH2CO2)2+	X	
YB(PROP)+2	YBCH3CH2CO2+2	X	
YB(PROP)2+	YB(CH3CH2CO2)2+	X	
YB(SO4)2-	YB(SO4)2-	X	X
YB+2	YB++	X	
YB+3	YB+3	X	X
YBCH3CO2+2	YBCH3CO2++	X	X

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
YBCL+2	YBCL+2	X	
YBCL2+	YBCL2+	X	
YBCL3-AQ	YBCL3,AQ	X	
YBCL4-	YBCL4-	X	
YBCO3+	YBCO3+	X	
YBF+2	YBF+2	X	
YBF2+	YBF2+	X	
YBF3	YBF3,AQ	X	
YBF4-	YBF4-	X	
YBH2PO4+2	YBH2PO4+2	X	
YBHCO3+2	YBHCO3+2	X	
YBNO3+2	YBNO3+2	X	
YBO+	YBO+	X	
YBO2-	YBO2-	X	
YBO2H	YBO2H,AQ	X	
YBOH+2	YBOH+2	X	
YBSO4+	YBSO4+	X	X

Aqueous Component Databanks: Zn

		Available in Databank	
Alias	**Name**	**AQ**	**AQ9**
ZN(ALA)+	ZN(C3H6NO2)+	X	
ZN(ALA)2	ZN(C3H6NO3)2	X	
ZN(BUT)+	ZNCH3(CH2)2CO2+	X	
ZN(BUT)2	ZN(CH3CH2CH2CO2)2	X	
ZN(C2O4)2-2	ZN(C2O4)2--	X	X
ZN(CH3COO)3-	ZN(CH3COO)3-	X	
ZN(CH3COOH)+	ZN(CH3COO)+	X	
ZN(CH3COOH)2	ZN(CH3COO)2	X	
ZN(CHO2)2	ZINC-FORMATE	X	X
ZN(CHO2)3-	ZN(CHO2)3-	X	X
ZN(CHO2)4-2	ZN(CHO2)4--	X	X
ZN(CN)4-2	ZN(CN)4--	X	X
ZN(FOR)+	ZNCHO2+	X	
ZN(GLY)+	ZN(C2H4NO2)+	X	
ZN(GLY)2	ZN(C2H4NO2)2	X	
ZN(GLYC)+	ZNCH3OCO2+	X	
ZN(GLYC)2	ZN(CH3OCO2)2	X	
ZN(LAC)+	ZNCH3CH2OCO2+	X	
ZN(LAC)2	ZN(CH3CH2OCO2)2	X	
ZN(N2H4)2+2	ZN(N2H4)2++	X	X
ZN(N2H4)3+2	ZN(N2H4)3++	X	X
ZN(N2H4)4+2	ZN(N2H4)4++	X	X
ZN(NH3)2+2	ZN(NH3)2++	X	X
ZN(NH3)3+2	ZN(NH3)3++	X	X
ZN(NH3)4+2	ZN(NH3)4++	X	X

Alias	Name	Available in Databank AQ	AQ9
ZN(OH)2	ZINC-HYDROXIDE	X	X
ZN(OH)3-	ZN(OH)3-	X	X
ZN(OH)4-2	ZN(OH)4--	X	X
ZN(OH)CL	ZN(OH)CL	X	X
ZN(PENT)+	ZNCH3(CH2)3CO2+	X	
ZN(PENT)2	ZN(CH3CH2CH2CH2CO2)2	X	
ZN(PROP)+	ZNCH3CH2CO2+	X	
ZN(PROP)2	ZN(CH3CH2CO2)2	X	
ZN(SCN)2	ZINC-THIOCYANATE	X	X
ZN(SCN)4-2	ZN(CNS)4--	X	X
ZN+2	ZN++	X	X
ZNBR+	ZNBR+	X	X
ZNBR2	ZINC-BROMIDE	X	X
ZNBR3-	ZNBR3-	X	X
ZNC2O4	ZINC-OXALATE	X	X
ZNCL+	ZNCL+	X	X
ZNCL2	ZINC-CHLORIDE	X	X
ZNCL3-	ZNCL3-	X	X
ZNCL4-2	ZNCL4--	X	X
ZNCLO4+	ZNCLO4+	X	X
ZNF+	ZNF+	X	X
ZNI+	ZNI+	X	X
ZNI2	ZINC-IODIDE	X	X
ZNI3-	ZNI3-	X	X
ZNI4-2	ZNI4--	X	X
ZNN2H4+2	ZNN2H4++	X	X
ZNN3+	ZNN3+	X	X
ZNN6	ZINC-AZIDE	X	X
ZNNH3+2	ZNNH3++	X	X
ZNO2-2	ZNO2--	X	X
ZNOH+	ZNOH+	X	X
ZNSO4	ZINC-SULFATE	X	X

Aqueous Component Databanks: Zr

Alias	Name	Available in Databank AQ	AQ9
ZR(OH)2+2	ZR(OH)2++	X	X
ZR(OH)3+	ZR(OH)3+	X	X
ZR(OH)4	ZIRCONIUM-TETRAHYDROXIDE	X	X
ZR(SO4)2	ZIRCONIUM-DISULFATE	X	X
ZR(SO4)3-2	ZR(SO4)3--	X	X
ZR+4	ZR+4	X	X
ZROH+3	ZR(OH)+++	X	X
ZRSO4+2	ZRSO4++	X	X

Aqueous Component Databanks: Other Elements

Alias	Name	Available in Databank AQ	AQ9
AR	ARGON	X	X
ASO+	ASO+	X	X
ASO2-	ASO2-	X	X
ASO3F-2	ASO3F--	X	X
ASO4-3	ASO4---	X	X
BE(AC)+	BECH3COO+	X	
BE(AC)2	BE(CH3COO)2	X	
BE+2	BE++	X	X
BEO2-2	BEO2--	X	X
BI(AC)+2	BICH3COO+2	X	
BI(AC)2+	BI(CH3COO)2+	X	
BI(AC)3	BI(CH3COO)3	X	
F-	F-	X	X
HE-4	HELIUM-4	X	X
KR	KRYPTON	X	X
MOO4-2	MOO4--	X	X
NBO2+	NBO2+	X	X
NBO3-	NBO3-	X	X
NE	NEON	X	X
OSO4	OSMIUM-TETROXIDE	X	X
RA(AC)+	RACH3COO+	X	
RA(AC)2	RA(CH3COO)2	X	
RA+2	RA++	X	X
RE-	RE-	X	X
RECL6-2	RECL6--	X	X
REO4-	REO4-	X	X
RN	RADON	X	
RUO4	RUTHENIUM-TETROXIDE	X	X
SB(OH)3	ANTIMONY-TRIHYDROXIDE	X	X
SB2S4-2	SB2S4--	X	X
SBO+	SBO+	X	X
SBO2-	SBO2-	X	X
SE-2	SE--	X	X
SEO3-2	SEO3--	X	X
SEO4-2	SEO4--	X	X
SIF6-2	SIF6--	X	X
SIO2	SILICON-DIOXIDE	X	
SIO4-4	SIO4----	X	X
TAO2+	TAO2+	X	X
TAO3-	TAO3-	X	X
TE(OH)3+	TE(OH)3+	X	X
WO4-2	WO4--	X	X
XE	XENON	X	X

Combust Component Databank

The COMBUST component databank contains data for these parameters:

Parameter Name	Description
CPIG	Ideal gas heat capacity coefficients
DGFORM	Standard free energy of formation
DHFORM	Standard enthalpy of formation
MW	Molecular weight
NATOM	Vector containing numbers of C, H, O, N, S, F, Cl, Br, I, Ar and He atoms

The table below lists the components present in the COMBUST component databank.

Alias	Name
AR	ARGON
BR	BROMINE-MONATOMIC-GAS
BR2	BROMINE
C	CARBON-GRAPHITE
C-2	CARBON-DIATOMIC-GAS
C-S	CARBON-MONOSULFIDE-GAS
C2H2	ACETYLENE
C2H4	ETHYLENE
C2N2	CYANOGEN
C3O2	CARBON-SUBOXIDE
CCL4	CARBON-TETRACHLORIDE
CH	METHYLIDYNE-GAS
CH2	METHYLENE-GAS
CH2CL2	DICHLOROMETHANE
CH2O	FORMALDEHYDE
CH3	METHYL-GAS
CH3CL	METHYL-CHLORIDE
CH4	METHANE
CHCL3	CHLOROFORM
CHN	HYDROGEN-CYANIDE
CHO	FORMYL-GAS
CL	CHLORINE-MONATOMIC-GAS
CL2	CHLORINE
CN	CYANO-GAS
CNO	NCO-RADICAL
CO	CARBON-MONOXIDE
CO2	CARBON-DIOXIDE
COS	CARBONYL-SULFIDE
CS2	CARBON-DISULFIDE

Alias	Name
F	FLUORINE-MONATOMIC-GAS
F2	FLUORINE
H	HYDROGEN-MONATOMIC-GAS
H2	HYDROGEN
H2N	AMIDOGEN
H2O	WATER
H2S	HYDROGEN-SULFIDE
H3N	AMMONIA
HBR	HYDROGEN-BROMIDE
HCL	HYDROGEN-CHLORIDE
HE-4	HELIUM-4
HF	HYDROGEN-FLUORIDE
HI	HYDROGEN-IODIDE
HNO	NITROXYL
HO2	HYDROPEROXYL
HS	HYDROGEN-MONOSULFIDE-GAS
I	IODINE-MONATOMIC-GAS
I2	IODINE
N	NITROGEN-MONATOMIC-GAS
N2	NITROGEN
N2O	NITROUS-OXIDE
NH	IMIDOGEN-GAS
NO	NITRIC-OXIDE
NO2	NITROGEN-DIOXIDE
O	OXYGEN-MONATOMIC-GAS
O2	OXYGEN
O2S	SULFUR-DIOXIDE
OH	HYDROXYL-GAS
S2	SULFUR-DIATOMIC-GAS
SO	SULFUR-MONOXIDE-GAS

Ethylene Component Databank

The ETHYLENE component databank contains data for these parameters:

Property	Description
SRKAIJ	Binary interaction parameter for the SRK equation of state model
SRKBIJ	Binary interaction parameter for the SRK equation of state model
SRKOMG	Acentric factor for the SRK equation of state
SRKPC	Critical pressure for the SRK equation of state
SRKTC	Critical temperature for the SRK equation of state

The table below lists the components present in the ETHYLENE component databank.

Alias	Name
AR	ARGON
CCL2F2	DICHLORODIFLUOROMETHANE
CH4	METHANE
CO	CARBON-MONOXIDE
CO2	CARBON-DIOXIDE
C2H2	ACETYLENE
C2H4	ETHYLENE
C2H6	ETHANE
C3H4-1	PROPADIENE
C3H4-2	METHYL-ACETYLENE
C3H6-2	PROPYLENE
C3H7NO	N,N-DIMETHYLFORMAMIDE
C3H8	PROPANE
C4H10-1	N-BUTANE
C4H10-2	ISOBUTANE
C4H4	VINYLACETYLENE
C4H6-4	1,3-BUTADIENE
C4H8-1	1-BUTENE
C4H8-2	CIS-2-BUTENE
C4H8-3	TRANS-2-BUTENE
C4H8-5	ISOBUTYLENE
C5H10-1	CYCLOPENTANE
C5H10-2	1-PENTENE
C5H12-1	N-PENTANE
C5H12-2	2-METHYL-BUTANE
C5H6	CYCLOPENTADIENE
C5H8	CIS-1,3-PENTADIENE
C5H8-1	CYCLOPENTENE
C5H8-3	1-TRANS-3-PENTADIENE

Alias	Name
C5H8-4	1,4-PENTADIENE
C5H8-6	2-METHYL-1,3-BUTADIENE
C6H10-2	CYCLOHEXENE
C6H12-1	CYCLOHEXANE
C6H12-3	1-HEXENE
C6H14-1	N-HEXANE
C6H14-5	2,3-DIMETHYL-BUTANE
C6H6	BENZENE
C7H14-6	METHYLCYCLOHEXANE
C7H14-7	1-HEPTENE
C7H16-1	N-HEPTANE
C7H16-2	2-METHYLHEXANE
C7H8	TOLUENE
C8H10-2	M-XYLENE
C8H10-4	ETHYLBENZENE
C8H16-1	1,1-DIMETHYLCYCLOHEXANE
C8H16-16	1-OCTENE
C8H18-1	N-OCTANE
C8H18-2	2-METHYLHEPTANE
C8H8	STYRENE
C9H10	ALPHA-METHYL-STYRENE
C9H12-5	1-METHYL-4-ETHYLBENZENE
C9H18-1	N-PROPYLCYCLOHEXANE
C9H18-3	1-NONENE
C9H20-1	N-NONANE
C9H20-D1	2-METHYLOCTANE
C9H8	INDENE
C10H14-9	1,2,4,5-TETRAMETHYLBENZENE
C10H20-1	N-BUTYLCYCLOHEXANE
C10H20-5	1-DECENE
C10H22-1	N-DECANE
C10H8	NAPHTHALENE
C11H10-1	1-METHYLNAPHTHALENE
C11H22-2	1-UNDECENE
C11H24	N-UNDECANE
C12H18-D2	P-DIISOPROPYLBENZENE
C12H24-2	1-DODECENE
C12H26	N-DODECANE
C13H10	FLUORENE
C13H26-2	1-TRIDECENE
C13H28	N-TRIDECANE
C14H10-1	ANTHRACENE
C14H28-2	1-TETRADECENE
C14H30	N-TETRADECANE
C15H24	N-NONYLBENZENE
C15H32	N-PENTADECANE
C16H12	1-PHENYLNAPHTHALENE

Alias	Name
C18H12	CHRYSENE
C20H16	TRIPHENYLETHYLENE
C26H20	TETRAPHENYLETHYLENE
H2	HYDROGEN
H2O	WATER
H2S	HYDROGEN-SULFIDE
N2	NITROGEN
O2	OXYGEN
O2S	SULFUR-DIOXIDE

SRKAIJ and SRKBIJ are used to compute the interaction parameter using this equation:

$$k_{ij} = a_{ij} + b_{ij}T$$

Where:

k_{ij} = Binary interaction parameter

a_{ij} = SRKAIJ

b_{ij} = SRKBIJ

T = Temperature

Inorganic Component Databank

The tables below list the components present in the INORGANIC component databank.

Components beginning with:

Ag	Al	As	Au	B	Ba	Be	Bi	C	Ca
Cd	Ce	Cl	Co	Cr	Cs	Cu	Dy	Er	Eu
Fe	Ga	Gd	Ge	H	Hf	Hg	Ho	In	Ir
K	La	Li	Mg	Mn	Mo	N	Na	Nb	Nd
Ni	Np	O	Os	P	Pb	Pd	Pr	Pt	Pu
Rb	Re	Rh	Ru	S	Sb	Sc	Se	Si	Sm
Sn	Sr	Ta	Tb	Te	Th	Ti	Tl	Tm	U
V	W	Y	Yb	Zn	Zr	Other Elements			

INORGANIC Component Databank Parameters

Parameter Name	Description
ATOMNO	Vector containing the atom types (atomic numbers) for a given molecule (e.g., H=1, C=6, O=8). Must use the vector NOATOM to define the number of occurrences of each atom.
CPIXP1	Ideal gas property parameters range 1
CPIXP2	Ideal gas property parameters range 2
CPIXP3	Ideal gas property parameters range 3
CPLXP1	Liquid property parameters range 1
CPLXP2	Liquid property parameters range 2
CPSXP1	Solid property parameters range 1
CPSXP2	Solid property parameters range 2
CPSXP3	Solid property parameters range 3
CPSXP4	Solid property parameters range 4
CPSXP5	Solid property parameters range 5
CPSXP6	Solid property parameters range 6
CPSXP7	Solid property parameters range 7
MW	Molecular weight
NOATOM	Vector containing the number of occurrences of each atom defined in ATOMNO for a given molecule. ATOMNO and NOATOM define the chemical formula of the molecule.
TB	Normal boiling temperature
TFP	Normal freezing temperature
VSPOLY	Molar volume parameters of solid

The properties enthalpy, entropy, Gibbs free energy and heat capacity can be calculated from the ideal gas, liquid, and solid parameters with names beginning with CP.

ATOMNO and NOATOM together form the chemical formula of the compound. They are used to calculate molecular weight and are used in RGIBBS.

INORGANIC Component Databank: Ag

Alias	Name
AG	SILVER
AG2CO3	SILVER-CARBONATE
AG2CRO4	SILVER-CHROMATE
AG2O	SILVER-OXIDE
AG2S	SILVER-SULFIDE
AG2S:A	SILVER-SULFIDE:SOL-A
AG2S:B	SILVER-SULFIDE:SOL-B
AG2S:C	SILVER-SULFIDE:SOL-C
AG2SE	SILVER-SELENIDE
AG2SE:A	SILVER-SELENIDE:SOL-A
AG2SE:B	SILVER-SELENIDE:SOL-B
AG2SE:C	SILVER-SELENIDE:SOL-C
AG2SO4	SILVER-SULFATE
AG2SO4:A	SILVER-SULFATE:SOL-A
AG2SO4:B	SILVER-SULFATE:SOL-B
AG2TE	SILVER-TELLURIDE
AG2TE:A	SILVER-TELLURIDE:SOL-A
AG2TE:B	SILVER-TELLURIDE:SOL-B
AG2WO4	SILVER-TUNGSTATE
AG3ASO4	SILVER-ARSENATE
AGBR	SILVER-BROMIDE
AGBRO3	SILVER-BROMATE
AGCL	SILVER-CHLORIDE
AGCLO3	SILVER-CHLORATE
AGCN	SILVER-CYANIDE
AGF	SILVER-FLUORIDE
AGI	SILVER-IODIDE
AGI:A	SILVER-IODIDE:SOL-A
AGI:B	SILVER-IODIDE:SOL-B
AGNO3	SILVER-NITRATE
AGNO3:A	SILVER-NITRATE:SOL-A
AGNO3:B	SILVER-NITRATE:SOL-B
AGP2	SILVER-DIPHOSPHIDE
AGP3	SILVER-TRIPHOSPHIDE

INORGANIC Component Databank: AI

Alias	Name
AL	ALUMINIUM
AL(OH)3-A	ALUMINIUM-HYDROXIDE-AMORPHOUS
AL18B4O33	18-ALUMINIUM-4-BORON-33-OXIDE
AL2(SO4)3	ALUMINIUM-SULFATE
AL2BR6	DIALUMINIUM-HEXABROMIDE-GAS
AL2CA	2-ALUMINIUM-CALCIUM
AL2CE	2-ALUMINIUM-CERIUM
AL2CL6	DIALUMINIUM-HEXACHLORIDE-GAS
AL2F6	DIALUMINIUM-HEXAFLUORIDE-GAS
AL2I6	DIALUMINIUM-HEXAIODIDE-GAS
AL2LA	2-ALUMINIUM-LANTHANUM
AL2O	DIALUMINIUM-OXIDE-GAS
AL2O2	DIALUMINIUM-DIOXIDE-GAS
AL2O3	ALUMINIUM-OXIDE-ALPHA-CORUNDUM
AL2O3*3H2O	GIBBSITE
AL2O3*H2O	DIASPORE
AL2O3*H2O-B	BOEHMITE
AL2O3-C	ALUMINIUM-OXIDE-GAMMA
AL2O3-D	ALUMINIUM-OXIDE-DELTA
AL2O3-K	ALUMINIUM-OXIDE-KAPPA
AL2S3	ALUMINIUM-SULFIDE
AL2SE2	DIALUMINIUM-DISELENIDE-GAS
AL2SE3	ALUMINIUM-SELENIDE
AL2SIO5	ALUMINIUM-SILICATE-KYANITE
AL2SIO5-A	ALUMINIUM-SILICATE-ANDALUSITE
AL2SIO5-S	ALUMINIUM-SILICATE-SILLIMANITE
AL2TE3	ALUMINIUM-TELLURIDE
AL2TIO5	DIALUMINIUM-TITANIUM-PENTAOXIDE
AL2U	2-ALUMINIUM-URANIUM
AL3NI	3-ALUMINIUM-NICKEL
AL3NI2	3-ALUMINIUM-2-NICKEL
AL3TH	3-ALUMINIUM-THORIUM
AL3TI	3-ALUMINIUM-TITANIUM
AL3U	3-ALUMINIUM-URANIUM
AL4B2O9	4-ALUMINIUM-2-BORON-9-OXIDE
AL4C3	TETRAALUMINIUM-TRICARBIDE
AL4CA	4-ALUMINIUM-CALCIUM
AL4CE	4-ALUMINIUM-CERIUM
AL4MG2SI5O18	CORDIERITE
AL4U	4-ALUMINIUM-URANIUM
AL5CO2	5-ALUMINIUM-2-COBALT
AL6SI2O13	MULLITE
ALAS	ALUMINIUM-ARSENIDE
ALASO4	ALUMINIUM-ARSENATE
ALB12	ALUMINIUM-DODECABORIDE
ALB2	ALUMINIUM-DIBORIDE
ALBR	ALUMINIUM-MONOBROMIDE-GAS

Alias	Name
ALBR3	ALUMINIUM-BROMIDE
ALCL	ALUMINIUM-MONOCHLORIDE-GAS
ALCL2	ALUMINIUM-DICHLORIDE-GAS
ALCL3	ALUMINIUM-CHLORIDE
ALCL3*6H2O	ALUMINIUM-CHLORIDE-HEXAHYDRATE
ALCO	ALUMINIUM-COBALT
ALF	ALUMINIUM-MONOFLUORIDE-GAS
ALF2	ALUMINIUM-DIFLUORIDE-GAS
ALF3	ALUMINIUM-FLUORIDE
ALF3:A	ALUMINIUM-FLUORIDE:SOL-A
ALF3:B	ALUMINIUM-FLUORIDE:SOL-B
ALH3	ALUMINIUM-HYDRIDE-HEXAGONAL
ALI3	ALUMINIUM-IODIDE
ALLI	ALUMINIUM-LITHIUM
ALN	ALUMINIUM-NITRIDE
ALNI	ALUMINIUM-NICKEL
ALNI3	ALUMINIUM-3-NICKEL
ALO	ALUMINIUM-MONOXIDE-GAS
ALO(OH)	BOEHMITE-ALO(OH)
ALO2	ALUMINIUM-DIOXIDE-GAS
ALOCL	ALUMINIUM-CHLORIDE-OXIDE
ALOF	ALUMINIUM-FLUORIDE-OXIDE-GAS
ALOF2	ALUMINIUM-DIFLUORIDE-OXIDE-GAS
ALP	ALUMINIUM-PHOSPHIDE
ALPO4	ALUMINIUM-PHOSPHATE
ALPO4:A	ALUMINIUM-PHOSPHATE:SOL-A
ALPO4:B	ALUMINIUM-PHOSPHATE:SOL-B
ALPO4:C	ALUMINIUM-PHOSPHATE:SOL-C
ALS	ALUMINIUM-MONOSULFIDE-GAS
ALSB	ALUMINIUM-ANTIMONY
ALTE	ALUMINIUM-MONOTELLURIDE-GAS
ALTI	ALUMINIUM-TITANIUM

INORGANIC Component Databank: As

Alias	Name
AS	ARSENIC
AS-2	ARSENIC-DIATOMIC
AS-3	ARSENIC-TRIATOMIC
AS-4	ARSENIC-4-ATOMIC
AS2O3-A	ARSENIC-OXIDE-ARSENOLITE
AS2O3-C	ARSENIC-OXIDE-CLAUDETITE
AS2O5	DIARSENIC-PENTAOXIDE
AS2S2	DIARSENIC-DISULFIDE
AS2S3	ARSENIC-SULFIDE
AS2S3:1	ARSENIC-SULFIDE:SOL-1
AS2S3:2	ARSENIC-SULFIDE:SOL-2
AS2SE3	ARSENIC-SELENIDE
AS2TE3	ARSENIC-TELLURIDE

Alias	Name
AS4O6	TETRAARSENIC-HEXAOXIDE-GAS
AS4S4	TETRAARSENIC-TETRASULFIDE
AS4S4-R	TETRAARSENIC-TETRASULFIDE-REALGA
ASBR3	ARSENIC-BROMIDE-GAS
ASCL3	ARSENIC-CHLORIDE
ASF3	ARSENIC-FLUORIDE
ASF5	ARSENIC-PENTAFLUORIDE-GAS
ASH3	ARSINE
ASI3	ARSENIC-IODIDE
ASO	ARSENIC-MONOXIDE-GAS
ASS	ARSENIC-MONOSULFIDE-GAS
ASSE	ARSENIC-MONOSELENIDE-GAS
ASTE	ARSENIC-MONOTELLURIDE-GAS

INORGANIC Component Databank: Au

Alias	Name
AU	GOLD
AU(OH)3-P	GOLD-TRIHYDROXIDE-PRECIPITATED
AU2O3	DIGOLD-TRIOXIDE
AU2P3	DIGOLD-TRIPHOSPHIDE
AU3ASO4	TRIGOLD-ARSENATE
AUBR	GOLD-MONOBROMIDE
AUCD	GOLD-CADMIUM
AUCL	GOLD-MONOCHLORIDE
AUCL3	GOLD-TRICHLORIDE
AUCU	GOLD-COPPER
AUCU3	GOLD-3-COPPER
AUCU3:11	GOLD-3-COPPER:SA-11
AUCU3:A	GOLD-3-COPPER:SOL-A
AUCU:12	GOLD-COPPER:SA-12
AUCU:22	GOLD-COPPER:SA-22
AUCU:A	GOLD-COPPER:SOL-A
AUF3	GOLD-TRIFLUORIDE
AUI	GOLD-MONOIODIDE
AUS	GOLD-MONOSULFIDE-GAS
AUSB2	GOLD-2-ANTIMONY
AUSE	GOLD-MONOSELENIDE-ALPHA
AUSE-B	GOLD-MONOSELENIDE-BETA
AUSN	GOLD-TIN
AUSN2	GOLD-2-TIN
AUSN4	GOLD-4-TIN
AUTE2	GOLD-DITELLURIDE

INORGANIC Component Databank: B

Alias	Name
B-B	BORON-BETA
B-GL	BORON-GLASS
B-I	BORON-MONOIODIDE-GAS
B-I2	BORON-DIIODIDE-GAS
B-I3	BORON-TRIIODIDE-GAS
B2H6	DIBORANE
B2O3	BORON-OXIDE
B2O3-GL	BORON-OXIDE-GLASS
B2S3	DIBORON-TRISULFIDE
B4C	TETRABORON-MONOCARBIDE
BBR	BORON-MONOBROMIDE-GAS
BBR2	BORON-DIBROMIDE-GAS
BBR3	BORON-TRIBROMIDE
BCL	BORON-MONOCHLORIDE-GAS
BCL2	BORON-DICHLORIDE-GAS
BCL3	BORON-TRICHLORIDE
BF	BORON-MONOFLUORIDE-GAS
BF2	BORON-DIFLUORIDE-GAS
BF3	BORON-TRIFLUORIDE
BH	BORON-MONOHYDRIDE-GAS
BN	BORON-NITRIDE
BOCL	BORON-CHLORIDE-OXIDE-GAS
BP	BORON-MONOPHOSPHIDE
BS	BORON-MONOSULFIDE-GAS

INORGANIC Component Databank: Ba

Alias	Name
BA	BARIUM
BA(NO3)2	BARIUM-NITRATE
BA(OH)2	BARIUM-HYDROXIDE
BA(OH)2:A	BARIUM-HYDROXIDE:SOL-A
BA(OH)2:B	BARIUM-HYDROXIDE:SOL-B
BA2SI3O8	DIBARIUM-TRISILICATE
BA2SIO4	BARIUM-ORTHOSILICATE
BA2SN	2-BARIUM-TIN
BA2TIO4	DIBARIUM-TITANIUM-TETRAOXIDE
BA3(ASO4)2	BARIUM-ARSENATE
BA3AL2O6	TRIBARIUM-DIALUMINIUM-HEXAOXIDE
BA3N2	TRIBARIUM-DINITRIDE
BAAL2O4	BARIUM-DIALUMINIUM-TETRAOXIDE
BABR2	BARIUM-BROMIDE
BAC2	BARIUM-DICARBIDE
BACL	BARIUM-MONOCHLORIDE-GAS
BACL2	BARIUM-CHLORIDE
BACL2:1	BARIUM-CHLORIDE:SOL-1
BACL2:2	BARIUM-CHLORIDE:SOL-2
BACO3	BARIUM-CARBONATE
BACO3:A	BARIUM-CARBONATE:SOL-A

Alias	Name
BACO3:B	BARIUM-CARBONATE:SOL-B
BACO3:C	BARIUM-CARBONATE:SOL-C
BACRO4	BARIUM-CHROMATE
BAF	BARIUM-MONOFLUORIDE-GAS
BAF2	BARIUM-FLUORIDE
BAF2:A	BARIUM-FLUORIDE:SOL-A
BAF2:B	BARIUM-FLUORIDE:SOL-B
BAF2:C	BARIUM-FLUORIDE:SOL-C
BAH	BARIUM-MONOHYDRIDE-GAS
BAH2	BARIUM-HYDRIDE
BAH2:1	BARIUM-HYDRIDE:SOL-1
BAH2:2	BARIUM-HYDRIDE:SOL-2
BAHFO3	BARIUM-HAFNIUM-TRIOXIDE
BAI	BARIUM-MONOIODIDE-GAS
BAI2	BARIUM-IODIDE
BAMOO4	BARIUM-MOLYBDATE
BAO	BARIUM-OXIDE
BAO2	BARIUM-PEROXIDE
BAS	BARIUM-SULFIDE
BASI2O5	BARIUM-DISILICATE
BASIO3	BARIUM-METASILICATE
BASO4	BARIUM-SULFATE
BASO4:1	BARIUM-SULFATE:SOL-1
BASO4:2	BARIUM-SULFATE:SOL-2
BATE	BARIUM-TELLURIDE
BATIO3	BARIUM-TITANIUM-TRIOXIDE
BATIO3:1	BARIUM-TITANIUM-TRIOXIDE:SOL-1
BATIO3:2	BARIUM-TITANIUM-TRIOXIDE:SOL-2
BATIO3:3	BARIUM-TITANIUM-TRIOXIDE:SOL-3
BAUO4	BARIUM-URANATE
BAWO4	BARIUM-TUNGSTATE
BAZRO3	BARIUM-ZIRCONIUM-TRIOXIDE

INORGANIC Component Databank: Be

Alias	Name
BE	BERYLLIUM
BE(OH)2	BERYLLIUM-HYDROXIDE-ALPHA
BE(OH)2-B	BERYLLIUM-HYDROXIDE-BETA
BE2C	DIBERYLLIUM-CARBIDE
BE2CL4	DIBERYLLIUM-TETRACHLORIDE-GAS
BE2SIO4	BERYLLIUM-SILICATE-PHENACITE
BE3(ASO4)2	BERYLLIUM-ARSENATE
BE3B2O6	TRIBERYLLIUM-DIBORATE
BE3N2	ALPHA-BERYLLIUM-NITRIDE
BEAL2O4	BERYLLIUM-DIALUMINIUM-TETRAOXIDE
BEAL6O10	BERYLLIUM-HEXAALUMINIUM-DECAOXID
BEBR	BERYLLIUM-MONOBROMIDE-GAS

Alias	Name
BEBR2	BERYLLIUM-BROMIDE
BECL	BERYLLIUM-MONOCHLORIDE-GAS
BECL2	BERYLLIUM-CHLORIDE
BECL2:A	BERYLLIUM-CHLORIDE:SOL-A
BECL2:B	BERYLLIUM-CHLORIDE:SOL-B
BEF	BERYLLIUM-MONOFLUORIDE-GAS
BEF2	BERYLLIUM-FLUORIDE
BEF2:2	BERYLLIUM-FLUORIDE:SOL-2
BEF2:A	BERYLLIUM-FLUORIDE:SOL-A
BEH	BERYLLIUM-MONOHYDRIDE-GAS
BEI	BERYLLIUM-MONOIODIDE-GAS
BEI2	BERYLLIUM-IODIDE
BEO	BERYLLIUM-OXIDE
BEO:A	BERYLLIUM-OXIDE:SOL-A
BEO:B	BERYLLIUM-OXIDE:SOL-B
BEOH	BERYLLIUM-MONOHYDROXIDE-GAS
BES	BERYLLIUM-SULFIDE
BESO4	BERYLLIUM-SULFATE
BESO4*2H2O	BERYLLIUM-SULFATE-DIHYDRATE
BESO4*4H2O	BERYLLIUM-SULFATE-TETRAHYDRATE
BESO4:A	BERYLLIUM-SULFATE:SOL-A
BESO4:B	BERYLLIUM-SULFATE:SOL-B
BESO4:C	BERYLLIUM-SULFATE:SOL-C
BEWO4	BERYLLIUM-TUNGSTATE

INORGANIC Component Databank: Bi

Alias	Name
BI	BISMUTH
BI2	BISMUTH-DIATOMIC-GAS
BI2(SO4)3	BISMUTH-SULFATE
BI2O3	BISMUTH-OXIDE
BI2O3:A	BISMUTH-OXIDE:SOL-A
BI2O3:B	BISMUTH-OXIDE:SOL-B
BI2S3	BISMUTH-SULFIDE
BI2SE3	BISMUTH-SELENIDE
BI2TE3	BISMUTH-TELLURIDE
BI2U	2-BISMUTH-URANIUM
BI4U3	4-BISMUTH-3-URANIUM
BIASO4	BISMUTH-ARSENATE
BIBR	BISMUTH-MONOBROMIDE-GAS
BIBR3	BISMUTH-BROMIDE
BIBR3:A	BISMUTH-BROMIDE:SOL-A
BIBR3:B	BISMUTH-BROMIDE:SOL-B
BICL	BISMUTH-MONOCHLORIDE-GAS
BICL3	BISMUTH-CHLORIDE
BIF	BISMUTH-MONOFLUORIDE-GAS
BIF3	BISMUTH-FLUORIDE
BII	BISMUTH-MONOIODIDE

	Alias	Name
	BII3	BISMUTH-IODIDE
	BII:A	BISMUTH-MONOIODIDE:SOL-A
	BII:B	BISMUTH-MONOIODIDE:SOL-B
	BIK3	BISMUTH-3-POTASSIUM
	BIK3:A	BISMUTH-3-POTASSIUM:SOL-A
	BIK3:B	BISMUTH-3-POTASSIUM:SOL-B
	BIMN	BISMUTH-MANGANESE
	BINI	BISMUTH-NICKEL
	BIOCL	BISMUTH-CHLORIDE-OXIDE
	BIU	BISMUTH-URANIUM
INORGANIC Component Databank: C	**Alias**	**Name**
	C	CARBON-GRAPHITE
	C-2	CARBON-DIATOMIC-GAS
	C-3	CARBON-TRIATOMIC-GAS
	C-D	CARBON-DIAMOND
	C-F	FLUOROMETHYLIDYNE-GAS
	C-S	CARBON-MONOSULFIDE-GAS
	C2CL4	TETRACHLOROETHYLENE
	C2CL6	HEXACHLOROETHANE
	C2F4	PERFLUOROETHENE
	C2F6	PERFLUOROETHANE
	C2H2	ACETYLENE
	C2H2O	KETENE
	C2H3CL	VINYL-CHLORIDE
	C2H4	ETHYLENE
	C2H4O-1	ACETALDEHYDE
	C2H5CL	ETHYL-CHLORIDE
	C2H6	ETHANE
	C2N2	CYANOGEN
	C3H4-1	PROPADIENE
	C3H4-2	METHYL-ACETYLENE
	C3H6-1	CYCLOPROPANE
	C3H6-2	PROPYLENE
	C3H8	PROPANE
	C4H10-1	N-BUTANE
	C4H6-1	1-BUTYNE
	C4H8-4	CYCLOBUTANE
	C4H8-5	ISOBUTYLENE
	C5H10-1	CYCLOPENTANE
	C5H12-1	N-PENTANE
	C5H8-1	CYCLOPENTENE
	C5H8-2	1,2-PENTADIENE
	C6H6O	PHENOL
	C8H14-D1	1-OCTYNE
	C9H16	NON-1-YNE
	CBR	BROMOMETHYLIDYNE-GAS

Alias	Name
CBR4	TETRABROMOMETHANE-GAS
CCL	CHLOROMETHYLIDYNE-GAS
CCL2	DICHLOROMETHYLENE-GAS
CCL2O	PHOSGENE
CCL3	TRICHLOROMETHYL-GAS
CF2	DIFLUOROMETHYLENE-GAS
CF3	TRIFLUOROMETHYL-GAS
CF4	CARBON-TETRAFLUORIDE
CH	METHYLIDYNE-GAS
CH2	METHYLENE-GAS
CH2CL2	DICHLOROMETHANE
CH2O	FORMALDEHYDE
CH3	METHYL-GAS
CH3CL	METHYL-CHLORIDE
CH4	METHANE
CHCL3	CHLOROFORM
CHN	HYDROGEN-CYANIDE
CHO	FORMYL-GAS
CN	CYANO-GAS
CN2	CARBON-NITRIDE-NCN-RADICAL-GAS
CO	CARBON-MONOXIDE
CO2	CARBON-DIOXIDE
COCL	CARBONYL-CHLORIDE-GAS
COF	CARBONYL-FLUORIDE-GAS
COF2-G	CARBONIC-DIFLUORIDE-GAS
COS	CARBONYL-SULFIDE
CS2	CARBON-DISULFIDE

INORGANIC Component Databank: Ca

Alias	Name
CA	CALCIUM
CA(NO3)2	CALCIUM-NITRATE
CA(OCL)CL	CALCIUM-CHLORIDE-HYPOCHLORITE
CA(OH)2	CALCIUM-HYDROXIDE
CA(VO3)2	CALCIUM-METAVANADATE
CA12AL14O33	(CAO)12*7AL2O3
CA2AL2O5	(CAO)2*AL2O3
CA2AL2SIO7	GEHLENITE
CA2B2O5	DICALCIUM-DIBORATE
CA2B2O5:A	DICALCIUM-DIBORATE:SOL-A
CA2B2O5:B	DICALCIUM-DIBORATE:SOL-B
CA2FE2O5	DICALCIUM-DIIRON-PENTAOXIDE
CA2MGSI2O7	AKERMANITE
CA2P2O7	CALCIUM-PYROPHOSPHATE
CA2P2O7:A	CALCIUM-PYROPHOSPHATE:SOL-A
CA2P2O7:B	CALCIUM-PYROPHOSPHATE:SOL-B
CA2P2O7:C	CALCIUM-PYROPHOSPHATE:SOL-C
CA2PB	2-CALCIUM-LEAD

Alias	Name
CA2SI	2-CALCIUM-SILICON
CA2SI3*5:2W	2-CALCIUM-3-SILICATE-5:2-HYDRATE
CA2SIO4	OLIVINE
CA2SIO4*7:6W	CALCIUM-ORTHOSILICATE-7:6-HYDRAT
CA2SIO4-B	LARNITE
CA2SIO4:A	OLIVINE:SOL-A
CA2SIO4:A1	OLIVINE:SOL-A1
CA2SIO4:C	OLIVINE:SOL-C
CA2SN	2-CALCIUM-TIN
CA2V2O7	CALCIUM-PYROVANADATE
CA3(ASO4)2	CALCIUM-ARSENATE
CA3(PO4)2	CALCIUM-PHOSPHATE
CA3(VO4)2	CALCIUM-ORTHOVANADATE
CA3AL2O6	(CAO)3*AL2O3
CA3AL2O6*6W	(CAO)3*AL2O3*6H2O
CA3AL2SI3O12	GROSSULAR
CA3B2O6	TRICALCIUM-DIBORATE
CA3MGSI2O8	MERWINITE
CA3N2	TRICALCIUM-DINITRIDE
CA3P2	TRICALCIUM-DIPHOSPHIDE
CA3PO4-2:1	CALCIUM-PHOSPHATE:SOL-1
CA3PO4-2:A	CALCIUM-PHOSPHATE:SOL-A
CA3PO4-2:B	CALCIUM-PHOSPHATE:SOL-B
CA3SB2	3-CALCIUM-2-ANTIMONY
CA3SI2O7	TRICALCIUM-DISILICATE-RANKINITE
CA3SI2O7*3W	TRICALCIUM-DISILICATE-TRIHYDRATE
CA3SIO5	TRICALCIUM-SILICATE
CA3TI2O7	(CAO)3*2TIO2
CA3WO6	CALCIUM-ORTHOTUNGSTATE
CA4SI3*3:2W	4-CALCIUM-3-SILICATE-3:2-HYDRATE
CA4TI3O10	4-CALCIUM-3-TITANIUM-10-OXIDE
CA5SI6*11:2W	5-CALCIUM-6-SILICATE-5.5-HYDRA
CA5SI6*21:2W	5-CALCIUM-6-SILICATE-10.5-HYDR
CA5SI6O17*3W	5-CALCIUM-6-SILICATE-3-HYDRATE
CA6SI6O18*W	6-CALCIUM-6-SILICATE-HYDRATE
CA:A	CALCIUM:SOL-A
CA:B	CALCIUM:SOL-B
CAAL2O4	CAO*AL2O3
CAAL2SI2O8	ANORTHITE
CAAL2SIO6	PYROXENE
CAAL4O7	CAO*2AL2O3
CAB2O4	CALCIUM-DIBORATE
CAB4O7	CALCIUM-TETRABORATE
CABR	CALCIUM-MONOBROMIDE-GAS
CABR2	CALCIUM-BROMIDE
CAC2	CALCIUM-DICARBIDE
CAC2:A	CALCIUM-DICARBIDE:SOL-A

Alias	Name
CAC2:B	CALCIUM-DICARBIDE:SOL-B
CACL	CALCIUM-MONOCHLORIDE-GAS
CACL2	CALCIUM-CHLORIDE
CACN2	CALCIUM-CYANAMIDE
CACO3	CALCIUM-CARBONATE-CALCITE
CACO3-A	CALCIUM-CARBONATE-ARAGONITE
CAF	CALCIUM-MONOFLUORIDE-GAS
CAF2	CALCIUM-FLUORIDE
CAF2:A	CALCIUM-FLUORIDE:SOL-A
CAF2:B	CALCIUM-FLUORIDE:SOL-B
CAFE2O4	CALCIUM-DIIRON-TETRAOXIDE
CAH	CALCIUM-MONOHYDRIDE-GAS
CAH2	CALCIUM-HYDRIDE
CAH2:A	CALCIUM-HYDRIDE:SOL-A
CAH2:B	CALCIUM-HYDRIDE:SOL-B
CAHFO3	CALCIUM-HAFNIUM-TRIOXIDE
CAHPO4	CALCIUM-HYDROGEN-PHOSPHATE
CAHPO4*2H2O	CALCIUM-HYDROGEN-PHOSPHATE-DIHYD
CAI	CALCIUM-MONOIODIDE-GAS
CAI2	CALCIUM-IODIDE
CAMG(CO3)2	DOLOMITE
CAMG2	CALCIUM-2-MAGNESIUM
CAMGO2	CALCIUM-MAGNESIUM-DIOXIDE
CAMGSI2O6	DIOPSIDE
CAMGSIO4	MONTICELLITE
CAMOO4	CALCIUM-MOLYBDATE
CANO3*2*2H2O	CALCIUM-NITRATE-DIHYDRATE
CANO3*2*3H2O	CALCIUM-NITRATE-TRIHYDRATE
CANO3*2*4H2O	CALCIUM-NITRATE-TETRAHYDRATE
CAO	CALCIUM-OXIDE
CAO2	CALCIUM-PEROXIDE
CAOH	CALCIUM-MONOHYDROXIDE-GAS
CAPB	CALCIUM-LEAD
CAS	CALCIUM-SULFIDE
CASE	CALCIUM-SELENIDE
CASI	CALCIUM-SILICON
CASI2	CALCIUM-2-SILICON
CASI2O5*2H2O	CALCIUM-2-SILICATE-2-HYDRATE
CASIO3	WOLLASTONITE
CASIO3-B	PSEUDOWOLLASTONITE
CASN	CALCIUM-TIN
CASO3	CALCIUM-SULFITE
CASO3*1:2W	CALCIUM-SULFITE-HEMIHYDRATE
CASO4	CALCIUM-SULFATE
CASO4*1:2W:A	CALCIUM-SULFATE-HEMIHYDRATE:S-A

Alias	Name
CASO4*2H2O	CALCIUM-SULFATE-DIHYDRATE-GYPSUM
CASO4:1	CALCIUM-SULFATE:SOL-1
CASO4:2	CALCIUM-SULFATE:SOL-2
CATE	CALCIUM-TELLURIDE
CATIO3-P	PEROVSKITE
CATIO3:A	PEROVSKITE:SOL-A
CATIO3:B	PEROVSKITE:SOL-B
CATISIO5	SPHENE
CAUO4	CALCIUM-URANATE
CAUO4:A	CALCIUM-URANATE:SOL-A
CAUO4:B	CALCIUM-URANATE:SOL-B
CAWO4	CALCIUM-TUNGSTATE
CAZN	CALCIUM-ZINC
CAZN2	CALCIUM-2-ZINC
CAZRO3	CALCIUM-ZIRCONIUM-TRIOXIDE

INORGANIC Component Databank: Cd

Alias	Name
CD	CADMIUM
CD(OH)2	CADMIUM-HYDROXIDE
CD11U	11-CADMIUM-URANIUM
CD3(ASO4)2	CADMIUM-ARSENATE
CD3AS2	CADMIUM-ARSENIDE
CDAL2O4	CADMIUM-DIALUMINIUM-TETRAOXIDE
CDBR2	CADMIUM-BROMIDE
CDCL2	CADMIUM-CHLORIDE
CDCO3	CADMIUM-CARBONATE
CDF2	CADMIUM-FLUORIDE
CDGA2O4	CADMIUM-DIGALLIUM-TETRAOXIDE
CDI2	CADMIUM-IODIDE
CDO	CADMIUM-OXIDE
CDS	CADMIUM-SULFIDE
CDSB	CADMIUM-ANTIMONY
CDSE	CADMIUM-SELENIDE
CDSEO3	CADMIUM-SELENITE
CDSIO3	CADMIUM-METASILICATE
CDSO4	CADMIUM-SULFATE
CDSO4:1	CADMIUM-SULFATE:SOL-1
CDSO4:A	CADMIUM-SULFATE:SOL-A
CDSO4:B	CADMIUM-SULFATE:SOL-B
CDTE	CADMIUM-TELLURIDE
CDTIO3	CADMIUM-TITANIUM-TRIOXIDE
CDTIO3:A	CADMIUM-TITANIUM-TRIOXIDE:SOL-A
CDTIO3:B	CADMIUM-TITANIUM-TRIOXIDE:SOL-B
CDWO4	CADMIUM-TUNGSTATE

INORGANIC Component Databank: Ce

Alias	Name
CE	CERIUM
CE2(SO4)3	CERIUM-SULFATE
CE2C3	DICERIUM-TRICARBIDE
CE2O3	CERIUM-OXIDE
CE2S3	CERIUM-SULFIDE
CE3S4	TRICERIUM-TETRASULFIDE
CE:C	CERIUM:SOL-C
CE:D	CERIUM:SOL-D
CEALO3	CERIUM-ALUMINIUM-TRIOXIDE
CEB6	CERIUM-HEXABORIDE
CEBR3	CERIUM-BROMIDE
CEC2	CERIUM-DICARBIDE
CECL3	CERIUM-CHLORIDE
CECRO3	CERIUM-CHROMIUM-TRIOXIDE
CEF3	CERIUM-FLUORIDE
CEH2	CERIUM-DIHYDRIDE
CEI3	CERIUM-IODIDE
CEMG	CERIUM-MAGNESIUM
CEN	CERIUM-NITRIDE
CEO	CERIUM-MONOXIDE-GAS
CEO2	CERIUM-DIOXIDE
CES	CERIUM-MONOSULFIDE
CETE	CERIUM-MONOTELLURIDE-GAS

INORGANIC Component Databank: Cl

Alias	Name
CL	CHLORINE-MONATOMIC-GAS
CL2	CHLORINE
CL2O-G	DICHLORINE-MONOXIDE-GAS
CLF	CHLORINE-MONOFLUORIDE-GAS
CLF3	CHLORINE-TRIFLUORIDE-GAS
CLO	CHLORINE-MONOXIDE-GAS

INORGANIC Component Databank: Co

Alias	Name
CO(OH)2	COBALT-HYDROXIDE-PRECIPITATED
CO-CL	COBALT-MONOCHLORIDE-GAS
CO-CL2	COBALT-DICHLORIDE
CO-F2	COBALT-DIFLUORIDE
CO2B	DICOBALT-BORIDE
CO2CL4	DICOBALT-TETRACHLORIDE-GAS
CO2P	DICOBALT-PHOSPHIDE
CO2SIO4	DICOBALT-SILICATE
CO2TIO4	DICOBALT-TITANIUM-TETRAOXIDE
CO3(ASO4)2	COBALT-ARSENATE
CO3N	TRICOBALT-NITRIDE
CO3O4	TRICOBALT-TETRAOXIDE
CO3S4	TRICOBALT-TETRASULFIDE
CO:A	COBALT:SOL-A

Alias	Name
CO:B	COBALT:SOL-B
COB	COBALT-MONOBORIDE
COBALT	COBALT
COBR2	COBALT-DIBROMIDE
COBR2:1	COBALT-DIBROMIDE:SOL-1
COBR2:21	COBALT-DIBROMIDE:SOL-21
COCL3	COBALT-TRICHLORIDE-GAS
COCO3	COBALT-CARBONATE
COCR2O4	COBALT-DICHROMIUM-TETRAOXIDE
COF3	COBALT-TRIFLUORIDE
COFE2O4	COBALT-DIIRON-TETRAOXIDE
COFE2O4:1	COBALT-DIIRON-TETRAOXIDE:SOL-1
COFE2O4:11	COBALT-DIIRON-TETRAOXIDE:SOL-11
COI2	COBALT-DIIODIDE
COO	COBALT-MONOXIDE
COP	COBALT-MONOPHOSPHIDE
COP3	COBALT-TRIPHOSPHIDE
COS0.89	COBALT-0.89-SULFIDE
COS2	COBALT-DISULFIDE
COSB0.98	COBALT-0.98-ANTIMONY
COSB2	COBALT-2-ANTIMONY
COSB3	COBALT-3-ANTIMONY
COSEO3	COBALT-SELENITE
COSN	COBALT-TIN
COSO4	COBALT-SULFATE
COSO4:A	COBALT-SULFATE:SOL-A
COSO4:B	COBALT-SULFATE:SOL-B
COTIO3	COBALT-TITANIUM-TRIOXIDE
COWO4	COBALT-TUNGSTATE
COWO4:A	COBALT-TUNGSTATE:SOL-A
COWO4:B	COBALT-TUNGSTATE:SOL-B

INORGANIC Component Databank: Cr

Alias	Name
CR	CHROMIUM
CR(CO)6	CHROMIUM-HEXACARBONYL
CR2(SO4)3	CHROMIUM-SULFATE
CR23C6	23-CHROMIUM-6-CARBIDE
CR2FEO4	DICHROMIUM-IRON-TETRAOXIDE
CR2MGO4	DICHROMIUM-MAGNESIUM-TETRAOXIDE
CR2N	DICHROMIUM-NITRIDE
CR2NB	2-CHROMIUM-NIOBIUM
CR2NIO4	DICHROMIUM-NICKEL-TETRAOXIDE
CR2O3	ESKOLAITE
CR2TA	2-CHROMIUM-TANTALUM
CR3(ASO4)2	TRICHROMIUM-ARSENATE
CR3C2	3-CHROMIUM-2-CARBIDE
CR3SI	3-CHROMIUM-SILICON

Alias	Name
CR5SI3	5-CHROMIUM-3-SILICON
CR7C3	7-CHROMIUM-3-CARBIDE
CRASO4	CHROMIUM-ARSENATE
CRB	CHROMIUM-MONOBORIDE
CRB2	CHROMIUM-DIBORIDE
CRBR2	CHROMIUM-DIBROMIDE
CRBR3	CHROMIUM-TRIBROMIDE
CRBR4	CHROMIUM-TETRABROMIDE-GAS
CRCL2	CHROMIUM-DICHLORIDE
CRCL3	CHROMIUM-TRICHLORIDE
CRCL4	CHROMIUM-TETRACHLORIDE-GAS
CRF2	CHROMIUM-DIFLUORIDE
CRF3	CHROMIUM-TRIFLUORIDE
CRF4	CHROMIUM-TETRAFLUORIDE
CRI2	CHROMIUM-DIIODIDE
CRI3	CHROMIUM-TRIIODIDE
CRN	CHROMIUM-NITRIDE
CRNAO2	CHROMIUM-SODIUM-DIOXIDE
CRO	CHROMIUM-MONOXIDE-GAS
CRO2	CHROMIUM-DIOXIDE
CRO2CL2	CHROMIUM-DICHLORIDE-DIOXIDE-GAS
CRO3	CHROMIUM-TRIOXIDE
CRS	CHROMIUM-MONOSULFIDE
CRS1.17	CHROMIUM-1.17-SULFIDE
CRS1.17:A	CHROMIUM-1.17-SULFIDE:SOL-A
CRS1.17:B	CHROMIUM-1.17-SULFIDE:SOL-B
CRS1.17:C	CHROMIUM-1.17-SULFIDE:SOL-C
CRS:1	CHROMIUM-MONOSULFIDE:SOL-1
CRS:2	CHROMIUM-MONOSULFIDE:SOL-2
CRSI	CHROMIUM-SILICON
CRSI2	CHROMIUM-2-SILICON

INORGANIC Component Databank: Cs

Alias	Name
CS	CESIUM
CS-2	CESIUM-DIATOMIC-GAS
CS2(OH)2	DICESIUM-DIHYDROXIDE-GAS
CS2CL2	DICESIUM-DICHLORIDE-GAS
CS2CO3	CESIUM-CARBONATE
CS2F2	DICESIUM-DIFLUORIDE-GAS
CS2O	CESIUM-OXIDE
CS2O3	DICESIUM-TRIOXIDE
CS2SO4	CESIUM-SULFATE
CS2SO4:A	CESIUM-SULFATE:SOL-A
CS2SO4:B	CESIUM-SULFATE:SOL-B
CS3ASO4	CESIUM-ARSENATE
CSBR	CESIUM-BROMIDE
CSCL	CESIUM-CHLORIDE

	Alias	Name
	CSCL:A	CESIUM-CHLORIDE:SOL-A
	CSCL:B	CESIUM-CHLORIDE:SOL-B
	CSF	CESIUM-FLUORIDE
	CSI	CESIUM-IODIDE
	CSO	CESIUM-MONOXIDE-GAS
	CSO2	CESIUM-DIOXIDE
	CSOH	CESIUM-HYDROXIDE
	CSOH:A	CESIUM-HYDROXIDE:SOL-A
	CSOH:B	CESIUM-HYDROXIDE:SOL-B
	CSOH:C	CESIUM-HYDROXIDE:SOL-C
INORGANIC Component Databank: Cu	**Alias**	**Name**
	CU	COPPER
	CU(OH)2	COPPER-HYDROXIDE
	CU2MG	2-COPPER-1-MAGNESIUM
	CU2O	DICOPPER-OXIDE
	CU2OSO4	DICOPPER-OXIDE-SULFATE
	CU2S	DICOPPER-SULFIDE
	CU2S:A	DICOPPER-SULFIDE:SOL-A
	CU2S:B	DICOPPER-SULFIDE:SOL-B
	CU2S:C	DICOPPER-SULFIDE:SOL-C
	CU2SB	2-COPPER-ANTIMONY
	CU2SB:1	2-COPPER-ANTIMONY:SOL-1
	CU2SB:11	2-COPPER-ANTIMONY:SOL-11
	CU2SE	DICOPPER-SELENIDE
	CU2SE:A	DICOPPER-SELENIDE:SOL-A
	CU2SE:B	DICOPPER-SELENIDE:SOL-B
	CU2SO4	DICOPPER-SULFATE
	CU2TE	DICOPPER-TELLURIDE
	CU2TE:A	DICOPPER-TELLURIDE:SOL-A
	CU2TE:B	DICOPPER-TELLURIDE:SOL-B
	CU2TE:C	DICOPPER-TELLURIDE:SOL-C
	CU2TE:D	DICOPPER-TELLURIDE:SOL-D
	CU2TE:E	DICOPPER-TELLURIDE:SOL-E
	CU2TE:Z	DICOPPER-TELLURIDE:SOL-Z
	CU3(ASO4)2	TRICOPPER-DIARSENATE
	CU3AS	TRICOPPER-ARSENIDE
	CU3ASO4	TRICOPPER-ARSENATE
	CU3BR3	TRICOPPER-TRIBROMIDE-GAS
	CU3CL3	TRICOPPER-TRICHLORIDE-GAS
	CU3I3	TRICOPPER-TRIIODIDE-GAS
	CU3P	TRICOPPER-PHOSPHIDE
	CU5FES4	PENTACOPPER-IRON-TETRASULFIDE
	CU5FES4:A	PENTACOPPER-IRON-TETRASULFIDE:A
	CU5FES4:B	PENTACOPPER-IRON-TETRASULFIDE:B
	CU5FES4:C	PENTACOPPER-IRON-TETRASULFIDE:C
	CUBR	COPPER-MONOBROMIDE

Alias	Name
CUBR2	COPPER-DIBROMIDE
CUBR:A	COPPER-MONOBROMIDE:SOL-A
CUBR:B	COPPER-MONOBROMIDE:SOL-B
CUBR:C	COPPER-MONOBROMIDE:SOL-C
CUCL	CUPROUS-CHLORIDE
CUCL2	COPPER-DICHLORIDE
CUCL2:A	COPPER-DICHLORIDE:SOL-A
CUCL2:B	COPPER-DICHLORIDE:SOL-B
CUCL:A	COPPER-MONOCHLORIDE:SOL-A
CUCL:B	COPPER-MONOCHLORIDE:SOL-B
CUCN	COPPER-CYANIDE
CUF	COPPER-MONOFLUORIDE
CUF2	COPPER-DIFLUORIDE
CUFE2O4	COPPER-DIIRON-TETRAOXIDE
CUFE2O4:A	COPPER-DIIRON-TETRAOXIDE:SOL-A
CUFE2O4:B	COPPER-DIIRON-TETRAOXIDE:SOL-B
CUFE2O4:C	COPPER-DIIRON-TETRAOXIDE:SOL-C
CUFEO2	COPPER-IRON-DIOXIDE
CUFEO2:A	COPPER-IRON-DIOXIDE:SOL-A
CUFEO2:B	COPPER-IRON-DIOXIDE:SOL-B
CUFES2	COPPER-IRON-DISULFIDE
CUFES2:A	COPPER-IRON-DISULFIDE:SOL-A
CUFES2:B	COPPER-IRON-DISULFIDE:SOL-B
CUFES2:C	COPPER-IRON-DISULFIDE:SOL-C
CUI	COPPER-MONOIODIDE
CUI:A	COPPER-MONOIODIDE:SOL-A
CUI:B	COPPER-MONOIODIDE:SOL-B
CUI:C	COPPER-MONOIODIDE:SOL-C
CUMG2	1-COPPER-2-MAGNESIUM
CUMOO4	COPPER-MOLYBDATE
CUO	COPPER-MONOXIDE
CUP2	COPPER-DIPHOSPHIDE
CUS	COPPER-SULFIDE
CUSE	COPPER-SELENIDE
CUSE:B	COPPER-SELENIDE:SOL-B
CUSE:O	COPPER-SELENIDE:SOL-O
CUSEO3	COPPER-SELENITE
CUSO4	COPPER-SULFATE
CUSO4*3H2O	COPPER-SULFATE-TRIHYDRATE
CUSO4*5H2O	COPPER-SULFATE-PENTAHYDRATE
CUSO4*H2O	COPPER-SULFATE-MONOHYDRATE
CUTE	COPPER-TELLURIDE

INORGANIC Component Databank: Dy

Alias	Name
DY	DYSPROSIUM
DY2O3	DYSPROSIUM-OXIDE
DY:A	DYSPROSIUM:SOL-A
DY:B	DYSPROSIUM:SOL-B
DYBR3	DYSPROSIUM-BROMIDE-GAS
DYCL3	DYSPROSIUM-CHLORIDE
DYCL3*6H2O	DYSPROSIUM-CHLORIDE-HEXAHYDRATE
DYF3	DYSPROSIUM-FLUORIDE
DYI3	DYSPROSIUM-IODIDE-GAS

INORGANIC Component Databank: Er

Alias	Name
ER	ERBIUM
ER2O3	ERBIUM-OXIDE-CUBIC
ERBR3	ERBIUM-BROMIDE-GAS
ERCL3	ERBIUM-CHLORIDE
ERCL3*6H2O	ERBIUM-CHLORIDE-HEXAHYDRATE
ERF3	ERBIUM-FLUORIDE
ERF3:A	ERBIUM-FLUORIDE:SOL-A
ERF3:B	ERBIUM-FLUORIDE:SOL-B
ERI3	ERBIUM-IODIDE-GAS

INORGANIC Component Databank: Eu

Alias	Name
EU	EUROPIUM
EU2O3	EUROPIUM-OXIDE-CUBIC
EU2O3-M	EUROPIUM-OXIDE-MONOCLINIC
EU2O3-M:M1	EUROPIUM-OXIDE-MONOCLINIC:SOL-M1
EU2O3-M:M2	EUROPIUM-OXIDE-MONOCLINIC:SOL-M2
EUBR2	EUROPIUM-DIBROMIDE
EUBR3	EUROPIUM-BROMIDE
EUCL3	EUROPIUM-CHLORIDE
EUCL3*6H2O	EUROPIUM-CHLORIDE-HEXAHYDRATE
EUF3	EUROPIUM-FLUORIDE
EUF3:A	EUROPIUM-FLUORIDE:SOL-A
EUF3:B	EUROPIUM-FLUORIDE:SOL-B
EUS	EUROPIUM-MONOSULFIDE

INORGANIC Component Databank: Fe

Alias	Name
FE	IRON
FE(CO)5	IRON-PENTACARBONYL
FE(OH)2	IRON-DIHYDROXIDE
FE(OH)3	IRON-TRIHYDROXIDE
FE(VO3)2	IRON-VANADATE
FE0.877S	PYRRHOTITE
FE0.877S:A	PYRRHOTITE:SOL-A
FE0.877S:B	PYRRHOTITE:SOL-B
FE0.947O	WUESTITE
FE2(SO4)3	DIIRON-TRISULFATE
FE2B	DIIRON-BORIDE

Alias	Name
FE2BR4	DIIRON-TETRABROMIDE-GAS
FE2CL4	DIIRON-TETRACHLORIDE-GAS
FE2CL6	DIIRON-HEXACHLORIDE-GAS
FE2I4	DIIRON-TETRAIODIDE-GAS
FE2MGO4	DIIRON-MAGNESIUM-TETRAOXIDE
FE2MNO4	DIIRON-MANGANESE-TETRAOXIDE
FE2MNO4:1	DIIRON-MANGANESE-TETRAOXIDE:S-1
FE2MNO4:2	DIIRON-MANGANESE-TETRAOXIDE:S-2
FE2NIO4	DIIRON-NICKEL-TETRAOXIDE
FE2NIO4:A	DIIRON-NICKEL-TETRAOXIDE:SOL-A
FE2NIO4:B	DIIRON-NICKEL-TETRAOXIDE:SOL-B
FE2O3	HEMATITE
FE2O3*H2O	IRON-TRIOXIDE-HYDRATE-GOETHITE
FE2O3:A	HEMATITE:SOL-A
FE2O3:B	HEMATITE:SOL-B
FE2SIO4	IRON-ORTHOSILICATE-FAYALITE
FE2TA	2-IRON-TANTALUM
FE2TIO4	DIIRON-TITANIUM-TETROXIDE
FE2U	2-IRON-URANIUM
FE2ZNO4	DIIRON-ZINC-TETRAOXIDE
FE3(ASO4)2	TRIIRON-DIARSENATE
FE3C	TRIIRON-CARBIDE
FE3C:A	TRIIRON-CARBIDE:SOL-A
FE3C:B	TRIIRON-CARBIDE:SOL-B
FE3MO2	3-IRON-2-MOLYBDENUM
FE3O4	MAGNETITE
FE3O4:A	MAGNETITE:SOL-A
FE3O4:B	MAGNETITE:SOL-B
FE4N	TETRAIRON-NITRIDE
FE4N:A	TETRAIRON-NITRIDE:SOL-A
FE4N:B	TETRAIRON-NITRIDE:SOL-B
FE:A	IRON:SOL-A
FE:B	IRON:SOL-B
FE:C	IRON:SOL-C
FE:D	IRON:SOL-D
FEAL2O4	IRON-DIALUMINIUM-TETRAOXIDE
FEASO4	IRON-ARSENATE
FEASO4:A	IRON-ARSENATE:SOL-A
FEASO4:B	IRON-ARSENATE:SOL-B
FEASO4:C	IRON-ARSENATE:SOL-C
FEB	IRON-MONOBORIDE
FEBR2	IRON-DIBROMIDE
FEBR2:1	IRON-DIBROMIDE:SOL-1
FEBR2:2	IRON-DIBROMIDE:SOL-2
FEBR3	IRON-TRIBROMIDE
FECL	IRON-MONOCHLORIDE-GAS
FECL2	FERROUS-CHLORIDE

Alias	Name
FECL3	FERRIC-CHLORIDE
FECO3	IRON-CARBONATE
FEF2	IRON-DIFLUORIDE
FEF3	IRON-TRIFLUORIDE
FEI2	IRON-DIIODIDE
FEI2:1	IRON-DIIODIDE:SOL-1
FEI2:2	IRON-DIIODIDE:SOL-2
FEMOO4	IRON-MOLYBDATE
FENAO2	IRON-SODIUM-DIOXIDE
FEO	FERROUS-OXIDE
FEOCL	IRON-CHLORIDE-OXIDE
FES	IRON-MONOSULFIDE
FES2	IRON-DISULFIDE-PYRITE
FES:A	IRON-MONOSULFIDE:SOL-A
FES:B	IRON-MONOSULFIDE:SOL-B
FES:C	IRON-MONOSULFIDE:SOL-C
FESE0.96	IRON-0.96-SELENIDE
FESE0.96:A	IRON-0.96-SELENIDE:SOL-A
FESE0.96:B	IRON-0.96-SELENIDE:SOL-B
FESI	IRON-SILICON
FESI2	LEBOITE-BETA
FESI2.33	LEBOITE-ALPHA
FESIO3	IRON-METASILICATE
FESO4	FERROUS-SULFATE
FETE0.9	IRON-0.9-TELLURIDE
FETE2	IRON-DITELLURIDE
FETI	IRON-TITANIUM
FETIO3	IRON-TITANIUM-TRIOXIDE-ILMENITE
FEV2O4	IRON-DIVANADIUM-TETRAOXIDE
FEWO4	IRON-TUNGSTATE

INORGANIC Component Databank: Ga

Alias	Name
GA	GALLIUM
GA2(SEO4)3	GALLIUM-SELENATE
GA2CL6	DIGALLIUM-HEXACHLORIDE-GAS
GA2O	DIGALLIUM-OXIDE-GAS
GA2O3	GALLIUM-OXIDE
GA2S	DIGALLIUM-SULFIDE-GAS
GA2S3	DIGALLIUM-TRISULFIDE
GA2SE3	DIGALLIUM-TRISELENIDE
GA2TE3	DIGALLIUM-TRITELLURIDE
GAAS	GALLIUM-ARSENIDE
GAASO4	GALLIUM-ARSENATE
GABR3	GALLIUM-BROMIDE
GACL	GALLIUM-MONOCHLORIDE-GAS
GACL2	GALLIUM-DICHLORIDE-GAS
GACL3	GALLIUM-TRICHLORIDE

	Alias	Name
	GAF	GALLIUM-MONOFLUORIDE-GAS
	GAF2	GALLIUM-DIFLUORIDE-GAS
	GAF3	GALLIUM-FLUORIDE
	GAI3	GALLIUM-IODIDE
	GAN	GALLIUM-NITRIDE
	GAO	GALLIUM-MONOXIDE-GAS
	GAP	GALLIUM-PHOSPHIDE
	GAS	GALLIUM-MONOSULFIDE
	GASB	GALLIUM-ANTIMONY
	GASE	GALLIUM-MONOSELENIDE
	GATE	GALLIUM-MONOTELLURIDE

INORGANIC Component Databank: Gd

Alias	Name
GD	GADOLINIUM
GD2O3	GADOLINIUM-OXIDE-CUBIC
GD2O3-M	GADOLINIUM-OXIDE-MONOCLINIC
GD:A	GADOLINIUM:SOL-A
GD:B	GADOLINIUM:SOL-B
GDBR3	GADOLINIUM-BROMIDE
GDCL3	GADOLINIUM-CHLORIDE
GDF3	GADOLINIUM-FLUORIDE
GDF3:A	GADOLINIUM-FLUORIDE:SOL-A
GDF3:B	GADOLINIUM-FLUORIDE:SOL-B
GDI3	GADOLINIUM-IODIDE
GDI3:A	GADOLINIUM-IODIDE:SOL-A
GDI3:B	GADOLINIUM-IODIDE:SOL-B
GDOCL	GADOLINIUM-CHLORIDE-OXIDE

INORGANIC Component Databank: Ge

Alias	Name
GE	GERMANIUM
GE2U	2-GERMANIUM-URANIUM
GE3U	3-GERMANIUM-URANIUM
GE3U5	3-GERMANIUM-5-URANIUM
GE5U3	5-GERMANIUM-3-URANIUM
GEBR4	GERMANIUM-TETRABROMIDE-GAS
GECL	GERMANIUM-MONOCHLORIDE-GAS
GECL2	GERMANIUM-DICHLORIDE-GAS
GECL3	GERMANIUM-TRICHLORIDE-GAS
GECL4	GERMANIUM-TETRACHLORIDE-GAS
GEF	GERMANIUM-MONOFLUORIDE-GAS
GEF2	GERMANIUM-DIFLUORIDE-GAS
GEF3	GERMANIUM-TRIFLUORIDE-GAS
GEF4	GERMANIUM-TETRAFLUORIDE-GAS
GEH4	GERMANIUM-TETRAHYDRIDE
GEI4	GERMANIUM-TETRAIODIDE-GAS
GEMG2	GERMANIUM-2-MAGNESIUM
GENI2	GERMANIUM-2-NICKEL

	Alias	Name
	GEO	GERMANIUM-MONOXIDE-GAS
	GEO2	GERMANIUM-DIOXIDE
	GEO2:A	GERMANIUM-DIOXIDE:SOL-A
	GEO2:B	GERMANIUM-DIOXIDE:SOL-B
	GEP	GERMANIUM-PHOSPHIDE
	GES	GERMANIUM-MONOSULFIDE
	GES2	GERMANIUM-DISULFIDE
	GESE	GERMANIUM-MONOSELENIDE
	GESE2	GERMANIUM-DISELENIDE
	GETE	GERMANIUM-MONOTELLURIDE
	GEU	GERMANIUM-URANIUM

INORGANIC Component Databank: H

Alias	Name
D	DEUTERIUM-MONATOMIC-GAS
D2	DEUTERIUM
D2O	DEUTERIUM-OXIDE
D2S	HYDROGEN-SULFIDE-D2-GAS
DCL	HYDROGEN-CHLORIDE-D1-GAS
DF	HYDROGEN-FLUORIDE-D1-GAS
DH	HYDROGEN-D1-GAS
DS	HYDROGEN-MONOSULFIDE-D1-GAS
H	HYDROGEN-MONATOMIC-GAS
1/2-H2	1/2-HYDROGEN
H2	HYDROGEN
H2O	WATER
H2O2	HYDROGEN-PEROXIDE
H2S	HYDROGEN-SULFIDE
H2S2	DIHYDROGEN-DISULFIDE-GAS
H2SE-G	HYDROGEN-SELENIDE-GAS
H2SO4	SULFURIC-ACID
H2TE	HYDROGEN-TELLURIDE-GAS
H2WO4	TUNGSTIC-ACID
H3BO3	HYDROGEN-ORTHOBORATE
H3N	AMMONIA
H3PO4	ORTHOPHOSPHORIC-ACID
H4N2	HYDRAZINE
HBO2	METABORIC-ACID
HBR	HYDROGEN-BROMIDE
HCL	HYDROGEN-CHLORIDE
HDO	WATER-D1-GAS
HF	HYDROGEN-FLUORIDE
HI	HYDROGEN-IODIDE
HNCO	ISOCYANIC-ACID-GAS
HNO3	NITRIC-ACID
HS	HYDROGEN-MONOSULFIDE-GAS

INORGANIC Component Databank: Hf

Alias	Name
HAFNIUM	HAFNIUM
HF:A	HAFNIUM:SOL-A
HF:B	HAFNIUM:SOL-B
HFB2	HAFNIUM-DIBORIDE
HFBR4	HAFNIUM-TETRABROMIDE
HFC	HAFNIUM-CARBIDE
HFCL2	HAFNIUM-DICHLORIDE-GAS
HFCL3	HAFNIUM-TRICHLORIDE-GAS
HFCL4	HAFNIUM-TETRACHLORIDE
HFF4	HAFNIUM-TETRAFLUORIDE
HFI4	HAFNIUM-TETRAIODIDE
HFN	HAFNIUM-NITRIDE
HFO2	HAFNIUM-DIOXIDE
HFO2:A	HAFNIUM-DIOXIDE:SOL-A
HFO2:B	HAFNIUM-DIOXIDE:SOL-B
HFSRO3	HAFNIUM-STRONTIUM-TRIOXIDE

INORGANIC Component Databank: Hg

Alias	Name
HG	MERCURY
HG2BR2	DIMERCURY-DIBROMIDE
HG2CL2	DIMERCURY-DICHLORIDE
HG2F2	DIMERCURY-DIFLUORIDE
HG2I2	DIMERCURY-DIIODIDE
HG2SO4	DIMERCURY-SULFATE
HG3(ASO4)2	TRIMERCURY-DIARSENATE
HGBR	MERCURY-MONOBROMIDE-GAS
HGBR2	MERCURY-DIBROMIDE
HGCL	MERCURY-MONOCHLORIDE-GAS
HGCL2	MERCURY-DICHLORIDE
HGF	MERCURY-MONOFLUORIDE-GAS
HGF2	MERCURY-DIFLUORIDE
HGH	MERCURY-MONOHYDRIDE-GAS
HGI	MERCURY-MONOIODIDE-GAS
HGI2	MERCURY-DIIODIDE
HGI2:A	MERCURY-DIIODIDE:SOL-A
HGI2:B	MERCURY-DIIODIDE:SOL-B
HGO	MERCURY-OXIDE-RED
HGS	MERCURY-SULFIDE-RED
HGS:B	MERCURY-SULFIDE-RED:SOL-B
HGS:R	MERCURY-SULFIDE-RED:SOL-R
HGSE	MERCURY-SELENIDE
HGSEO3	MERCURY-SELENITE
HGSO4	MERCURY-SULFATE
HGTE	MERCURY-TELLURIDE

INORGANIC Component Databank: Ho

Alias	Name
HO-1	HOLMIUM
HO2O3	HOLMIUM-OXIDE
HO:A	HOLMIUM:SOL-A
HO:B	HOLMIUM:SOL-B
HOBR3	HOLMIUM-BROMIDE
HOCL3	HOLMIUM-CHLORIDE
HOCL3*6H2O	HOLMIUM-CHLORIDE-HEXAHYDRATE
HOF3	HOLMIUM-FLUORIDE
HOF3:A	HOLMIUM-FLUORIDE:SOL-A
HOF3:B	HOLMIUM-FLUORIDE:SOL-B

INORGANIC Component Databank: In

Alias	Name
IN	INDIUM
IN2(SO4)3	DIINDIUM-TRISULFATE
IN2CL6	DIINDIUM-HEXACHLORIDE-GAS
IN2O	DIINDIUM-OXIDE-GAS
IN2O3	DIINDIUM-TRIOXIDE
IN2S3	DIINDIUM-TRISULFIDE
IN2S3:A	DIINDIUM-TRISULFIDE:SOL-A
IN2S3:B	DIINDIUM-TRISULFIDE:SOL-B
IN2S3:C	DIINDIUM-TRISULFIDE:SOL-C
IN2SE3	DIINDIUM-TRISELENIDE
IN2SE3:A	DIINDIUM-TRISELENIDE:SOL-A
IN2SE3:B	DIINDIUM-TRISELENIDE:SOL-B
IN2TE	DIINDIUM-TELLURIDE
IN2TE3	DIINDIUM-TRITELLURIDE
IN2TE3:A	DIINDIUM-TRITELLURIDE:SOL-A
IN2TE3:B	DIINDIUM-TRITELLURIDE:SOL-B
IN5S6	PENTAINDIUM-HEXASULFIDE
INAS	INDIUM-ARSENIDE
INASO4	INDIUM-ARSENATE
INBR	INDIUM-MONOBROMIDE
INBR3	INDIUM-TRIBROMIDE
INCL	INDIUM-MONOCHLORIDE
INCL2	INDIUM-DICHLORIDE
INCL2:1	INDIUM-DICHLORIDE:SOL-1
INCL2:2	INDIUM-DICHLORIDE:SOL-2
INCL3	INDIUM-TRICHLORIDE
INCL:A	INDIUM-MONOCHLORIDE:SOL-A
INCL:B	INDIUM-MONOCHLORIDE:SOL-B
INF	INDIUM-MONOFLUORIDE-GAS
INF2	INDIUM-DIFLUORIDE-GAS
INF3	INDIUM-TRIFLUORIDE
INI	INDIUM-MONOIODIDE
INI2	INDIUM-DIIODIDE-GAS
INI3	INDIUM-TRIIODIDE
INN	INDIUM-NITRIDE

	Alias	Name
	INP	INDIUM-PHOSPHIDE
	INP:A	INDIUM-PHOSPHIDE:SOL-A
	INP:B	INDIUM-PHOSPHIDE:SOL-B
	INS	INDIUM-MONOSULFIDE
	INSB	INDIUM-ANTIMONY
	INSE	INDIUM-MONOSELENIDE
	INTE	INDIUM-MONOTELLURIDE

INORGANIC Component Databank: Ir

Alias	Name
IR	IRIDIUM
IR2S3	DIIRIDIUM-TRISULFIDE
IRBR3	IRIDIUM-TRIBROMIDE
IRCL3	IRIDIUM-TRICHLORIDE
IRF6	IRIDIUM-HEXAFLUORIDE-GAS
IRI	IRIDIUM-MONOIODIDE
IRI2	IRIDIUM-DIIODIDE
IRO2	IRIDIUM-DIOXIDE
IRO3	IRIDIUM-TRIOXIDE-GAS
IRS2	IRIDIUM-DISULFIDE

INORGANIC Component Databank: K

Alias	Name
K	POTASSIUM
K2	POTASSIUM-DIATOMIC-GAS
K2(CN)2	DIPOTASSIUM-DICYANIDE-GAS
K2(OH)2	DIPOTASSIUM-DIHYDROXIDE-GAS
K2B407	DIPOTASSIUM-TETRABORATE
K2B6O10	DIPOTASSIUM-HEXABORATE
K2B8O13	DIPOTASSIUM-OCTABORATE
K2BR2	DIPOTASSIUM-DIBROMIDE-GAS
K2CL2	DIPOTASSIUM-DICHLORIDE-GAS
K2CO3	POTASSIUM-CARBONATE
K2CRO4	POTASSIUM-CHROMATE
K2CRO4:A	POTASSIUM-CHROMATE:SOL-A
K2CRO4:B	POTASSIUM-CHROMATE:SOL-B
K2F2	DIPOTASSIUM-DIFLUORIDE-GAS
K2HPO4	DIPOTASSIUM-PHOSPHATE
K2I2	DIPOTASSIUM-DIIODIDE-GAS
K2O	POTASSIUM-OXIDE
K2O2	DIPOTASSIUM-PEROXIDE
K2S	POTASSIUM-SULFIDE
K2S:1	POTASSIUM-SULFIDE:SOL-1
K2S:2	POTASSIUM-SULFIDE:SOL-2
K2SI2O5	POTASSIUM-DISILICATE
K2SI2O5:B	POTASSIUM-DISILICATE:SOL-B
K2SI2O5:C	POTASSIUM-DISILICATE:SOL-C
K2SI4O9	POTASSIUM-TETRASILICATE
K2SI4O9:A	POTASSIUM-TETRASILICATE:SOL-A

Alias	Name
K2SI4O9:B	POTASSIUM-TETRASILICATE:SOL-B
K2SIO3	POTASSIUM-METASILICATE
K2SO3	POTASSIUM-SULFITE
K2SO4	POTASSIUM-SULFATE
K2SO4:A	POTASSIUM-SULFATE:SOL-A
K2SO4:B	POTASSIUM-SULFATE:SOL-B
K3ALCL6	TRIPOTASSIUM-HEXACHLOROALUMINATE
K3ALF6	TRIPOTASSIUM-HEXAFLUOROALUMINATE
K3ASO4	POTASSIUM-ARSENATE
K3PO4	POTASSIUM-PHOSPHATE
KAL(SO4)2	POTASSIUM-ALUMINIUM-SULFATE
KALCL4	POTASSIUM-TETRACHLOROALUMINATE
KALSI2O6	LEUCITE
KALSI3O8	SANIDINE
KALSI3O8-A	ADULARIA
KALSI3O8-M	MICROCLINE
KALSIO4	KALIOPHILITE
KALSO4*2*12W	POTASSIUM-ALUMINIUM-SULFATE-12-H
KALSO4*2*3W	POTASSIUM-ALUMINIUM-SULFATE-3-HY
KBO2	POTASSIUM-METABORATE
KBR	POTASSIUM-BROMIDE
KCL	POTASSIUM-CHLORIDE
KCLO4	POTASSIUM-PERCHLORATE
KCLO4:1	POTASSIUM-PERCHLORATE:SOL-1
KCLO4:2	POTASSIUM-PERCHLORATE:SOL-2
KCN	POTASSIUM-CYANIDE
KF	POTASSIUM-FLUORIDE
KH	POTASSIUM-HYDRIDE
KH2PO4	POTASSIUM-DIHYDROGEN-PHOSPHATE
KH2PO4:1	POTASSIUM-DIHYDROGEN-PHOS:SOL-1
KH2PO4:2	POTASSIUM-DIHYDROGEN-PHOS:SOL-2
KI	POTASSIUM-IODIDE
KNO3	POTASSIUM-NITRATE
KNO3:A	POTASSIUM-NITRATE:SOL-A
KNO3:B	POTASSIUM-NITRATE:SOL-B
KO	POTASSIUM-MONOXIDE-GAS
KO2	POTASSIUM-DIOXIDE
KOH	POTASSIUM-HYDROXIDE
KOH:A	POTASSIUM-HYDROXIDE:SOL-A
KOH:B	POTASSIUM-HYDROXIDE:SOL-B

INORGANIC Component Databank: La

Alias	Name
LA	LANTHANUM
LA2O3	LANTHANUM-OXIDE
LA2S3	LANTHANUM-SULFIDE

Alias	Name
LA2SE3	LANTHANUM-SELENIDE
LA2TE3	LANTHANUM-TELLURIDE
LA:A	LANTHANUM:SOL-A
LA:B	LANTHANUM:SOL-B
LA:C	LANTHANUM:SOL-C
LAASO4	LANTHANUM-ARSENATE
LABR3	LANTHANUM-BROMIDE
LACL3	LANTHANUM-CHLORIDE
LAF3	LANTHANUM-FLUORIDE
LAH2	LANTHANUM-DIHYDRIDE
LAI3	LANTHANUM-IODIDE
LAMG	LANTHANUM-MAGNESIUM
LAN	LANTHANUM-NITRIDE
LAO	LANTHANUM-MONOXIDE-GAS
LAOCL	LANTHANUM-CHLORIDE-OXIDE
LAS	LANTHANUM-MONOSULFIDE
LASE	LANTHANUM-MONOSELENIDE

INORGANIC Component Databank: Li

Alias	Name
LI	LITHIUM
LI2	LITHIUM-DIATOMIC-GAS
LI2(OH)2	DILITHIUM-DIHYDROXIDE-GAS
LI2B4O7	DILITHIUM-TETRABORATE
LI2B6O10	DILITHIUM-HEXABORATE
LI2BEF4	DILITHIUM-TETRAFLUOROBERYLLATE
LI2BR2	DILITHIUM-DIBROMIDE-GAS
LI2CL2	DILITHIUM-DICHLORIDE-GAS
LI2CO3	LITHIUM-CARBONATE
LI2CO3:A	LITHIUM-CARBONATE:SOL-A
LI2CO3:B	LITHIUM-CARBONATE:SOL-B
LI2CO3:C	LITHIUM-CARBONATE:SOL-C
LI2F2	DILITHIUM-DIFLUORIDE-GAS
LI2I2	DILITHIUM-DIIODIDE-GAS
LI2O	LITHIUM-OXIDE
LI2O2	DILITHIUM-PEROXIDE
LI2S	LITHIUM-SULFIDE
LI2SE	LITHIUM-SELENIDE
LI2SI2O5	LITHIUM-DISILICATE
LI2SI2O5:A	LITHIUM-DISILICATE:SOL-A
LI2SI2O5:B	LITHIUM-DISILICATE:SOL-B
LI2SIO3	LITHIUM-METASILICATE
LI2SO4	LITHIUM-SULFATE
LI2SO4:A	LITHIUM-SULFATE:SOL-A
LI2SO4:B	LITHIUM-SULFATE:SOL-B
LI2TE	LITHIUM-TELLURIDE
LI2TIO3	DILITHIUM-TITANIUM-TRIOXIDE
LI2TIO3:A	DILITHIUM-TITANIUM-TRIOXIDE:S-A

Alias	Name
LI2TIO3:B	DILITHIUM-TITANIUM-TRIOXIDE:S-B
LI2ZRO3	DILITHIUM-ZIRCONIUM-TRIOXIDE
LI3ALF6	TRILITHIUM-HEXAFLUOROALUMINATE
LI3ALF6:B	TRILITHIUM-6-FLUOROALUMINATE:S-B
LI3ALF6:C	TRILITHIUM-6-FLUOROALUMINATE:S-C
LI3ALF6:D	TRILITHIUM-6-FLUOROALUMINATE:S-D
LI3ALF6:E	TRILITHIUM-6-FLUOROALUMINATE:S-E
LI3ASO4	LITHIUM-ARSENATE
LI3F3	TRILITHIUM-TRIFLUORIDE-GAS
LI3N	TRILITHIUM-NITRIDE
LI4SIO4	LITHIUM-ORTHOSILICATE
LIALF4	LITHIUM-TETRAFLUOROALUMINATE-GAS
LIALO2	LITHIUM-ALUMINATE
LIALSI2O6	ALPHA-SPODUMENE
LIALSI2O6-B	BETA-SPODUMENE
LIALSIO4	EUCRYPTITE
LIALSIO4:B	EUCRYPTITE:SOL-B
LIALSIO4:C	EUCRYPTITE:SOL-C
LIBEF3	LITHIUM-TRIFLUOROBERYLLATE
LIBO2	LITHIUM-METABORATE
LIBR	LITHIUM-BROMIDE
LICL	LITHIUM-CHLORIDE
LICLO	LITHIUM-HYPOCHLORITE-GAS
LICLO4	LITHIUM-PERCHLORATE
LIF	LITHIUM-FLUORIDE
LIFEO2	LITHIUM-IRON-DIOXIDE
LIFO	LITHIUM-HYPOFLUORITE-GAS
LIH	LITHIUM-HYDRIDE
LII	LITHIUM-IODIDE
LIO	LITHIUM-MONOXIDE-GAS
LIOH	LITHIUM-HYDROXIDE

INORGANIC Component Databank: Mg

Alias	Name
MG	MAGNESIUM
MG(NO3)2	MAGNESIUM-NITRATE
MG(OH)2	MAGNESIUM-HYDROXIDE
MG(OH)CL	MAGNESIUM-CHLORIDE-HYDROXIDE
MG(VO3)2	MAGNESIUM-METAVANADATE
MG2BR4	DIMAGNESIUM-TETRABROMIDE-GAS
MG2C3	DIMAGNESIUM-TRICARBIDE
MG2F4	DIMAGNESIUM-TETRAFLUORIDE-GAS
MG2PB	2-MAGNESIUM-LEAD
MG2SI	2-MAGNESIUM-SILICON
MG2SIO4	MAGNESIUM-ORTHOSILICATE
MG2TH	2-MAGNESIUM-THORIUM
MG2TIO4	DIMAGNESIUM-TITANIUM-TETRAOXIDE

Alias	Name
MG2V2O7	MAGNESIUM-PYROVANADATE
MG3(ASO4)2	MAGNESIUM-ARSENATE
MG3(PO4)2	MAGNESIUM-ORTHOPHOSPHATE
MG3N2	TRIMAGNESIUM-DINITRIDE
MG3N2:A	TRIMAGNESIUM-DINITRIDE:SOL-A
MG3N2:B	TRIMAGNESIUM-DINITRIDE:SOL-B
MG3N2:C	TRIMAGNESIUM-DINITRIDE:SOL-C
MGAL2O4	MAGNESIUM-DIALUMINIUM-TETRAOXIDE
MGB2	MAGNESIUM-DIBORIDE
MGB4	MAGNESIUM-TETRABORIDE
MGBR	MAGNESIUM-MONOBROMIDE-GAS
MGBR2	MAGNESIUM-BROMIDE
MGC2	MAGNESIUM-DICARBIDE
MGCL	MAGNESIUM-MONOCHLORIDE-GAS
MGCL2	MAGNESIUM-CHLORIDE
MGCO3	MAGNESIUM-CARBONATE
MGF	MAGNESIUM-MONOFLUORIDE-GAS
MGF2	MAGNESIUM-FLUORIDE
MGH2	MAGNESIUM-HYDRIDE
MGI	MAGNESIUM-MONOIODIDE-GAS
MGI2	MAGNESIUM-IODIDE
MGMOO4	MAGNESIUM-MOLYBDATE
MGNI2	MAGNESIUM-2-NICKEL
MGO	MAGNESIUM-OXIDE
MGOH	MAGNESIUM-MONOHYDROXIDE-GAS
MGS	MAGNESIUM-SULFIDE
MGSE	MAGNESIUM-SELENIDE
MGSEO3	MAGNESIUM-SELENITE
MGSIO3	MAGNESIUM-METASILICATE
MGSIO3:1	MAGNESIUM-METASILICATE:SOL-1
MGSIO3:2	MAGNESIUM-METASILICATE:SOL-2
MGSIO3:3	MAGNESIUM-METASILICATE:SOL-3
MGSO4	MAGNESIUM-SULFATE
MGTE	MAGNESIUM-TELLURIDE
MGTI2O5	MAGNESIUM-DITITANIUM-PENTOXIDE
MGTIO3	MAGNESIUM-TITANIUM-TRIOXIDE
MGWO4	MAGNESIUM-TUNGSTATE

INORGANIC Component Databank: Mn

Alias	Name
MN	MANGANESE
MN15C4	15-MANGANESE-4-CARBID
MN2O3	DIMANGANESE-TRIOXIDE
MN2P	DIMANGANESE-PHOSPHIDE
MN2SB	2-MANGANESE-ANTIMONY
MN2SB:1	2-MANGANESE-ANTIMONY:SOL-1
MN2SB:2	2-MANGANESE-ANTIMONY:SOL-2

Alias	Name
MN2SIO4	TEPHROITE
MN2TIO4	DIMANGANESE-TITANIUM-TETRAOXIDE
MN3(ASO4)2	MANGANESE-ARSENATE
MN3C	TRIMANGANESE-CARBIDE
MN3O4	TRIMANGANESE-TETRAOXIDE
MN3O4:A	TRIMANGANESE-TETRAOXIDE:SOL-A
MN3O4:B	TRIMANGANESE-TETRAOXIDE:SOL-B
MN3SI	3-MANGANESE-SILICON
MN3SI:1	3-MANGANESE-SILICON:SOL-1
MN3SI:2	3-MANGANESE-SILICON:SOL-2
MN4N	TETRAMANGANESE-MONONITRIDE
MN5N2	PENTAMANGANESE-DINITRIDE
MN5SI3	5-MANGANESE-3-SILICON
MN7C3	HEPTAMANGANESE-TRICARBIDE
MN:A	MANGANESE:SOL-A
MN:B	MANGANESE:SOL-B
MN:C	MANGANESE:SOL-C
MN:D	MANGANESE:SOL-D
MNAL2O4	MANGANESE-DIALUMINIUM-TETRAOXIDE
MNAS	MANGANESE-ARSENIDE
MNAS:1	MANGANESE-ARSENIDE:SOL-1
MNAS:2	MANGANESE-ARSENIDE:SOL-2
MNAS:3	MANGANESE-ARSENIDE:SOL-3
MNB	MANGANESE-MONOBORIDE
MNB2	MANGANESE-DIBORIDE
MNBR2	MANGANESE-DIBROMIDE
MNCL2	MANGANESE-DICHLORIDE
MNCO3	MANGANESE-CARBONATE
MNF2	MANGANESE-DIFLUORIDE
MNF2:A	MANGANESE-DIFLUORIDE:SOL-A
MNF2:B	MANGANESE-DIFLUORIDE:SOL-B
MNF3	MANGANESE-TRIFLUORIDE
MNI2	MANGANESE-DIIODIDE
MNMOO4	MANGANESE-MOLYBDATE
MNO	MANGANESE-OXIDE
MNO2	MANGANESE-DIOXIDE
MNP	MANGANESE-MONOPHOSPHIDE
MNP3	MANGANESE-TRIPHOSPHIDE
MNS	MANGANESE-MONOSULFIDE-GREEN
MNS2	MANGANESE-DISULFIDE
MNSB	MANGANESE-ANTIMONY
MNSE	MANGANESE-SELENIDE
MNSI	MANGANESE-SILICON
MNSI1.7	MANGANESE-1.7-SILICON
MNSIO3	RHODONITE
MNSN2	MANGANESE-2-TIN

	Alias	Name
	MNSO4	MANGANESE-SULFATE
	MNTE	MANGANESE-TELLURIDE
	MNTE2	MANGANESE-DITELLURIDE
	MNTE:A	MANGANESE-TELLURIDE:SOL-A
	MNTE:B	MANGANESE-TELLURIDE:SOL-B
	MNTIO3	MANGANESE-TITANIUM-TRIOXIDE
	MNWO4	MANGANESE-TUNGSTATE

INORGANIC Component Databank: Mo

Alias	Name
MO	MOLYBDENUM
MO(CO)6	MOLYBDENUM-HEXACARBONYL
MO2C	DIMOLYBDENUM-CARBIDE
MO2N	DIMOLYBDENUM-NITRIDE
MO2S3	MOLYBDENUM-SESQUISULFIDE
MO3SI	3-MOLYBDENUM-SILICON
MO5SI3	5-MOLYBDENUM-3-SILICON
MOASO4	MOLYBDENUM-ARSENATE
MOC	MOLYBDENUM-MONOCARBIDE-GAMMA
MOO	MOLYBDENUM-MONOXIDE-GAS
MOO2	MOLYBDENUM-DIOXIDE
MOO2CL2	MOLYBDENUM-DICHLORIDE-DIOXIDE
MOO3	MOLYBDENUM-TRIOXIDE
MOS2	MOLYBDENUM-DISULFIDE
MOS3	MOLYBDENUM-TRISULFIDE
MOSI2	MOLYBDENUM-2-SILICON

INORGANIC Component Databank: N

Alias	Name
N	NITROGEN-MONATOMIC-GAS
N-D	IMIDOGEN-D1-GAS
1/2-N2	1/2-NITROGEN
N2	NITROGEN
N2O	NITROUS-OXIDE
N2O3	NITROGEN-TRIOXIDE
N2O5	NITROGEN-PENTOXIDE
NCO	NCO-RADICAL-GAS
ND3	AMMONIA-D3-GAS
ND2	AMIDOGEN-D2-GAS
NH	IMIDOGEN-GAS
NH2	AMIDOGEN-GAS
NH4CL	AMMONIUM-CHLORIDE
NH4CL:1	AMMONIUM-CHLORIDE:SOL-1
NH4CL:2	AMMONIUM-CHLORIDE:SOL-2
NH4CLO4	AMMONIUM-PERCHLORATE
NH4I	AMMONIUM-IODIDE
(NH4)2SO4	AMMONIUM-SULFATE
NO	NITRIC-OXIDE
NO2	NITROGEN-DIOXIDE

	Alias	Name
	NO2CL	NITRYL-CHLORIDE-GAS
	NO3	NITROGEN-TRIOXIDE-GAS
	NOBR	NITROSYL-BROMIDE-GAS
	NOCL-G	NITROSYL-CHLORIDE-GAS
	NOF	NITROSYL-FLUORIDE-GAS

INORGANIC Component Databank: Na

Alias	Name
NA	SODIUM
NA2	SODIUM-DIATOMIC-GAS
NA2(CN)2	DISODIUM-DICYANIDE-GAS
NA2(OH)2	DISODIUM-DIHYDROXIDE-GAS
NA2B4O7	DISODIUM-TETRABORATE
NA2BR2	DISODIUM-DIBROMIDE-GAS
NA2CL2	DISODIUM-DICHLORIDE-GAS
NA2CO3	SODIUM-CARBONATE
NA2CO3:1	SODIUM-CARBONATE:SOL-1
NA2CO3:2	SODIUM-CARBONATE:SOL-2
NA2CRO4	SODIUM-CHROMATE
NA2CRO4:A	SODIUM-CHROMATE:SOL-A
NA2CRO4:B	SODIUM-CHROMATE:SOL-B
NA2F2	DISODIUM-DIFLUORIDE-GAS
NA2MOO4	SODIUM-MOLYBDATE
NA2MOO4:A	SODIUM-MOLYBDATE:SOL-A
NA2MOO4:B	SODIUM-MOLYBDATE:SOL-B
NA2MOO4:C	SODIUM-MOLYBDATE:SOL-C
NA2MOO4:D	SODIUM-MOLYBDATE:SOL-D
NA2O	SODIUM-OXIDE
NA2O2	SODIUM-PEROXIDE
NA2O2:A	DISODIUM-PEROXIDE:SOL-A
NA2O2:B	DISODIUM-PEROXIDE:SOL-B
NA2O:A	SODIUM-OXIDE:SOL-A
NA2O:B	SODIUM-OXIDE:SOL-B
NA2O:C	SODIUM-OXIDE:SOL-C
NA2S	SODIUM-SULFIDE
NA2S2	DISODIUM-DISULFIDE
NA2S3	DISODIUM-TRISULFIDE
NA2S4	DISODIUM-TETRASULFIDE
NA2S:1	SODIUM-SULFIDE:SOL-1
NA2S:2	SODIUM-SULFIDE:SOL-2
NA2SI2O5	SODIUM-DISILICATE
NA2SI2O5:A	SODIUM-DISILICATE:SOL-A
NA2SI2O5:B	SODIUM-DISILICATE:SOL-B
NA2SI2O5:C	SODIUM-DISILICATE:SOL-C
NA2SIO3	SODIUM-SILICATE
NA2SO3	SODIUM-SULFITE
NA2SO4	SODIUM-SULFATE
NA2SO4-III	SODIUM-SULFATE-III

Alias	Name
NA2SO4:1	SODIUM-SULFATE:SOL-1
NA2SO4:4	SODIUM-SULFATE:SOL-4
NA2SO4:5	SODIUM-SULFATE:SOL-5
NA2TE	DISODIUM-TELLURIDE
NA2TI2O5	DISODIUM-DITITANIUM-PENTAOXIDE
NA2TI3O7	DISODIUM-TRITITANIUM-HEPTAOXIDE
NA2TIO3	DISODIUM-TITANIUM-TRIOXIDE
NA2TIO3:A	DISODIUM-TITANIUM-TRIOXIDE:SOL-A
NA2TIO3:B	DISODIUM-TITANIUM-TRIOXIDE:SOL-B
NA2WO4	SODIUM-TUNGSTATE
NA2WO4:1	SODIUM-TUNGSTATE:SOL-1
NA2WO4:2	SODIUM-TUNGSTATE:SOL-2
NA3ALCL6	TRISODIUM-HEXACHLOROALUMINATE
NA3ALF6	CRYOLITE
NA3ALF6:A	CRYOLITE:SOL-A
NA3ALF6:B	CRYOLITE:SOL-B
NA3ALF6:C	CRYOLITE:SOL-C
NA3AS	TRISODIUM-ARSENIDE
NA3ASO4	SODIUM-ARSENATE
NA3PO4	TRISODIUM-PHOSPHATE
NA3VO4	SODIUM-ORTHOVANADATE
NA4SIO4	SODIUM-ORTHOSILICATE
NA4V2O7	SODIUM-PYROVANADATE
NA6SI2O7	HEXASODIUM-DISILICON-HEPTAOXIDE
NAALCL4	SODIUM-TETRACHLOROALUMINATE
NAALO2	SODIUM-ALUMINATE
NAALO2:A	SODIUM-ALUMINATE:SOL-A
NAALO2:B	SODIUM-ALUMINATE:SOL-B
NAALSI2O6	JADEITE
NAALSI2O6-D	DEHYDRATED-ANALCITE
NAALSI3O8	ALBITE
NAALSI3O8-A	ANALBITE
NAALSIO4	NEPHELINE
NAALSIO4:A	NEPHELINE:SOL-A
NAALSIO4:B	NEPHELINE:SOL-B
NAALSIO4:C	NEPHELINE:SOL-C
NAB3O5	SODIUM-TRIBORATE
NABO2	SODIUM-METABORATE
NABR	SODIUM-BROMIDE
NACL	SODIUM-CHLORIDE
NACLO4	SODIUM-PERCHLORATE
NACLO4:A	SODIUM-PERCHLORATE:SOL-A
NACLO4:B	SODIUM-PERCHLORATE:SOL-B
NACN	SODIUM-CYANIDE
NAF	SODIUM-FLUORIDE
NAH	SODIUM-HYDRIDE
NAHCO3	SODIUM-BICARBONATE

Alias	Name
NAI	SODIUM-IODIDE
NANO2	SODIUM-NITRITE
NANO3	SODIUM-NITRATE
NANO3:1	SODIUM-NITRATE:SOL-1
NANO3:2	SODIUM-NITRATE:SOL-2
NAO	SODIUM-MONOXIDE-GAS
NAO2	SODIUM-SUPEROXIDE
NAOH	SODIUM-HYDROXIDE
NAOH:A	SODIUM-HYDROXIDE:SOL-A
NAOH:B	SODIUM-HYDROXIDE:SOL-B
NATE	SODIUM-TELLURIDE
NATE3	SODIUM-TRITELLURIDE
NAVO3	SODIUM-METAVANADATE
NAVO3:1	SODIUM-METAVANADATE:SOL-1
NAVO3:2	SODIUM-METAVANADATE:SOL-2

INORGANIC Component Databank: Nb

Alias	Name
NB	NIOBIUM
NB2C	DINIOBIUM-CARBIDE
NB2N	DINIOBIUM-NITRIDE
NB2O5	DINIOBIUM-PENTAOXIDE
NB5SI3	5-NIOBIUM-3-SILICON
NBB2	NIOBIUM-DIBORIDE
NBBR5	NIOBIUM-PENTABROMIDE
NBC	NIOBIUM-CARBIDE
NBC0.702	NIOBIUM-0.702-CARBIDE
NBC0.825	NIOBIUM-0.825-CARBIDE
NBCL2	NIOBIUM-DICHLORIDE
NBCL2.33	NIOBIUM-2.33-CHLORIDE
NBCL2.67	NIOBIUM-2.67-CHLORIDE
NBCL3	NIOBIUM-TRICHLORIDE
NBCL3.13	NIOBIUM-3.13-CHLORIDE
NBCL4	NIOBIUM-TETRACHLORIDE
NBCL5	NIOBIUM-PENTACHLORIDE
NBF5	NIOBIUM-PENTAFLUORIDE
NBFE2	NIOBIUM-2-IRON
NBI5	NIOBIUM-PENTAIODIDE
NBN	NIOBIUM-NITRIDE
NBN:A	NIOBIUM-NITRIDE:SOL-A
NBN:B	NIOBIUM-NITRIDE:SOL-B
NBO	NIOBIUM-MONOXIDE
NBO2	NIOBIUM-DIOXIDE
NBO2:A	NIOBIUM-DIOXIDE:SOL-A
NBO2:B	NIOBIUM-DIOXIDE:SOL-B
NBO2:C	NIOBIUM-DIOXIDE:SOL-C
NBO2CL	NIOBIUM-CHLORIDE-DIOXIDE
NBOCL2	NIOBIUM-DICHLORIDE-OXIDE

	Alias	Name
	NBOCL3	NIOBIUM-TRICHLORIDE-OXIDE
	NBSI2	NIOBIUM-2-SILICON

INORGANIC Component Databank: Nd

Alias	Name
ND	NEODYMIUM
ND2(SO4)3	NEODYMIUM-SULFATE
ND2O3	NEODYMIUM-OXIDE
ND2O3:A	NEODYMIUM-OXIDE:SOL-A
ND2O3:B	NEODYMIUM-OXIDE:SOL-B
ND2S3	NEODYMIUM-SULFIDE
ND2SE3	NEODYMIUM-SELENIDE
ND2TE3	NEODYMIUM-TELLURIDE
ND2ZR2O7	NEODYMIUM-ZIRCONIUM-HEPTAOXIDE
ND:A	NEODYMIUM:SOL-A
ND:B	NEODYMIUM:SOL-B
NDBR3	NEODYMIUM-BROMIDE
NDCL3	NEODYMIUM-CHLORIDE
NDF3	NEODYMIUM-FLUORIDE
NDH2	NEODYMIUM-DIHYDRIDE
NDI3	NEODYMIUM-IODIDE
NDI3:A	NEODYMIUM-IODIDE:SOL-A
NDI3:B	NEODYMIUM-IODIDE:SOL-B
NDOCL	NEODYMIUM-CHLORIDE-OXIDE
NDS	NEODYMIUM-MONOSULFIDE
NDSE	NEODYMIUM-MONOSELENIDE
NDTE	NEODYMIUM-MONOTELLURIDE

INORGANIC Component Databank: Ni

Alias	Name
NI	NICKEL
NI(CO)4	NICKEL-TETRACARBONYL-GAS
NI11AS8	11-NICKEL-8-ARSENIDE
NI2P	DINICKEL-PHOSPHIDE
NI2SIO4	DINICKEL-ORTHOSILICATE
NI3(ASO4)2	NICKEL-ARSENATE
NI3C	TRINICKEL-CARBIDE
NI3P	TRINICKEL-PHOSPHIDE
NI3S2	TRINICKEL-DISULFIDE
NI3S2:1	TRINICKEL-DISULFIDE:SOL-1
NI3S2:2	TRINICKEL-DISULFIDE:SOL-2
NI3S4	TRINICKEL-TETRASULFIDE
NI3SN	3-NICKEL-TIN
NI3SN2	3-NICKEL-2-TIN
NI3TI	3-NICKEL-TITANIUM
NI4B3	TETRANICKEL-TRIBORIDE
NI5AS2	5-NICKEL-2-ARSENIDE
NI5P2	PENTANICKEL-DIPHOSPHIDE
NI7SI13	7-NICKEL-13-SILICON

Alias	Name
NIAL2O4	NICKEL-DIALUMINIUM-TETRAOXIDE
NIAS	NICKEL-ARSENIDE
NIB	NICKEL-MONOBORIDE
NIBR	NICKEL-MONOBROMIDE-GAS
NIBR2	NICKEL-BROMIDE
NICL	NICKEL-MONOCHLORIDE-GAS
NICL2	NICKEL-CHLORIDE
NICO3	NICKEL-CARBONATE
NIF	NICKEL-MONOFLUORIDE-GAS
NIF2	NICKEL-FLUORIDE
NII	NICKEL-MONOIODIDE-GAS
NII2	NICKEL-IODIDE
NIO	NICKEL-OXIDE
NIO:A	NICKEL-OXIDE:SOL-A
NIO:B	NICKEL-OXIDE:SOL-B
NIO:C	NICKEL-OXIDE:SOL-C
NIS	NICKEL-SULFIDE
NIS0.84	NICKEL-0.84-SULFIDE
NIS2	NICKEL-DISULFIDE
NIS:A	NICKEL-SULFIDE:SOL-A
NIS:B	NICKEL-SULFIDE:SOL-B
NISB	NICKEL-ANTIMONY
NISE1.05	NICKEL-1.05-SELENIDE
NISE1.143	NICKEL-1.143-SELENIDE
NISE1.25	NICKEL-1.25-SELENIDE
NISE1.25:A	NICKEL-1.25-SELENIDE:SOL-A
NISE1.25:B	NICKEL-1.25-SELENIDE:SOL-B
NISE1.25:C	NICKEL-1.25-SELENIDE:SOL-C
NISE2	NICKEL-DISELENIDE
NISEO3	NICKEL-SELENITE
NISI	NICKEL-SILICON
NISO4	NICKEL-SULFATE
NITE1.1	NICKEL-1.1-TELLURIDE
NITI	NICKEL-TITANIUM
NITI2	NICKEL-2-TITANIUM
NITIO3	NICKEL-TITANIUM-TRIOXIDE
NIWO4	NICKEL-TUNGSTATE

INORGANIC Component Databank: Np

Alias	Name
NP	NEPTUNIUM
NP:A	NEPTUNIUM:SOL-A
NP:B	NEPTUNIUM:SOL-B
NP:C	NEPTUNIUM:SOL-C
NPCL3	NEPTUNIUM-TRICHLORIDE
NPCL4	NEPTUNIUM-TETRACHLORIDE
NPF3	NEPTUNIUM-TRIFLUORIDE
NPF6	NEPTUNIUM-HEXAFLUORIDE

	Alias	Name
	NPO2	NEPTUNIUM-DIOXIDE
	NPO3*H2O	NEPTUNIUM-TRIOXIDE-HYDRATE
	NPOCL2	NEPTUNIUM-DICHLORIDE-OXIDE

INORGANIC Component Databank: O

Alias	Name
O	OXYGEN-MONATOMIC-GAS
1/2-O2	1/2-OXYGEN
O2	OXYGEN
O2S	SULFUR-DIOXIDE
O3	OZONE
O3S	SULFUR-TRIOXIDE
OD	HYDROXYL-D1-GAS
OF2	OXYGEN-DIFLUORIDE-GAS
OH	HYDROXYL-GAS

INORGANIC Component Databank: Os

Alias	Name
OS	OSMIUM
OSO2	OSMIUM-DIOXIDE
OSO4-Y	OSMIUM-TETRAOXIDE-YELLOW
OSP2	OSMIUM-DIPHOSPHIDE
OSS2	OSMIUM-DISULFIDE
OSSE2	OSMIUM-DISELENIDE

INORGANIC Component Databank: P

Alias	Name
1/2-P2	1/2-PHOSPHORUS-P2
1/4-P4	1/4-PHOSPHORUS-P4
P-O	PHOSPHORUS-MONOXIDE-GAS
P-R	PHOSPHORUS-RED
P-W	PHOSPHORUS-WHITE
P2	PHOSPHORUS-DIATOMIC-GAS
P2O5-L	DIPHOSPHORUS-PENTAOXIDE-LIQID
P4	PHOSPHORUS-4-ATOMIC-GAS
P4O10	TETRAPHOSPHORUS-DECAOXIDE
P4O6	TETRAPHOSPHORUS-HEXAOXIDE-GAS
P4S10	PHOSPHORUS-PENTASULFIDE
P4S3	TETRAPHOSPHORUS-TRISULFIDE
P4S3:A	TETRAPHOSPHORUS-TRISULFIDE:SOL-A
P4S3:B	TETRAPHOSPHORUS-TRISULFIDE:SOL-B
P4S5	TETRAPHOSPHORUS-PENTASULFIDE
P4S6	TETRAPHOSPHORUS-HEXASULFIDE
P4S7	TETRAPHOSPHORUS-HEPTASULFIDE
PBR3	PHOSPHORUS-TRIBROMIDE-GAS
PCL3-G	PHOSPHORUS-TRICHLORIDE-GAS
PCL5-G	PHOSPHORUS-PENTACHLORIDE-GAS
PF3	PHOSPHORUS-TRIFLUORIDE-GAS
PF5	PHOSPHORUS-PENTAFLUORIDE-GAS
PH3	PHOSPHINE
PI3	PHOSPHORUS-TRIIODIDE-GAS

	Alias	Name
	PN	PHOSPHORUS-MONONITRIDE-GAS
	PO2	PHOSPHORUS-DIOXIDE-GAS
	POBR3	PHOSPHORUS-TRIBROMIDE-OXIDE-GAS
	POCL3	PHOSPHORUS-OXYCHLORIDE
	PS	PHOSPHORUS-MONOSULFIDE-GAS

INORGANIC Component Databank: Pb

Alias	Name
PB	LEAD
PB2	LEAD-DIATOMIC-GAS
PB2I4	DILEAD-TETRAIODIDE-GAS
PB2SIO4	DILEAD-ORTHOSILICATE
PB3(ASO4)2	LEAD-ARSENATE
PB3O4	TRILEAD-TETRAOXIDE
PB4SIO6	TETRALEAD-SILICATE
PBB2O4	LEAD-DIBORATE
PBB4O7	LEAD-TETRABORATE
PBBR	LEAD-MONOBROMIDE-GAS
PBBR2	LEAD-DIBROMIDE
PBBR4	LEAD-TETRABROMIDE-GAS
PBCL	LEAD-MONOCHLORIDE-GAS
PBCL2	LEAD-DICHLORIDE
PBCL4	LEAD-TETRACHLORIDE-GAS
PBCO3	LEAD-CARBONATE
PBF	LEAD-MONOFLUORIDE-GAS
PBF2	LEAD-DIFLUORIDE
PBF2:A	LEAD-DIFLUORIDE:SOL-A
PBF2:B	LEAD-DIFLUORIDE:SOL-B
PBF4	LEAD-TETRAFLUORIDE-GAS
PBH	LEAD-MONOHYDRIDE-GAS
PBI	LEAD-MONOIODIDE-GAS
PBI2	LEAD-DIIODIDE
PBI4	LEAD-TETRAIODIDE-GAS
PBMOO4	LEAD-MOLYBDATE
PBO*PBCO3	DILEAD-OXIDE-CARBONATE
PBO*PBSO4	DILEAD-OXIDE-SULFATE
2PBO*PBSO4	TRILEAD-DIOXIDE-SULFATE
3PBO*PBSO4	TETRALEAD-TRIOXIDE-SULFATE
4PBO*PBSO4	PENTALEAD-TETRAOXIDE-SULFATE
PBO-R	LEAD-OXIDE-RED
PBO-Y	LEAD-OXIDE-YELLOW-MASSICOT
PBO2	LEAD-DIOXIDE
PBS	LEAD-SULFIDE
PBSE	LEAD-SELENIDE
PBSEO3	LEAD-SELENITE
PBSEO4	LEAD-SELENATE
PBSIO3	LEAD-METASILICATE
PBSO4	LEAD-SULFATE

	Alias	Name
	PBSO4:A	LEAD-SULFATE:SOL-A
	PBSO4:B	LEAD-SULFATE:SOL-B
	PBTE	LEAD-TELLURIDE
	PBTIO3	LEAD-TITANIUM-TRIOXIDE
	PBTIO3:A	LEAD-TITANIUM-TRIOXIDE:SOL-A
	PBTIO3:B	LEAD-TITANIUM-TRIOXIDE:SOL-B
	PBWO4	LEAD-TUNGSTATE

INORGANIC Component Databank: Pd

Alias	Name
PD	PALLADIUM
PD4S	TETRAPALLADIUM-SULFIDE
PDCL2	PALLADIUM-CHLORIDE
PDF2	PALLADIUM-FLUORIDE
PDI2	PALLADIUM-IODIDE
PDI2:A	PALLADIUM-IODIDE:SOL-A
PDI2:B	PALLADIUM-IODIDE:SOL-B
PDO	PALLADIUM-OXIDE
PDS	PALLADIUM-SULFIDE
PDS2	PALLADIUM-DISULFIDE
PDTE	PALLADIUM-TELLURIDE

INORGANIC Component Databank: Pr

Alias	Name
PR	PRASEODYMIUM
PR2O3	PRASEODYMIUM-OXIDE
PR3S4	TRIPRASEODYMIUM-TETRASULFIDE
PR7O12	7-PRASEODYMIUM-12-OXIDE
PR:A	PRASEODYMIUM:SOL-A
PR:B	PRASEODYMIUM:SOL-B
PRBR3	PRASEODYMIUM-BROMIDE
PRCL3	PRASEODYMIUM-CHLORIDE
PRF3	PRASEODYMIUM-FLUORIDE
PRH2	PRASEODYMIUM-DIHYDRIDE
PRI3	PRASEODYMIUM-IODIDE
PRO1.833	PRASEODYMIUM-1.833-OXIDE
PRO1.833:A	PRASEODYMIUM-1.833-OXIDE:SOL-A
PRO1.833:B	PRASEODYMIUM-1.833-OXIDE:SOL-B
PRO2	PRASEODYMIUM-DIOXIDE
PRS	PRASEODYMIUM-MONOSULFIDE

INORGANIC Component Databank: Pt

Alias	Name
PT	PLATINUM
PT5SE4	PENTAPLATINUM-TETRASELENIDE
PTBR2	PLATINUM-DIBROMIDE
PTBR3	PLATINUM-TRIBROMIDE
PTBR4	PLATINUM-TETRABROMIDE
PTCL2	PLATINUM-DICHLORIDE
PTCL3	PLATINUM-TRICHLORIDE
PTCL4	PLATINUM-TETRACHLORIDE

	Alias	Name
	PTI4	PLATINUM-TETRAIODIDE
	PTO2	PLATINUM-DIOXIDE-GAS
	PTS	PLATINUM-MONOSULFIDE
	PTS2	PLATINUM-DISULFIDE

INORGANIC Component Databank: Pu

Alias	Name
PU	PLUTONIUM
PU(SO4)2	PLUTONIUM-DISULFATE
PU2C3	DIPLUTONIUM-TRICARBIDE
PU2O3	DIPLUTONIUM-TRIOXIDE-ALPHA
PU2O3-B	DIPLUTONIUM-TRIOXIDE-BETA
PU2S3	DIPLUTONIUM-TRISULFIDE
PU:A	PLUTONIUM:SOL-A
PU:B	PLUTONIUM:SOL-B
PU:C	PLUTONIUM:SOL-C
PU:D	PLUTONIUM:SOL-D
PU:D1	PLUTONIUM:S.-D1
PU:E	PLUTONIUM:SOL-E
PUBR3	PLUTONIUM-TRIBROMIDE
PUC0.88	PLUTONIUM-0.88-CARBIDE
PUC2	PLUTONIUM-DICARBIDE
PUCL3	PLUTONIUM-TRICHLORIDE
PUF3	PLUTONIUM-TRIFLUORIDE
PUF4	PLUTONIUM-TETRAFLUORIDE
PUF6	PLUTONIUM-HEXAFLUORIDE
PUH2	PLUTONIUM-DIHYDRIDE
PUH3	PLUTONIUM-TRIHYDRIDE
PUI3	PLUTONIUM-TRIIODIDE
PUN	PLUTONIUM-NITRIDE
PUO	PLUTONIUM-OXIDE
PUO2	PLUTONIUM-DIOXIDE
PUOBR	PLUTONIUM-BROMIDE-OXIDE
PUOCL	PLUTONIUM-CHLORIDE-OXIDE
PUOF	PLUTONIUM-FLUORIDE-OXIDE
PUOI	PLUTONIUM-IODIDE-OXIDE
PUS	PLUTONIUM-MONOSULFIDE

INORGANIC Component Databank: Rb

Alias	Name
RB	RUBIDIUM
RB2	RUBIDIUM-DIATOMIC-GAS
RB2CL2	DIRUBIDIUM-DICHLORIDE-GAS
RB2CO3	RUBIDIUM-CARBONATE
RB2CO3:1	RUBIDIUM-CARBONATE:SOL-1
RB2CO3:2	RUBIDIUM-CARBONATE:SOL-2
RB2F2	DIRUBIDIUM-DIFLUORIDE-GAS
RB2O	RUBIDIUM-OXIDE
RB2O:A	RUBIDIUM-OXIDE:SOL-A

	Alias	Name
	RB2O:B	RUBIDIUM-OXIDE:SOL-B
	RB2O:C	RUBIDIUM-OXIDE:SOL-C
	RB2SI2O5	RUBIDIUM-DISILICATE
	RB2SI4O9	RUBIDIUM-TETRASILICATE
	RB2SIO3	RUBIDIUM-METASILICATE
	RB2SO4	RUBIDIUM-SULFATE
	RB2SO4:A	RUBIDIUM-SULFATE:SOL-A
	RB2SO4:B	RUBIDIUM-SULFATE:SOL-B
	RB3ASO4	RUBIDIUM-ARSENATE
	RBBR	RUBIDIUM-BROMIDE
	RBCL	RUBIDIUM-CHLORIDE
	RBF	RUBIDIUM-FLUORIDE
	RBI	RUBIDIUM-IODIDE
	RBO2	RUBIDIUM-PEROXIDE

INORGANIC Component Databank: Re

Alias	Name
RE	RHENIUM
RE2O7	DIRHENIUM-HEPTAOXIDE
RE2O7:A	DIRHENIUM-HEPTAOXIDE:SOL-A
RE2O7:B	DIRHENIUM-HEPTAOXIDE:SOL-B
RE2S7	DIRHENIUM-HEPTASULFIDE
RE2TE5	DIRHENIUM-PENTATELLURIDE
RE2Y	2-RHENIUM-YTTRIUM
RE3AS7	TRIRHENIUM-HEPTAARSENIDE
RE5SI3	5-RHENIUM-3-SILICON
REASO4	RHENIUM-ARSENATE
REBR3	RHENIUM-TRIBROMIDE
RECL3	RHENIUM-TRICHLORIDE
REO2	RHENIUM-DIOXIDE
REO3	RHENIUM-TRIOXIDE
RES2	RHENIUM-DISULFIDE
RESI	RHENIUM-SILICON
RESI2	RHENIUM-2-SILICON

INORGANIC Component Databank: Rh

Alias	Name
RH	RHODIUM
RH2O3	DIRHODIUM-TRIOXIDE
RH3U	3-RHODIUM-URANIUM
RHCL2	RHODIUM-DICHLORIDE-GAS
RHCL3	RHODIUM-TRICHLORIDE
RHO2	RHODIUM-DIOXIDE-GAS

INORGANIC Component Databank: Ru

Alias	Name
RU	RUTHENIUM
RU3U	3-RUTHENIUM-URANIUM
RUCL3	RUTHENIUM-TRICHLORIDE
RUCL4	RUTHENIUM-TETRACHLORIDE-GAS
RUF5	RUTHENIUM-PENTAFLUORIDE

	Alias	Name
	RUO2	RUTHENIUM-DIOXIDE
	RUO3	RUTHENIUM-TRIOXIDE-GAS
	RUO4-G	RUTHENIUM-TETROXIDE-GAS
	RUS2	RUTHENIUM-DISULFIDE
	RUSE2	RUTHENIUM-DISELENIDE

INORGANIC Component Databank: S

Alias	Name
S	SULFUR
S-N	SULFUR-MONONITRIDE-GAS
1/2-S2	1/2-SULFUR-S2
S2	SULFUR-DIATOMIC-GAS
S2BR2	DISULFUR-DIBROMIDE-GAS
S2CL	DISULFUR-CHLORIDE-RADICAL-GAS
S2CL2	DISULFUR-DICHLORIDE
S2F10	DISULFUR-DECAFLUORIDE-GAS
S2O	DISULFUR-OXIDE-GAS
S3	SULFUR-TRIATOMIC-GAS
S4	SULFUR-4-ATOMIC-GAS
S5	SULFUR-5-ATOMIC-GAS
S6	SULFUR-6-ATOMIC-GAS
S7	SULFUR-7-ATOMIC-GAS
S8	SULFUR-8-ATOMIC-GAS
S:MO	SULFUR-RHOMBIC-MONOCLINIC:S.MO
S:RH	SULFUR-RHOMBIC-MONOCLINIC:S.RH
SCL	SULFUR-MONOCHLORIDE-GAS
SCL2-G	SULFUR-DICHLORIDE-GAS
SF	SULFUR-MONOFLUORIDE-GAS
SF2	SULFUR-DIFLUORIDE-GAS
SF3	SULFUR-TRIFLUORIDE-GAS
SF4	SULFUR-TETRAFLUORIDE-GAS
SF5	SULFUR-PENTAFLUORIDE-GAS
SF6-G	SULFUR-HEXAFLUORIDE-GAS
SO	SULFUR-MONOXIDE-GAS
SO2CL2-G	SULFONYL-DICHLORIDE-GAS
SO2F2	SULFONYL-DIFLUORIDE-GAS
SOCL2-G	SULFINYL-DICHLORIDE-GAS
SOF2	SULFINYL-DIFLUORIDE-GAS
SSF2	SULFINOTHIOYL-DIFLUORIDE-GAS

INORGANIC Component Databank: Sb

Alias	Name
SB	ANTIMONY
SB2	ANTIMONY-DIATOMIC-GAS
SB2(SO4)3	DIANTIMONY-TRISULFATE
SB2O3	DIANTIMONY-TRIOXIDE-CUBIC
SB2O3-O	DIANTIMONY-TRIOXIDE-ORTHORHOMBIC
SB2O3:A	DIANTIMONY-TRIOXIDE-CUBIC:SOL-A
SB2O3:B	DIANTIMONY-TRIOXIDE-CUBIC:SOL-B

Alias	Name
SB2O4	DIANTIMONY-TETRAOXIDE
SB2O5	DIANTIMONY-PENTAOXIDE
SB2S3	DIANTIMONY-TRISULFIDE-BLACK
SB2S4	DIANTIMONY-TETRASULFIDE-GAS
SB2SE3	DIANTIMONY-TRISELENIDE
SB2TE3	DIANTIMONY-TRITELLURIDE
SB3S2	TRIANTIMONY-DISULFIDE-GAS
SB4	ANTIMONY-4-ATOMIC-GAS
SB4O6	TETRAANTIMONY-HEXAOXIDE-GAS
SB4S3	TETRAANTIMONY-TRISULFIDE-GAS
SBBR3	ANTIMONY-TRIBROMIDE
SBCL	ANTIMONY-MONOCHLORIDE-GAS
SBCL3	ANTIMONY-TRICHLORIDE
SBCL5	ANTIMONY-PENTACHLORIDE-GAS
SBF	ANTIMONY-MONOFLUORIDE-GAS
SBF3	ANTIMONY-TRIFLUORIDE
SBH3	ANTIMONY-TRIHYDRIDE-GAS
SBI3	ANTIMONY-TRIIODIDE
SBO	ANTIMONY-OXIDE-GAS
SBOCL	ANTIMONY-CHLORIDE-OXIDE
SBR2	SULFUR-DIBROMIDE-GAS
SBS	ANTIMONY-SULFIDE-GAS
SBSE	ANTIMONY-SELENIDE-GAS
SBZN	ANTIMONY-ZINC

INORGANIC Component Databank: Sc

Alias	Name
SC	SCANDIUM
SC2O3	SCANDIUM-OXIDE
SC:A	SCANDIUM:SOL-A
SC:B	SCANDIUM:SOL-B
SCASO4	SCANDIUM-ARSENATE
SCBR3	SCANDIUM-BROMIDE
SCCL3	SCANDIUM-CHLORIDE
SCF3	SCANDIUM-FLUORIDE
SCN	SCANDIUM-NITRIDE

INORGANIC Component Databank: Se

Alias	Name
SE	SELENIUM
SE2	SELENIUM-DIATOMIC-GAS
SE2BR2	DISELENIUM-DIBROMIDE-GAS
SE2CL2	DISELENIUM-DICHLORIDE
SE3	SELENIUM-TRIATOMIC-GAS
SE4	SELENIUM-4-ATOMIC-GAS
SE5	SELENIUM-5-ATOMIC-GAS
SE6	SELENIUM-6-ATOMIC-GAS
SE7	SELENIUM-7-ATOMIC-GAS
SE8	SELENIUM-8-ATOMIC-GAS

	Alias	Name
	SEBR2	SELENIUM-DIBROMIDE-GAS
	SECL2	SELENIUM-DICHLORIDE-GAS
	SECL4	SELENIUM-TETRACHLORIDE
	SEF	SELENIUM-FLUORIDE-GAS
	SEF2	SELENIUM-DIFLUORIDE-GAS
	SEF4	SELENIUM-TETRAFLUORIDE-GAS
	SEF5	SELENIUM-PENTAFLUORIDE-GAS
	SEF6	SELENIUM-HEXAFLUORIDE-GAS
	SEO	SELENIUM-OXIDE-GAS
	SEO2	SELENIUM-DIOXIDE

INORGANIC Component Databank: Si

Alias	Name
SI	SILICON
SI2	SILICON-DIATOMIC-GAS
SI2H6-G	DISILANE-GAS
SI2TA	2-SILICON-TANTALUM
SI2TH	2-SILICON-THORIUM
SI2TH3	2-SILICON-3-THORIUM
SI2TI	2-SILICON-TITANIUM
SI2U	2-SILICON-URANIUM
SI2U3	2-SILICON-3-URANIUM
SI2V	2-SILICON-VANADIUM
SI2W	2-SILICON-TUNGSTEN
SI2ZR	2-SILICON-ZIRCONIUM
SI3	SILICON-TRIATOMIC-GAS
SI3N4	TRISILICON-TETRANITRIDE-ALPHA
SI3TA5	3-SILICON-5-TANTALUM
SI3TI5	3-SILICON-5-TITANIUM
SI3U	3-SILICON-URANIUM
SI3V5	3-SILICON-5-VANADIUM
SI3W5	3-SILICON-5-TUNGSTEN
SI3ZR5	3-SILICON-5-ZIRCONIUM
SI5TH3	5-SILICON-3-THORIUM
SI5U3	5-SILICON-3-URANIUM
SIBR	SILICON-MONOBROMIDE-GAS
SIBR2	SILICON-DIBROMIDE-GAS
SIBR3	SILICON-TRIBROMIDE-GAS
SIBR4	SILICON-TETRABROMIDE
SIC-C	SILICON-CARBIDE-CUBIC
SICL	SILICON-CHLORIDE-GAS
SICL2	SILICON-DICHLORIDE-GAS
SICL3	SILICON-TRICHLORIDE-GAS
SICL4-G	SILICON-TETRACHLORIDE-GAS
SIF	SILICON-FLUORIDE-GAS
SIF2	SILICON-DIFLUORIDE-GAS
SIF3	SILICON-TRIFLUORIDE-GAS
SIF4-G	SILICON-TETRAFLUORIDE-GAS

Alias	Name
SIH	SILICON-HYDRIDE-GAS
SIH4-G	SILANE-GAS
SII	SILICON-IODIDE-GAS
SII2	SILICON-DIIODIDE-GAS
SII3	SILICON-TRIIODIDE-GAS
SII4	SILICON-TETRAIODIDE
SIO	SILICON-OXIDE-GAS
SIO2	SILICON-DIOXIDE
SIO2-CR	SILICON-DIOXIDE-CRISTOBALITE
SIO2:HC	SILICON-DIOXIDE:S-HC
SIO2:HQ	SILICON-DIOXIDE:S-HQ
SIO2:LQ	SILICON-DIOXIDE:S-LQ
SIOF2	SILICON-DIFLUORIDE-OXIDE-GAS
SIP	SILICON-PHOSPHIDE
SIS	SILICON-SULFIDE-GAS
SIS2	SILICON-DISULFIDE
SISE	SILICON-SELENIDE-GAS
SITA2	SILICON-2-TANTALUM
SITH	SILICON-THORIUM
SITI	SILICON-TITANIUM
SIU	SILICON-URANIUM
SIU3	SILICON-3-URANIUM
SIV3	SILICON-3-VANADIUM
SIZR	SILICON-ZIRCONIUM
SIZR2	SILICON-2-ZIRCONIUM

INORGANIC Component Databank: Sm

Alias	Name
SM	SAMARIUM
SM2O3	DISAMARIUM-TRIOXIDE-CUBIC
SM2O3-M	DISAMARIUM-TRIOXIDE-MONOCLINIC
SM2O3-M:M1	DISAMARIUM-3-OXIDE-MONOCLINIC:M1
SM2O3-M:M2	DISAMARIUM-3-OXIDE-MONOCLINIC:M2
SM2ZR2O7	DISAMARIUM-DIZIRCONIUM-HEPTAOXID
SM:A	SAMARIUM:SOL-A
SM:B	SAMARIUM:SOL-B
SMC2	SAMARIUM-DICARBIDE
SMC2:A	SAMARIUM-DICARBIDE:SOL-A
SMC2:B	SAMARIUM-DICARBIDE:SOL-B
SMCL2	SAMARIUM-DICHLORIDE
SMCL3	SAMARIUM-TRICHLORIDE
SMOF	SAMARIUM-FLUORIDE-OXIDE
SMOF:A	SAMARIUM-FLUORIDE-OXIDE:SOL-A
SMOF:B	SAMARIUM-FLUORIDE-OXIDE:SOL-B

INORGANIC Component Databank: Sn

Alias	Name
SN	TIN-WHITE
SN(SO4)2	TIN-DISULFATE
SN2I4	DITIN-TETRAIODIDE-GAS
SN2S3	DITIN-TRISULFIDE
SN3(ASO4)2	TRITIN-ARSENATE
SN3S4	TRITIN-TETRASULFIDE
SNBR2	TIN-DIBROMIDE
SNBR4	TIN-TETRABROMIDE
SNCL	TIN-MONOCHLORIDE-GAS
SNCL2	TIN-DICHLORIDE
SNCL4	TIN-TETRACHLORIDE
SNF	TIN-MONOFLUORIDE-GAS
SNF2	TIN-DIFLUORIDE
SNH4	TIN-TETRAHYDRIDE-GAS
SNI2	TIN-DIIODIDE
SNI4	TIN-TETRAIODIDE
SNO	TIN-MONOXIDE
SNO2	TIN-DIOXIDE
SNS	TIN-MONOSULFIDE
SNS2	TIN-DISULFIDE
SNS:A	TIN-MONOSULFIDE:SOL-A
SNS:B	TIN-MONOSULFIDE:SOL-B
SNSE	TIN-MONOSELENIDE
SNSE2	TIN-DISELENIDE
SNSO4	TIN-MONOSULFATE
SNTE	TIN-MONOTELLURIDE

INORGANIC Component Databank: Sr

Alias	Name
SR	STRONTIUM
SR(OH)2	STRONTIUM-HYDROXIDE
SR2SIO4	STRONTIUM-ORTHOSILICATE
SR2TIO4	DISTRONTIUM-TITANIUM-TETRAOXIDE
SR2TIO4:1	DISTRONTIUM-TITANIUM-4-OXIDE:S-1
SR2TIO4:2	DISTRONTIUM-TITANIUM-4-OXIDE:S-2
SR3(ASO4)2	STRONTIUM-ARSENATE
SR3N2	TRISTRONTIUM-DINITRIDE
SR4TI3O10	TETRASTRONTIUM-TRITITANIUM-DECAO
SR:A	STRONTIUM:SOL-A
SR:C	STRONTIUM:SOL-C
SRAL2O4	STRONTIUM-DIALUMINIUM-TETRAOXIDE
SRAL2O4:A	STRONTIUM-DIALUMINIUM-4-OXIDE:A
SRAL2O4:B	STRONTIUM-DIALUMINIUM-4-OXIDE:B
SRBR	STRONTIUM-MONOBROMIDE-GAS
SRBR2	STRONTIUM-BROMIDE
SRBR2:A	STRONTIUM-BROMIDE:SOL-A
SRBR2:B	STRONTIUM-BROMIDE:SOL-B
SRC2	STRONTIUM-DICARBIDE

	Alias	Name
	SRCL	STRONTIUM-MONOCHLORIDE-GAS
	SRCL2	STRONTIUM-CHLORIDE
	SRCO3	STRONTIUM-CARBONATE
	SRCO3:A	STRONTIUM-CARBONATE:SOL-A
	SRCO3:B	STRONTIUM-CARBONATE:SOL-B
	SRF2	STRONTIUM-FLUORIDE
	SRF2:1	STRONTIUM-FLUORIDE:SOL-1
	SRF2:2	STRONTIUM-FLUORIDE:SOL-2
	SRF2:3	STRONTIUM-FLUORIDE:SOL-3
	SRH2	STRONTIUM-HYDRIDE
	SRI2	STRONTIUM-IODIDE
	SRMOO4	STRONTIUM-MOLYBDATE
	SRO	STRONTIUM-OXIDE
	SRO2	STRONTIUM-PEROXIDE
	SROH	STRONTIUM-MONOHYDROXIDE-GAS
	SRS	STRONTIUM-SULFIDE
	SRSIO3	STRONTIUM-METASILICATE
	SRSO4	STRONTIUM-SULFATE
	SRSO4:1	STRONTIUM-SULFATE:SOL-1
	SRSO4:2	STRONTIUM-SULFATE:SOL-2
	SRTIO3	STRONTIUM-TITANIUM-TRIOXIDE
	SRWO4	STRONTIUM-TUNGSTATE
	SRZRO3	STRONTIUM-ZIRCONIUM-TRIOXIDE

INORGANIC Component Databank: Ta

Alias	Name
TA	TANTALUM
TA2C	DITANTALUM-CARBIDE
TA2N	DITANTALUM-NITRIDE
TA2O5	DITANTALUM-PENTOXIDE
TAB2	TANTALUM-DIBORIDE
TABR5	TANTALUM-PENTABROMIDE
TAC	TANTALUM-MONOCARBIDE
TACL	TANTALUM-MONOCHLORIDE-GAS
TACL2	TANTALUM-DICHLORIDE-GAS
TACL2.5	TANTALUM-2.5-CHLORIDE
TACL3	TANTALUM-TRICHLORIDE
TACL4	TANTALUM-TETRACHLORIDE
TACL5	TANTALUM-PENTACHLORIDE
TAF5	TANTALUM-PENTAFLUORIDE
TAI5	TANTALUM-PENTAIODIDE
TAN	TANTALUM-MONONITRIDE
TAO	TANTALUM-MONOXIDE-GAS
TAO2	TANTALUM-DIOXIDE-GAS
TAO2CL	TANTALUM-CHLORIDE-DIOXIDE
TAOCL3	TANTALUM-TRICHLORIDE-OXIDE
TAS	TANTALUM-MONOSULFIDE-GAS
TAS2	TANTALUM-DISULFIDE

INORGANIC Component Databank: Tb

Alias	Name
TB	TERBIUM
TB2O3	DITERBIUM-TRIOXIDE
TB:A	TERBIUM:SOL-A
TB:B	TERBIUM:SOL-B
TBBR3	TERBIUM-TRIBROMIDE-GAS
TBCL3	TERBIUM-TRICHLORIDE
TBCL3:A	TERBIUM-TRICHLORIDE:SOL-A
TBCL3:B	TERBIUM-TRICHLORIDE:SOL-B
TBO1.72	TERBIUM-1.72-OXIDE
TBO1.81	TERBIUM-1.81-OXIDE
TBO2	TERBIUM-DIOXIDE
TBS	TERBIUM-SULFIDE-GAS
TBSE	TERBIUM-SELENIDE-GAS
TBTE	TERBIUM-TELLURIDE-GAS

INORGANIC Component Databank: Te

Alias	Name
TE	TELLURIUM
TE2	TELLURIUM-DIATOMIC-GAS
TE2O2	DITELLURIUM-DIOXIDE-GAS
TEBR4	TELLURIUM-TETRABROMIDE
TECL2	TELLURIUM-DICHLORIDE-GAS
TECL4	TELLURIUM-TETRACHLORIDE
TEF	TELLURIUM-MONOFLUORIDE-GAS
TEF2	TELLURIUM-DIFLUORIDE-GAS
TEF4	TELLURIUM-TETRAFLUORIDE-GAS
TEF5	TELLURIUM-PENTAFLUORIDE-GAS
TEF6	TELLURIUM-HEXAFLUORIDE-GAS
TEO	TELLURIUM-MONOXIDE-GAS
TEO2	TELLURIUM-DIOXIDE

INORGANIC Component Databank: Th

Alias	Name
TH	THORIUM
TH(SO4)2	THORIUM-DISULFATE
TH2N2O	DITHORIUM-DINITRIDE-MONOXIDE
TH2S3	DITHORIUM-TRISULFIDE
TH3N4	TRITHORIUM-TETRANITRIDE
TH3P4	TRITHORIUM-TETRAPHOSPHIDE
TH:A	THORIUM:SOL-A
TH:B	THORIUM:SOL-B
THBR4	THORIUM-TETRABROMIDE
THBR4:A	THORIUM-TETRABROMIDE:SOL-A
THBR4:B	THORIUM-TETRABROMIDE:SOL-B
THC1.94	THORIUM-1.94-CARBIDE
THC1.94:A	THORIUM-1.94-CARBIDE:SOL-A
THC1.94:B	THORIUM-1.94-CARBIDE:SOL-B
THC1.94:C	THORIUM-1.94-CARBIDE:SOL-C
THCL4	THORIUM-TETRACHLORIDE

Alias	Name
THCL4:A	THORIUM-TETRACHLORIDE:SOL-A
THCL4:B	THORIUM-TETRACHLORIDE:SOL-B
THF2	THORIUM-DIFLUORIDE-GAS
THF3	THORIUM-TRIFLUORIDE-GAS
THF4	THORIUM-TETRAFLUORIDE
THH2	THORIUM-DIHYDRIDE
THI4	THORIUM-TETRAIODIDE
THN	THORIUM-MONONITRIDE
THO	THORIUM-MONOXIDE-GAS
THO2	THORIUM-DIOXIDE
THOBR2	THORIUM-DIBROMIDE-OXIDE
THOCL2	THORIUM-DICHLORIDE-OXIDE
THOF2	THORIUM-DIFLUORIDE-OXIDE
THOI2	THORIUM-DIIODIDE-OXIDE
THP	THORIUM-MONOPHOSPHIDE
THRE2	THORIUM-2-RHENIUM
THS	THORIUM-MONOSULFIDE
THS2	THORIUM-DISULFIDE

INORGANIC Component Databank: Ti

Alias	Name
TI	TITANIUM
TI2O3	DITITANIUM-TRIOXIDE
TI2O3:A	DITITANIUM-TRIOXIDE:SOL-A
TI2O3:B	DITITANIUM-TRIOXIDE:SOL-B
TI3(ASO4)2	TRITITANIUM-DIARSENATE
TI3O5	TRITITANIUM-PENTOXIDE
TI3O5:A	TRITITANIUM-PENTOXIDE:SOL-A
TI3O5:B	TRITITANIUM-PENTOXIDE:SOL-B
TI4O7	TETRATITANIUM-HEPTAOXIDE
TI:A	TITANIUM:SOL-A
TI:B	TITANIUM:SOL-B
TIB	TITANIUM-MONOBORIDE
TIB2	TITANIUM-DIBORIDE
TIBR	TITANIUM-MONOBROMIDE-GAS
TIBR2	TITANIUM-DIBROMIDE
TIBR3	TITANIUM-TRIBROMIDE
TIBR4	TITANIUM-TETRABROMIDE
TIC	TITANIUM-MONOCARBIDE
TICL	TITANIUM-MONOCHLORIDE-GAS
TICL2	TITANIUM-DICHLORIDE
TICL3	TITANIUM-TRICHLORIDE
TICL4	TITANIUM-TETRACHLORIDE
TIF	TITANIUM-MONOFLUORIDE-GAS
TIF2	TITANIUM-DIFLUORIDE-GAS
TIF3	TITANIUM-TRIFLUORIDE
TIF4	TITANIUM-TETRAFLUORIDE
TIH2	TITANIUM-DIHYDRIDE

Alias	Name
TII	TITANIUM-MONOIODIDE-GAS
TII2	TITANIUM-DIIODIDE
TII3	TITANIUM-TRIIODIDE
TII4	TITANIUM-TETRAIODIDE
TII4:A	TITANIUM-TETRAIODIDE:SOL-A
TII4:B	TITANIUM-TETRAIODIDE:SOL-B
TIN	TITANIUM-MONONITRIDE
TIO	TITANIUM-MONOXIDE
TIO2	TITANIUM-DIOXIDE-RUTILE
TIO2-A	TITANIUM-DIOXIDE-ANATASE
TIO:A	TITANIUM-MONOXIDE:SOL-A
TIO:B	TITANIUM-MONOXIDE:SOL-B
TIOCL	TITANIUM-CHLORIDE-OXIDE-GAS
TIOCL2	TITANIUM-DICHLORIDE-OXIDE-GAS
TIOF	TITANIUM-FLUORIDE-OXIDE-GAS
TIOF2	TITANIUM-DIFLUORIDE-OXIDE-GAS
TIS	TITANIUM-MONOSULFIDE
TIS2	TITANIUM-DISULFIDE
TIS2:A	TITANIUM-DISULFIDE:SOL-A
TIS2:B	TITANIUM-DISULFIDE:SOL-B

INORGANIC Component Databank: TI

Alias	Name
TL	THALLIUM
TL2CL2	DITHALLIUM-DICHLORIDE-GAS
TL2F2	DITHALLIUM-DIFLUORIDE-GAS
TL2O	THALLIUM-OXIDE
TL2O3	DITHALLIUM-TRIOXIDE
TL2S	THALLIUM-SULFIDE
TL2SE	DITHALLIUM-SELENIDE
TL2SO4	THALLIUM-SULFATE
TL2SO4:A	THALLIUM-SULFATE:SOL-A
TL2SO4:B	THALLIUM-SULFATE:SOL-B
TL2TE	THALLIUM-TELLURIDE
TL:A	THALLIUM:SOL-A
TL:B	THALLIUM:SOL-B
TLASO4	THALLIUM-ARSENATE
TLBR	THALLIUM-BROMIDE
TLCL	THALLIUM-CHLORIDE
TLCL3	THALLIUM-TRICHLORIDE
TLF	THALLIUM-FLUORIDE
TLF:A	THALLIUM-FLUORIDE:SOL-A
TLF:B	THALLIUM-FLUORIDE:SOL-B
TLI	THALLIUM-IODIDE
TLI:A	THALLIUM-IODIDE:SOL-A
TLI:B	THALLIUM-IODIDE:SOL-B
TLSE	THALLIUM-SELENIDE
TLSE:A	THALLIUM-SELENIDE:SOL-A

	Alias	Name
	TLSE:B	THALLIUM-SELENIDE:SOL-B

INORGANIC Component Databank: Tm

Alias	Name
TM	THULIUM
TM2O3	DITHULIUM-TRIOXIDE
TM2O3:A	DITHULIUM-TRIOXIDE:SOL-A
TM2O3:B	DITHULIUM-TRIOXIDE:SOL-B
TMBR3	THULIUM-TRIBROMIDE-GAS
TMCL3	THULIUM-TRICHLORIDE
TMF3	THULIUM-TRIFLUORIDE
TMF3:A	THULIUM-TRIFLUORIDE:SOL-A
TMF3:B	THULIUM-TRIFLUORIDE:SOL-B
TMI3	THULIUM-TRIIODIDE-GAS

INORGANIC Component Databank: U

Alias	Name
U	URANIUM
U(SO4)2	URANIUM-DISULFATE
U2C3	DIURANIUM-TRICARBIDE
U2S3	DIURANIUM-TRISULFIDE
U3O8	TRIURANIUM-OCTAOXIDE-ORTHORHOMBI
U4O9	TETRAURANIUM-NONAOXIDE
U4O9:1	TETRAURANIUM-NONAOXIDE:SOL-1
U4O9:2	TETRAURANIUM-NONAOXIDE:SOL-2
U4O9:3	TETRAURANIUM-NONAOXIDE:SOL-3
U:A	URANIUM:SOL-A
U:B	URANIUM:SOL-B
U:C	URANIUM:SOL-C
UB12	URANIUM-DODECABORIDE
UB2	URANIUM-DIBORIDE
UB4	URANIUM-TETRABORIDE
UBR3	URANIUM-TRIBROMIDE
UBR4	URANIUM-TETRABROMIDE
UBR5	URANIUM-PENTABROMIDE
UC	URANIUM-MONOCARBIDE
UC1.94	URANIUM-1.94-CARBIDE
UCL3	URANIUM-TRICHLORIDE
UCL4	URANIUM-TETRACHLORIDE
UCL5	URANIUM-PENTACHLORIDE
UCL6	URANIUM-HEXACHLORIDE
UF3	URANIUM-TRIFLUORIDE
UF4	URANIUM-TETRAFLUORIDE
UF4.25	URANIUM-4.25-FLUORIDE
UF4.5	URANIUM-4.5-FLUORIDE
UF5	URANIUM-PENTAFLUORIDE
UF6	URANIUM-HEXAFLUORIDE
UH3-B	URANIUM-TRIHYDRIDE-BETA
UI3	URANIUM-TRIIODIDE

Alias	Name
UI4	URANIUM-TETRAIODIDE
UN	URANIUM-NITRIDE
UO2	URANIUM-DIOXIDE
UO2(NO3)2	URANIUM-DINITRATE-DIOXIDE
UO2BR2	URANIUM-DIBROMIDE-DIOXIDE
UO2CL2	URANIUM-DICHLORIDE-DIOXIDE
UO2F2	URANIUM-DIFLUORIDE-DIOXIDE
UO2SO4	URANIUM-SULFATE-DIOXIDE
UO3	URANIUM-TRIOXIDE-ORTHORHOMBIC
UO3*2H2O	URANIUM-TRIOXIDE-DIHYDRATE
UO3*H2O	URANIUM-TRIOXIDE-MONOHYDRATE
UOBR2	URANIUM-DIBROMIDE-OXIDE
UOBR3	URANIUM-TRIBROMIDE-OXIDE
UOCL	URANIUM-CHLORIDE-OXIDE
UOCL2	URANIUM-DICHLORIDE-OXIDE
UOCL3	URANIUM-TRICHLORIDE-OXIDE
US	URANIUM-SULFIDE
US2	URANIUM-DISULFIDE
USE	URANIUM-SELENIDE

INORGANIC Component Databank: V

Alias	Name
V	VANADIUM
V2C	DIVANADIUM-CARBIDE
V2O3	DIVANADIUM-TRIOXIDE
V2O4	DIVANADIUM-TETRAOXIDE
V2O4:1	DIVANADIUM-TETRAOXIDE:SOL-1
V2O4:2	DIVANADIUM-TETRAOXIDE:SOL-2
V2O5	DIVANADIUM-PENTAOXIDE
V3B2	TRIVANADIUM-DIBORIDE
V3B4	TRIVANADIUM-TETRABORIDE
VB	VANADIUM-BORIDE
VB2	VANADIUM-DIBORIDE
VBR2	VANADIUM-DIBROMIDE
VBR3	VANADIUM-TRIBROMIDE
VBR4	VANADIUM-TETRABROMIDE-GAS
VC0.88	VANADIUM-0.88-CARBIDE
VCL2	VANADIUM-DICHLORIDE
VCL3	VANADIUM-TRICHLORIDE
VCL4	VANADIUM-TETRACHLORIDE
VF3	VANADIUM-TRIFLUORIDE
VF4	VANADIUM-TETRAFLUORIDE
VF5	VANADIUM-PENTAFLUORIDE-GAS
VI2	VANADIUM-DIIODIDE
VI3	VANADIUM-TRIIODIDE
VN	VANADIUM-NITRIDE
VN0.465	VANADIUM-0.465-NITRIDE
VO	VANADIUM-OXIDE

	Alias	Name
	VO2	VANADIUM-DIOXIDE-GAS
	VOCL3	VANADIUM-TRICHLORIDE-OXIDE

INORGANIC Component Databank: W

Alias	Name
W	TUNGSTEN
W(CO)6	TUNGSTEN-HEXACARBONYL
W2C	DITUNGSTEN-CARBIDE
W2CL10	DITUNGSTEN-DECACHLORIDE-GAS
W2O6	DITUNGSTEN-HEXAOXIDE-GAS
W3O8	TRITUNGSTEN-OCTAOXIDE-GAS
W3O9	TRITUNGSTEN-NONAOXIDE-GAS
W4O12	TETRATUNGSTEN-DODECAOXIDE-GAS
WBR	TUNGSTEN-BROMIDE-GAS
WBR5	TUNGSTEN-PENTABROMIDE
WBR6	TUNGSTEN-HEXABROMIDE
WC	TUNGSTEN-CARBIDE
WCL	TUNGSTEN-CHLORIDE-GAS
WCL2	TUNGSTEN-DICHLORIDE
WCL4	TUNGSTEN-TETRACHLORIDE
WCL5	TUNGSTEN-PENTACHLORIDE
WCL6	TUNGSTEN-HEXACHLORIDE
WCL6:A1	TUNGSTEN-HEXACHLORIDE:S.-A1
WCL6:A2	TUNGSTEN-HEXACHLORIDE:S.-A2
WCL6:B	TUNGSTEN-HEXACHLORIDE:SOL-B
WF	TUNGSTEN-FLUORIDE-GAS
WF6	TUNGSTEN-HEXAFLUORIDE-GAS
WO	TUNGSTEN-OXIDE-GAS
WO2	TUNGSTEN-DIOXIDE
WO2.72	TUNGSTEN-2.72-OXIDE
WO2.90	TUNGSTEN-2.90-OXIDE
WO2.96	TUNGSTEN-2.96-OXIDE
WO2CL2	TUNGSTEN-DICHLORIDE-DIOXIDE
WO2I2	TUNGSTEN-DIIODIDE-DIOXIDE-GAS
WO3	TUNGSTEN-TRIOXIDE
WO3:1	TUNGSTEN-TRIOXIDE:SOL-1
WO3:2	TUNGSTEN-TRIOXIDE:SOL-2
WOCL4	TUNGSTEN-TETRACHLORIDE-OXIDE
WOF4	TUNGSTEN-TETRAFLUORIDE-OXIDE
WS2	TUNGSTEN-DISULFIDE

INORGANIC Component Databank: Y

Alias	Name
Y	YTTRIUM
Y2O3	DIYTTRIUM-TRIOXIDE
Y2O3:A	DIYTTRIUM-TRIOXIDE:SOL-A
Y2O3:B	DIYTTRIUM-TRIOXIDE:SOL-B
Y2ZR2O7	DIYTTRIUM-DIZIRCONIUM-HEPTAOXIDE
Y:A	YTTRIUM:SOL-A

	Alias	Name
	Y:B	YTTRIUM:SOL-B
	YASO4	YTTRIUM-ARSENATE
	YCL3	YTTRIUM-TRICHLORIDE
	YF3	YTTRIUM-TRIFLUORIDE
	YF3:A	YTTRIUM-TRIFLUORIDE:SOL-A
	YF3:B	YTTRIUM-TRIFLUORIDE:SOL-B
	YI3	YTTRIUM-TRIIODIDE
	YN	YTTRIUM-NITRIDE

INORGANIC Component Databank: Yb

Alias	Name
YB	YTTERBIUM
YB2O3	DIYTTERBIUM-TRIOXIDE
YB2O3:A	DIYTTERBIUM-TRIOXIDE:SOL-A
YB2O3:B	DIYTTERBIUM-TRIOXIDE:SOL-B
YB:A	YTTERBIUM:SOL-A
YB:B	YTTERBIUM:SOL-B
YBCL2	YTTERBIUM-DICHLORIDE
YBCL3	YTTERBIUM-TRICHLORIDE

INORGANIC Component Databank: Zn

Alias	Name
ZN	ZINC
ZN2SIO4	ZINC-ORTHOSILICATE-WILLEMITE
ZN2TIO4	DIZINC-TITANIUM-TETRAOXIDE
ZN3(ASO4)2	ZINC-ARSENATE
ZN3(PO4)2	ZINC-PHOSPHATE
ZN3AS2	ZINC-ARSENIDE
ZN3AS2:1	ZINC-ARSENIDE:SOL-1
ZN3AS2:2	ZINC-ARSENIDE:SOL-2
ZN3AS2:3	ZINC-ARSENIDE:SOL-3
ZN3N2	ZINC-NITRIDE
ZN3O(SO4)2	TRIZINC-DISULFATE-OXIDE
ZN3P2	TRIZINC-DIPHOSPHIDE
ZN3P2:1	TRIZINC-DIPHOSPHIDE:SOL-1
ZN3P2:2	TRIZINC-DIPHOSPHIDE:SOL-2
ZN3PO4-2:A	ZINC-PHOSPHATE:SOL-A
ZN3PO4-2:B	ZINC-PHOSPHATE:SOL-B
ZNBR2	ZINC-BROMIDE
ZNCL2	ZINC-CHLORIDE
ZNCO3	ZINC-CARBONATE
ZNF2	ZINC-FLUORIDE
ZNF2:A	ZINC-FLUORIDE:SOL-A
ZNF2:B	ZINC-FLUORIDE:SOL-B
ZNI2	ZINC-IODIDE
ZNO	ZINC-OXIDE
ZNP2	ZINC-DIPHOSPHIDE
ZNS	ZINC-SULFIDE-WURTZITE
ZNS-S	ZINC-SULFIDE-SPHALERITE

	Alias	Name
	ZNSE	ZINC-SELENIDE
	ZNSEO3	ZINC-SELENITE
	ZNSIO3	ZINC-METASILICATE
	ZNSO4	ZINC-SULFATE
	ZNSO4*2H2O	ZINC-SULFATE-DIHYDRATE
	ZNSO4*6H2O	ZINC-SULFATE-HEXAHYDRATE
	ZNSO4*7H2O	ZINC-SULFATE-HEPTAHYDRATE
	ZNSO4*H2O	ZINC-SULFATE-MONOHYDRATE
	ZNSO4:1	ZINC-SULFATE:SOL-1
	ZNSO4:2	ZINC-SULFATE:SOL-2
	ZNTE	ZINC-TELLURIDE
	ZNWO4	ZINC-TUNGSTATE

INORGANIC Component Databank: Zr

Alias	Name
ZR	ZIRCONIUM
ZR:A	ZIRCONIUM:SOL-A
ZR:B	ZIRCONIUM:SOL-B
ZRB2	ZIRCONIUM-DIBORIDE
ZRBR	ZIRCONIUM-MONOBROMIDE-GAS
ZRBR2	ZIRCONIUM-DIBROMIDE
ZRBR3	ZIRCONIUM-TRIBROMIDE
ZRBR4	ZIRCONIUM-TETRABROMIDE
ZRC	ZIRCONIUM-CARBIDE
ZRCL	ZIRCONIUM-MONOCHLORIDE-GAS
ZRCL2	ZIRCONIUM-DICHLORIDE
ZRCL3	ZIRCONIUM-TRICHLORIDE
ZRCL4	ZIRCONIUM-TETRACHLORIDE
ZRF	ZIRCONIUM-MONOFLUORIDE-GAS
ZRF2	ZIRCONIUM-DIFLUORIDE
ZRF3	ZIRCONIUM-TRIFLUORIDE
ZRF4	ZIRCONIUM-TETRAFLUORIDE
ZRF4:A	ZIRCONIUM-TETRAFLUORIDE:SOL-A
ZRF4:B	ZIRCONIUM-TETRAFLUORIDE:SOL-B
ZRH	ZIRCONIUM-HYDRIDE-GAS
ZRI	ZIRCONIUM-MONOIODIDE-GAS
ZRI2	ZIRCONIUM-DIIODIDE
ZRI3	ZIRCONIUM-TRIIODIDE
ZRI4	ZIRCONIUM-TETRAIODIDE
ZRN	ZIRCONIUM-NITRIDE
ZRO	ZIRCONIUM-MONOXIDE-GAS
ZRO2	ZIRCONIUM-DIOXIDE
ZRO2:A	ZIRCONIUM-DIOXIDE:SOL-A
ZRO2:B	ZIRCONIUM-DIOXIDE:SOL-B
ZRS	ZIRCONIUM-MONOSULFIDE-GAS
ZRS2	ZIRCONIUM-DISULFIDE
ZRSIO4	ZIRCONIUM-ORTHOSILICATE

INORGANIC Component Databank: Other Elements

Alias	Name
ALBITE-HIGH	NAALSI3O8-H
ALUNITE	KAL3(OH)6(SO4)2
AM	AMERICIUM
AM:A	AMERICIUM:SOL-A
AM:B	AMERICIUM:SOL-B
AM:C	AMERICIUM:SOL-C
ANALCITE	NAALSI2O6*H2O
ANDRADITE	CA3FE2SI3O12
ANNITE	KFE3(ALSI3)O10(OH)2
ANTHOPHYLLIT	ANTHOPHYLLITE
ANTIGORITE	MG48SI34O85(OH)62
AR	ARGON
ARTINITE	MG2(OH)2(CO3)*3H2O
AZURITE	CU3(OH)2(CO3)2
BR	BROMINE-MONATOMIC-GAS
BR2	BROMINE
CHRYSOTILE	MG3SI2O5(OH)4
CLINOCHL-14A	MG5AL(ALSI3)O10(OH)8-14A
CLINOCHLO-7A	MG5AL(ALSI3)O10(OH)8-7A
CLINOZOISITE	CA2AL3SI3O12(OH)-C
CORDIERITE-H	MG2AL3(ALSI5)O18*H20
DIASPORE-D	ALO(OH)-D
DICKITE	AL2SI2O7*2H2O-D
DOLOMITE-D	CAMG(CO3)2-D
DOLOMITE-O	CAMG(CO3)2-O
E-	ELECTRON-GAS
EPIDOTE	CA2FEAL2SI3O12(OH)
EPIDOTE-O	CA2FEAL2SI3O12(OH)-O
F	FLUORINE-MONATOMIC-GAS
F2	FLUORINE
HALLOYSITE	AL2SI2O7*2H2O-H
HE	HELIUM
HEDENBERGITE	CAFE(SIO3)2
HUNTITE	CAMG3(CO3)4
HYDROMAGNES I	MG5(OH)2(CO3)4*4H20
I	IODINE-MONATOMIC-GAS
I2	IODINE
KAOLINITE	AL2SI2O7*2H2O
KR	KRYPTON
LAUMONTITE	CA(AL2SI4)O12*4H2O
LAWSONITE	CAAL2SI2O8*2H2O
LU	LUTETIUM
LU2O3	LUTETIUM-OXIDE
MALACHITE	CU2(OH)2(CO3)
MARGARITE	CAAL2(AL2SI2)O10(OH)2
MUSCOVITE	KAL3SI3O10(OH)2

Alias	Name
NE	NEON
NESQUEHONITE	MGCO3*3H2O
PA	PROTACTINIUM
PA:A	PROTACTINIUM:SOL-A
PA:B	PROTACTINIUM:SOL-B
PARAGONITE	NAAL2(ALSI3)O10(OH)2
PARGASITE	NA(CA2MG4AL)(AL2SI6)O22(OH)2
PHLOGOPITE	KMG3(ALSI3)O10(OH)2
PREHNITE	CA2AL2SI3O10(OH)2
PYROPHYLLITE	AL2SI4O10(OH)2
RN-G	RADON-MONATOMIC-GAS
SEPIOLITE	MG4SI6O15(OH)2(H2O)2*4H2O
TALC	MG3SI4O10(OH)2
TC	TECHNETIUM
TC2O7	DITECHNETIUM-HEPTAOXIDE
TCO2	TECHNETIUM-DIOXIDE
TCO3	TECHNETIUM-TRIOXIDE
TREMOLITE	CA2MG5SI8O23*H2O
WAIRAKITE	CA(AL2SI4)O12*2H2O
XE	XENON
ZOISITE	CA2AL3SI3O12(OH)-A

Solids Component Databank

The tables below list the components present in the SOLIDS component databank.

Components beginning with:

Ag	Al	Au	B	Ba	Be	Bi	C	Ca	Cd
Ce	Co	Cr	Cs	Cu	Dy	Er	Eu	Fe	Ga
Gd	H	Hg	Ho	In	K	La	Li	Lu	Mg
Mn	Mo	N	Na	Nb	Nd	Ni	P	Pa	Pb
Pd	Pr	Pt	Ra	Rb	Sb	Sc	Si	Sm	Sn
Sr	Tb	Th	Ti	Tl	U	V	W	Y	Yb
Zn	Zr	Other Elements							

SOLIDS Component Databank Parameters

Parameter Name	Description
ATOMNO	Vector containing the atom types (atomic numbers) for a given molecule (e.g., H=1, C=6, O=8). Must use the vector NOATOM to define the number of occurrences of each atom.
CPIG	Ideal gas heat capacity coefficient
CPSPO1	Solid heat capacity coefficients
DGFORM	Standard free energy of formation
DGSFRM	Solids free energy of formation at 25ºC
DHFORM	Standard heat of formation
DHLSF	Heat of fusion at TFP
DHSFRM	Solids heat of formation at 25ºC
DHVLB	Heat of vaporization at TB
DHVLWT	Watson heat of vaporization parameters
MW	Molecular weight
NOATOM	Vector containing the number of occurrences of each atom defined in ATOMNO for a given molecule. ATOMNO and NOATOM define the chemical formula of the molecule.
OMEGA	Pitzer acentric factor
PC	Critical pressure
PLXANT	Antoine liquid vapor pressure coefficients
PSANT	Antoine solid vapor pressure coefficients
TB	Boiling point
TC	Critical temperature
TFP	Freezing point

Parameter Name	Description
VC	Critical volume
VSPOLY	Solid molar volume coefficients
ZC	Critical compressibility factor

Vectors ATOMNO and NOATOM together form the chemical formula of the compound. They are used to calculate molecular weight and are used in RGIBBS

DGFORM and DHFORM are calculated for Ideal gas at 25°C

SOLIDS Component Databank: Ag

Alias	Name
AG	SILVER
AG2C2	AG2C2
AG2C2O4	AG2C2O4
AG2H3IO6	AG2H3IO6
AG2HGI4	AG2HGI4
AG2HVO4	AG2HVO4
AG2MOO4	AG2MOO4
AG2N2O2	AG2N2O2
AG2PTBR6	AG2PTBR6
AG2PTCL6	AG2PTCL6
AG2S2O6*2W	AG2S2O6*2H2O
AG2SEO3	AG2SEO3
AG2SEO4	AG2SEO4
AG2SO3	AG2SO3
AG3C2CL	AG2C2*AGCL
AG3C2I	AG2C2*AGI
AG3C2NO3	AG2C2*AGNO3
AG3H2VO5	AG2HVO4*AGOH
AG3I4H*7W	(AGI)3*HI*7H2O
AG3IN2O6	AG3I(NO3)2
AG3N	AG3N
AG3P3O9*W	(AGPO3)3*H2O
AG3PO4	AG3PO4
AG4C2I2	AG2C2*2AGI
AG4C2SO4	AG2C2*AG2SO4
AG4FEC6N6*W	AG4FE(CN)6*H2O
AG4P2O7	AG4P2O7
AG5C4CL	(AG2C2)2*AGCL
AG6C4SO4	(AG2C2)2*AG2SO4
AGAUF4	AGAUF4
AGBR	SILVER-BROMIDE
AGBR*1.5NH3	AGBR*1.5NH3
AGBR4AL	AGBR*ALBR3
AGBR7AL2	AGBR*2ALBR3
AGBRCH5N	AGBR*CH3NH2
AGBRNH3	AGBR*NH3

Alias	Name
AGCH3CO2	SILVER-ACETATE
AGCL	SILVER-CHLORIDE
AGCL*1.5NH3	AGCL*1.5NH3
AGCL*NH3	AGCL*NH3
AGCL4AL	AGCL*ALCL3
AGCLCH5N	AGCL*CH3NH2
AGCLO2	AGCLO2
AGCLO4	AGCLO4
AGCN2	SILVER-CYANAMIDE
AGCN2H3	AGCN*NH3
AGF*2W	AGF*2H2O
AGF*4W	AGF*4H2O
AGF2	AGF2
AGI	SILVER-IODIDE
AGI*0.5NH3	AGI*0.5NH3
AGI*0.5PH3	AGI*0.5PH3
AGINH3	AGI*NH3
AGIO3	AGIO3
AGN2H6CLO4	AG(NH3)2CLO4
AGN3	AGN3
AGN3H6O3	AG(NH3)2NO3
AGN3H9BR	AG(NH3)3BR
AGN3H9CL	AG(NH3)3CL
AGN3H9CLO4	AG(NH3)3CLO4
AGN4H9O3	AG(NH3)3NO3
AGNO2	AGNO2
AGOCN	SILVER-CYANATE
AGONC	SILVER-FULMINATE
AGREO4	AGREO4
AGSCN	SILVER-THIOCYANATE
AGVO3	AGVO3

SOLIDS Component Databank: AI

Alias	Name
AL	ALUMINIUM
AL(OH)3	ALUMINIUM-HYDROXIDE
AL2CL9ZN1.5	AL2CL6*1.5ZNCL2
AL2NABR6CL	(ALBR3)2*NACL
AL2NABR7	(ALBR3)2*NABR
AL2O3	ALUMINIUM-OXIDE-ALPHA-CORUNDUM
AL2O3-2	ALUMINIUM-OXIDE-ALUMINA
AL2S3O12*18W	AL2(SO4)3*18H2O
AL2S3O12*6W	ALUMINUM-SULFATE-HEXAHYDRATE
AL2SIO5-S	ALUMINIUM-SILICATE-SILLIMANITE
AL6SI2O13	MULLITE
ALB12-A	ALB12-ALPHA
ALBR3*14NH3	ALBR3*14NH3
ALBR3*3NH3	ALBR3*3NH3

Alias	Name
ALBR3*5NH3	ALBR3*5NH3
ALBR3*6NH3	ALBR3*6NH3
ALBR3*7NH3	ALBR3*7NH3
ALBR3*9NH3	ALBR3*9NH3
ALBR3*H2S	ALBR3*H2S
ALBR3*NABR	ALBR3*NABR
ALBR3*NACL	ALBR3*NACL
ALBR3*NH3	ALBR3*NH3
ALBR3*PH3	ALBR3*PH3
ALC3H9	AL(CH3)3
ALC6H9O6	ALUMINUM-ACETATE
ALCL3*0.5SO2	ALCL3*0.5SO2
ALCL3*14NH3	ALCL3*14NH3
ALCL3*3NH3	ALCL3*3NH3
ALCL3*5NH3	ALCL3*5NH3
ALCL3*6NH3	ALCL3*6NH3
ALCL3*7NH3	ALCL3*7NH3
ALCL3*H2S	ALCL3*H2S
ALCL3*NABR	ALCL3*NABR
ALCL3*NACL	ALCL3*NACL
ALCL3*NH3	ALCL3*NH3
ALCL3*NH4CL	ALCL3*NH4CL
ALCL3*PH3	ALCL3*PH3
ALCL3*SO2	ALCL3*SO2
ALCL4N7H22	ALCL3*NH4CL*6NH3
ALI3*13NH3	ALI3*13NH3
ALI3*20NH3	ALI3*20NH3
ALI3*2H2S	ALI3*2H2S
ALI3*3NH3	ALI3*3NH3
ALI3*5NH3	ALI3*5NH3
ALI3*6NH3	ALI3*6NH3
ALI3*7NH3	ALI3*7NH3
ALI3*9NH3	ALI3*9NH3
ALI3*NH3	ALI3*NH3
ALN3O9*6W	ALUMINUM-NITRATE-HEXAHYDRATE
ALN3O9*9W	ALUMINUM-NITRATE-NONAHYDRATE
ALO(OH)	BOEHMITE-ALO(OH)

SOLIDS Component Databank: Au

Alias	Name
AU	GOLD
AU2PB	AU2PB
AUBR*2NH3	AUBR*2NH3
AUBR*3NH3	AUBR*3NH3
AUBR*4NH3	AUBR*4NH3
AUBR*6NH3	AUBR*6NH3
AUBR*NH3	AUBR*NH3
AUBR3	AUBR3

Alias	Name
AUCL*2NH3	AUCL*2NH3
AUCL*NH3	AUCL*NH3
AUCL3*2W	AUCL3*2H2O
AUI*2NH3	AUI*2NH3
AUI*3NH3	AUI*3NH3
AUI*6NH3	AUI*6NH3
AUI*NH3	AUI*NH3
AUI*PH3	AUI*PH3
AUIN	AUIN
AUIN2	AUIN2
AUPB2	AUPB2

SOLIDS Component Databank: B

Alias	Name
B	BORON
B10H14	DECABORANE
B13P2	B13P2
B2O3	BORON-OXIDE
B3N3H3CL3	TRICHLOROBORAZOLE-BETA
BC4H12NH2	B(CH3)3*NH2CH3
BF3*PC3H9	BF3*P(CH3)3
BH3NH2CH3	BH3NH2CH3
BO3C3H9*NH3	B(OCH3)3*NH3
BO3C6H12N	TRIETHANOLAMINE-BORATE

SOLIDS Component Databank: Ba

Alias	Name
BA	BARIUM
BA(C2H5O)2	BA(C2H5O)2
BA(CH3CO2)2	BA(CH3CO2)2
BA(CH3CO3)2	BA(CH2OHCO2)2
BA(CN)2	BA(CN)2
BA(CN)2*2W	BA(CN)2*2H2O
BA(CN)2*W	BA(CN)2*H2O
BA(CNO)2	BA(CNO)2
BA(H2PO2)2*W	BA(H2PO2)2*H2O
BA(H2PO4)2	BA(H2PO4)2
BA(HCO2)2	BA(HCO2)2
BA(IO3)2	BA(IO3)2
BA(IO3)2*W	BA(IO3)2*H2O
BA(NH2)2	BA(NH2)2
BA(NH3)6	BA(NH3)6
BA(NO2)2	BA(NO2)2
BA(NO2)2*W	BA(NO2)2*H2O
BA(REO4)2*4W	BA(REO4)2*4H2O
BA2AL2O5*5W	(BAO)2*AL2O3*5H2O
BA2N	BA2N
BA2NBR	BA2NBR
BA2NCL	BA2NCL

Alias	Name
BA2TL(NO2)5	(BA(NO2)2)2*TLNO2
BA3(ASO4)2-P	BARIUM-ARSENATE-PRECIPITATE
BA3(RHCL6)2	BA3(RHCL6)2
BA3AL4CL18	(BACL2)3*2AL2CL6
BA3P2O8	BA3(PO4)2-COLLOIDAL
BA3WO6	BA3WO6
BA6NI9	BA6NI9
BAAL4	BAAL4
BABR2*2NH3	BABR2*2NH3
BABR2*2W	BABR2*2H2O
BABR2*4NH3	BABR2*4NH3
BABR2*8NH3	BABR2*8NH3
BABR2*BAO*2W	BABR2*BAO*2H2O
BABR2*BAO*5W	BABR2*BAO*5H2O
BABR2*NH3	BABR2*NH3
BABR2*W	BABR2*H2O
BABR2O6	BA(BRO3)2
BABR2O6*W	BA(BRO3)2*H2O
BAC2O4	BAC2O4
BAC2O4*0.5W	BAC2O4*0.5H2O
BAC2O4*2W	BAC2O4*2H2O
BAC2O4*3.5W	BAC2O4*3.5H2O
BAC4H14S2O10	BA(C2H5SO4)2*2H2O
BAC4H6O4*3W	BA(CH3CO2)2*3H2O
BACA(CO3)2	BACA(CO3)2
BACL2*2W	BACL2*2H2O
BACL2*8NH3	BACL2*8NH3
BACL2*AL2CL6	BACL2*AL2CL6
BACL2*BAO*3W	BACL2*BAO*3H2O
BACL2*BAO*5W	BACL2*BAO*5H2O
BACL2*BAO*8W	BACL2*BAO*8H2O
BACL2*W	BACL2*H2O
BACL2O4	BA(CLO2)2
BACL2O4*3.5W	BA(CLO2)2*3.5H2O
BACL2O6	BA(CLO3)2
BACL2O6*W	BA(CLO3)2*H2O
BACL2O8	BA(CLO4)2
BACL2O8*2NH3	BA(CLO4)2*2NH3
BACL2O8*3W	BA(CLO4)2*3H2O
BACL2O8*6NH3	BA(CLO4)2*6NH3
BACLF	BACLF
BACLH	BACLH
BACN2	BACN2
BACO3	BARIUM-CARBONATE
BACS3	BACS3
BAF2	BARIUM-FLUORIDE
BAH4AS2O8*2W	BA(H2ASO4)2*2H2O

Alias	Name
BAH4P2O4	BA(H2PO2)2
BAH4S3O12*W	BASO4*2H2SO4*H2O
BAHASO4*W	BAHASO4*H2O
BAHPO4	BAHPO4
BAI2*10NH3	BAI2*10NH3
BAI2*2.5W	BAI2*2.5H2O
BAI2*2NH3	BAI2*2NH3
BAI2*2PBI	BAI2*2PBI2
BAI2*2SO2	BAI2*2SO2
BAI2*2W	BAI2*2H2O
BAI2*4NH3	BAI2*4NH3
BAI2*4SO2	BAI2*4SO2
BAI2*6NH3	BAI2*6NH3
BAI2*7W	BAI2*7H2O
BAI2*8NH3	BAI2*8NH3
BAI2*9NH3	BAI2*9NH3
BAI2*BAO*2W	BAI2*BAO*2H2O
BAI2*BAO*9W	BAI2*BAO*9H2O
BAI2*W	BAI2*H2O
BAIH	BAIH
BAMG2	BAMG2
BAMNO4	BAMNO4
BAMOO3	BAMOO3
BAN2	BAN2
BAN6*W	BA(N3)2*H2O
BANH	BANH
BAO*2SIO2	BAO*2SIO2
BAO*AL2O3	BAO*AL2O3
BAO*AL2O3*2W	BAO*AL2O3*2H2O
BAO*AL2O3*4W	BAO*AL2O3*4H2O
BAO*AL2O3*7W	BAO*AL2O3*7H2O
BAO*AL2O3*W	BAO*AL2O3*H2O
BAO*GEO2	BAO*GEO2
BAO*SIO2	BAO*SIO2
(BAO)2*3SIO2	(BAO)2*3SIO2
(BAO)2*GEO2	(BAO)2*GEO2
(BAO)2*SIO2	(BAO)2*SIO2
(BAO)3*AL2O3	(BAO)3*AL2O3
(BAO)3*GEO2	(BAO)3*GEO2
3BAO*4C2H6O	(BAO)3*4C2H5OH
3BAO*4CH4O	(BAO)3*4CH3OH
BAO2H2*3W	BA(OH)2*3H2O
BAO2H2*8W	BA(OH)2*8H2O
BAO2H2*W	BA(OH)2*H2O
BAOSCL6	BAOSCL6
BAPB2I6*7W	BAI2*2PBI2*7H2O
BAPDCL4	BAPDCL4

Alias	Name
BAPTCL6	BAPTCL6
BAPTCL6*6W	BAPTCL6*6H2O
BARUO4*W	BARUO4*H2O
BAS2O3	BAS2O3
BAS2O6*2W	BAS2O6*2H2O
BAS2O8*4W	BAS2O8*4H2O
BAS4O6*2W	BAS4O6*2H2O
BASE	BASE
BASEO3	BASEO3
BASEO4	BASEO4
BASIF6	BASIF6
BASO3	BASO3
BASO4	BARIUM-SULFATE
BASO4*H2SO4	BASO4*H2SO4
BASRTIO4	BASRTIO4

SOLIDS Component Databank: Be

Alias	Name
BE	BERYLLIUM
BE2SIO4	BERYLLIUM-SILICATE-PHENACITE
BE3B2O6	TRIBERYLLIUM-DIBORATE
BEBR2*10NH3	BEBR2*10NH3
BEBR2*2H2S	BEBR2*2H2S
BEBR2*4NH3	BEBR2*4NH3
BEBR2*6NH3	BEBR2*6NH3
BECL2*12NH3	BECL2*12NH3
BECL2*2NH3	BECL2*2NH3
BECL2*4NH3	BECL2*4NH3
BECL2*4W	BECL2*4H2O
BECL2*6NH3	BECL2*6NH3
BECO3	BECO3
BEH2	BEH2
BEI2*13NH3	BEI2*13NH3
BEI2*2H2S	BEI2*2H2S
BEI2*4NH3	BEI2*4NH3
BEI2*6NH3	BEI2*6NH3
BEMOO4	BEMOO4
BEO*3AL2O3	BEO*3AL2O3
BEO*AL2O3	BEO*AL2O3
BESEO4	BESEO4
BESEO4*2W	BESEO4*2H2O
BESEO4*4W	BESEO4*4H2O
BESO4	BERYLLIUM-SULFATE
BESO4*W	BESO4*H2O

SOLIDS Component Databank: Bi

Alias	Name
BI	BISMUTH
BI(OH)2CL	BI(OH)2CL
BI(OH)3	BISMUTH-HYDROXIDE
BIOBR	BIOBR
BIONO3	BIONO3
BIOOH	BIOOH

SOLIDS Component Databank: C

Alias	Name
C	CARBON-GRAPHITE
C2H4O8S2K2	C2H2O2*2KHSO3
C2H5OK	C2H5OK
C2O3.5H4NA	CH2OHCOONA*0.5H2O
C2O4H3NA	CH(OH)2COONA
C3H9AS*BC3H9	(CH3)3AS*B(CH3)3
C3H9AS*BF3	(CH3)3AS*BF3
C3H9B*NH3	(CH3)3B*NH3
C3H9N*ALBR3	(CH3)3N*ALBR3
C3H9N*ALCL3	(CH3)3N*ALCL3
C3H9N*BC3H9	(CH3)3N*B(CH3)3
C3H9N*BH3	(CH3)3N*BH3
C3H9NB3H7	(CH3)3NB3H7
C3H9P*BC3H9	(CH3)3P*B(CH3)3
C4H11N*BC3H9	(C2H5)2NH*B(CH3)3
C4H11O2CS	C2H5OCS*C2H5OH
C4H11O2K	C2H5OK*C2H5OH
C4H12N*BH4	(CH3)4N*BH4
CCL3COONA	CCL3COONA
CH2OHCOONA	CH2OHCOONA
CH2SO4	METHYLENE-SULFATE
CH3COOK	CH3COOK
CH3COONH4	AMMONIUM-ACETATE

SOLIDS Component Databank: Ca

Alias	Name
CA	CALCIUM
CA(OH)2	CALCIUM-HYDROXIDE
CA10P6O24F2	CA10(PO4)6F2
CA10P6O26H2	CA10(PO4)6(OH)2
CA12AL14O33	(CAO)12*7AL2O3
CA2AL2O5	(CAO)2*AL2O3
CA2AL2O5*5W	(CAO)2*AL2O3*5H2O
CA2AL2SIO7	GEHLENITE
CA2B2O5	DICALCIUM-DIBORATE
CA2B2SI2O9	(CAO)2*B2O3*2SIO2
CA2B2SI2O9*W	(CAO)2*B2O3*2SIO2*H2O
CA2B6O11	(CAO)2*3B2O3
CA2B6O11*13W	(CAO)2*3B2O3*13H2O
CA2FE2O5	DICALCIUM-DIIRON-PENTAOXIDE

Alias	Name
CA2GEO4	(CAO)2*GEO2
CA2MGSI2O7	AKERMANITE
CA2N2O10.5H7	CA(NO3)2*CA(OH)2*2.5H2O
CA2N2O8H2	CA(NO3)2*CA(OH)2
CA2SIO4-B	LARNITE
CA2V2O7	CALCIUM-PYROVANADATE
CA3AL2O6	(CAO)3*AL2O3
CA3AL2O6*6W	(CAO)3*AL2O3*6H2O
CA3AL2SI2O10	(CAO)3*AL2O3*2SIO2
CA3AL4CL18	(CACL2)3*4ALCL3
CA3B2O6	TRICALCIUM-DIBORATE
CA3BI2	CA3BI2
CA3CL2O2	CACL2*2CAO
CA3GEO5	(CAO)3*GEO2
CA3MGSI2O8	MERWINITE
CA3O7C8H24	(CAO)3*4C2H5OH
CA3P2O8-A	CA3(PO4)2-ALPHA
CA3P2O8-B	CA3(PO4)2-BETA
CA3TI2O7	(CAO)3*2TIO2
CA3V2O8	(CAO)3*V2O5
CA4AL2O7	(CAO)4*AL2O3
CA4BR2O19H32	CABR2*3CAO*16H2O
CA4CL2O3	CACL2*3CAO
CA4CL2O3*16W	CACL2*3CAO*16H2O
CA4CL2O3*3W	CACL2*3CAO*3H2O
CA4I2O19H32	CAI2*3CAO*16H2O
CA4SI2O7F2	(CAO)3*2SIO2*CAF2
CA5I2O12	CA5(IO6)2
CA8H12P6O29	CA8H2(PO4)6*5H2O
CAAL2	CAAL2
CAAL2O4	CAO*AL2O3
CAAL2SI2O8	ANORTHITE
CAAL2SI6O16	CAO*AL2O3*6SIO2
CAAL2SIO6	PYROXENE
CAAL4	CAAL4
CAAL4O7	CAO*2AL2O3
CAALGASI2O8	CAALGASI2O8
CAB2F8	CA(BF4)2
CAB2O4	CALCIUM-DIBORATE
CAB4O7	CALCIUM-TETRABORATE
CABR2*2NH3	CABR2*2NH3
CABR2*6NH3	CABR2*6NH3
CABR2*6W	CABR2*6H2O
CABR2*8NH3	CABR2*8NH3
CABR2*NH3	CABR2*NH3
CABR2O6	CA(BRO3)2
CABRH	CABRH

Alias	Name
CAC2N2	CA(CN)2
CAC2O4	CAC2O4
CAC2O4*W	CAC2O4*H2O
CAC4H10O2	CA(C2H5O)2
CAC4H6O4	CA(CH3CO2)2
CAC4H6O4*W	CA(CH3CO2)2*H2O
CAC4H6O6	CA(CH2OHCO2)2
CAC4H6O6*3W	CA(CH2OHCO2)2*3H2O
CAC4H6O6*5W	CA(CH2OHCO2)2*5H2O
CAC8H22O4	CA(C2H5O)2*2C2H5OH
CACL2	CALCIUM-CHLORIDE
CACL2*2NH3	CACL2*2NH3
CACL2*2W	CACL2*2H2O
CACL2*4NH3	CACL2*4NH3
CACL2*4W	CACL2*4H2O
CACL2*6W	CACL2*6H2O
CACL2*8NH3	CACL2*8NH3
CACL2*NH3	CACL2*NH3
CACL2*W	CACL2*H2O
CACL2C6H18O3	CACL2*3C2H5OH
CACL2C8H24O4	CACL2*4C2H5OH
CACL2O4	CA(CLO2)2
CACL2O8	CA(CLO4)2
CACL2O8*4W	CA(CLO4)2*4H2O
CACL2O8*6NH3	CA(CLO4)2*6NH3
CACLH	CACLH
CACO3	CALCIUM-CARBONATE-CALCITE
CACO3-A	CALCIUM-CARBONATE-ARAGONITE
CAFESIO4	CAFESIO4
CAGEO3	CAO*GEO2
CAH12P2O9N2	CA(H2PO4)2*H2O*2NH3
CAH18P2O9N4	CA(H2PO4)2*H2O*4NH3
CAH2	CALCIUM-HYDRIDE
CAH2C2O4	CA(HCOO)2
CAH4P2O4	CA(H2PO2)2
CAH4P2O8	CA(H2PO4)2
CAH6P2O9	CA(H2PO4)2*H2O
CAH9P2O9N	CA(H2PO4)2*H2O*NH3
CAI2*2NH3	CAI2*2NH3
CAI2*6NH3	CAI2*6NH3
CAI2*8NH3	CAI2*8NH3
CAI2*8W	CAI2*8H2O
CAI2*NH3	CAI2*NH3
CAI2O6	CA(IO3)2
CAI2O6*6W	CA(IO3)2*6H2O
CAI2O6*W	CA(IO3)2*H2O
CAIH	CAIH

Alias	Name
CAMG(CO3)2	DOLOMITE
CAMG2CL6*2W	CACL2*2MGCL2*2H2O
CAMOO3	CAMOO3
CAN2H4	CA(NH2)2
CAN2O2*4W	CAN2O2*4H2O
CAN2O4	CA(NO2)2
CAN2O4*4W	CA(NO2)2*4H2O
CAN2O8C2H8	CA(NO3)2*2CH3OH
CAN6	CA(N3)2
CAN6*0.5W	CA(N3)2*0.5H2O
CAN6*1.5W	CA(N3)2*1.5H2O
CAN6*2N2H4	CA(N3)2*2N2H4
CAN6*4W	CA(N3)2*4H2O
CAN6*N2H4	CA(N3)2*N2H4
CAO	CALCIUM-OXIDE
CAO*FE2O3	CAO*FE2O3
CAO4H4	CA(OH)2*H2O2
CAOCL2	CA(OCL)CL
CAP2O6-B	CA(PO3)2-BETA
CAPB2I6	CAI2*2PBI2
CAPB2I6*7W	CAI2*2PBI2*7H2O
CAPB3	CAPB3
CAS2O6*4W	CAS2O6*4H2O-DITHIONATE
CASEO3*2W-1	CASEO3*2H2O
CASEO3*2W-2	CASEO3*2H2O-PRECIPITATED
CASEO4	CASEO4
CASEO4*2W	CASEO4*2H2O
CASO4	CALCIUM-SULFATE
CASO4*0.5W-B	CASO4*0.5H2O-BETA
CASO4-A	CASO4-SOLUBLE-ALPHA
CASO4-B	CASO4-SOLUBLE-BETA
2(CASO4)*W	2(CASO4)*H2O
CATIO3	CAO*TIO2
CATL	CATL
CAV2O6	CAO*V2O5

SOLIDS Component Databank: Cd

Alias	Name
CD	CADMIUM
CD2I6PB	(CDI2)2*PBI2
CD3C4N4O6H10	(CD(CN)2)2*CDO*5H2O
CD3N2	CADMIUM-NITRIDE
CD3P2	CADMIUM-PHOSPHIDE
CD3P2O8	CD3(PO4)2
CD3S2O10H2	(CDSO4)2*CD(OH)2
CD3SB2	CD3SB2
CD3SO8H4	CDSO4*2CD(OH)2
CDAS2	CDAS2

Alias	Name
CDB2O4	CD(BO2)2
CDBR2*4W	CADMIUM-BROMIDE-TETRAHYDRATE
CDBR2N12H36	CDBR2*12NH3
CDBR2N2H6	CDBR2*2NH3
CDBR2N6H18	CDBR2*6NH3
CDBR2NH3	CDBR2*NH3
CDBR3NH5O0.5	CDBR2*NH4BR*0.5H2O
CDBROH	CDBROH
CDC2N2	CADMIUM-CYANIDE
CDC2N2S2	CD(CNS)2
CDC2O4	CADMIUM-OXALATE
CDC2O7H6	CADMIUM-OXALATE-TRIHYDRATE
CDCL2*2.5W	CDCL2*2.5H2O
CDCL2*W	CADMIUM-CHLORIDE-HYDRATE
CDCL2N10H30	CDCL2*10NH3
CDCL2N2H6	CDCL2*2NH3
CDCL2N4H12	CDCL2*4NH3
CDCL2N6H18	CDCL2*6NH3
CDCL2NH3	CDCL2*NH3
CDCL2O8*6W	CADMIUM-PERCHLORATE-HEXAHYDRATE
CDCL3NH5O0.5	CDCL2*NH4CL*0.5H2O
CDCL4H2*7W	CDCL2*2HCL*7H2O
CDCL6N4H16	CDCL2*4NH4CL
CDH5S3.5O14	CDSO4*2.5H2SO4
CDI2N2H6	CDI2*2NH3
CDI2N6H18	CDI2*6NH3
CDI2O6	CADMIUM-IODATE
CDI3NH5O0.5	CDI2*NH4I*0.5H2O
CDIOH	CDIOH
CDN2H4	CADMIUM-AMIDE
CDN2O6	CADMIUM-NITRATE
CDN2O6*2W	CADMIUM-NITRATE-DIHYDRATE
CDN2O6*4W	CADMIUM-NITRATE-TETRAHYDRATE
CDN6	CADMIUM-AZIDE
CDO2N2C2	CADMIUM-FULMINATE
CDOHCL	CD(OH)CL
CDSEO4	CADMIUM-SELENATE
CDSEO4*W	CADMIUM-SELENATE-HYDRATE
CDSO4*W	CADMIUM-SULFATE-HYDRATE

SOLIDS Component Databank: Ce

Alias	Name
CE	CERIUM
CE2C6O12*10W	CE2(C2O4)3*10H2O
CE2S3O12*5W	CE2(SO4)3*5H2O
CE2S3O12*8W	CE2(SO4)3*8H2O
CE2SE3O9*10W	CE2(SEO3)3*10H2O

Alias	Name
CE3AL	CE3AL
CEAL2	CEAL2
CEAL4	CEAL4
CEAS	CEAS
CECL3*12NH3	CECL3*12NH3
CECL3*20NH3	CECL3*20NH3
CECL3*2NH3	CECL3*2NH3
CECL3*4NH3	CECL3*4NH3
CECL3*7W	CECL3*7H2O
CECL3*8NH3	CECL3*8NH3
CEF3*W	CEF3*H2O
CEHG4	CEHG4
CEI3O9	CE(IO3)3
CEI3O9*2W	CE(IO3)3*2H2O
CEN3O9	CE(NO3)3
CEN3O9*3W	CE(NO3)3*3H2O
CEN3O9*4W	CE(NO3)3*4H2O
CEN3O9*6W	CE(NO3)3*6H2O
CEOCL	CEOCL
CES2	CES2
CEZN	CEZN

SOLIDS Component Databank: Co

Alias	Name
CO2AL5	CO2AL5
CO2AS	CO2AS
CO2AS3	CO2AS3
CO2C	CO2C
CO2N11H17O13	(CO(NH3)5H2O)(CO(NO2)6)
CO2N12H18O12	(CO(NH3)6)(CO(NO2)6)
CO2S3	CO2S3
CO2SI	CO2SI
CO2SIO4	DICOBALT-SILICATE
CO3AS2	CO3AS2
CO3N18H27O18	(CO(NH3)5NO2)(CO(NH3)2(NO2)4)2
CO3P2O8	CO3(PO4)2
CO3TE4	CO3TE4
CO3W	CO3W
CO4N24H36O24	(CO(NH3)6)(CO(NH3)2(NO2)4)3
CO4SO10H6	COSO4*3CO(OH)2
CO5AS2	CO5AS2
CO5N30H45O30	(CO(NH3)5NO2)3(CO(NO2)6)2
CO5TE6	CO5TE6
COAL	COAL
COAL2	COAL2
COAL4	COAL4
COAS	COAS
COAS2	COAS2

Alias	Name
COB2O4	CO(BO2)2
COBALT	COBALT
COBR2*2N2H4	COBR2*2N2H4
COBR2*2NH3	COBR2*2NH3-ROSE
COBR2*6W	COBR2*6H2O
COBR2*NH3	COBR2*NH3
COBR2C2H8O2	COBR2*2CH3OH
COBR2C4H12O2	COBR2*2C2H5OH
COBR2C4H12O4	COBR2*2C2H4(OH)2
COBR2C6H18O3	COBR2*3C2H5OH
COBR2C6H18O6	COBR2*3C2H4(OH)2
COC2N2O2	CO(CNO)2
COC2N2S2	CO(CNS)2
COC2O4	COBALT-OXALATE
COCL2	COCL2
COCL2*2N2H4	COCL2*2N2H4
COCL2*2NH3	COCL2*2NH3-ROSE
COCL2*2W	COCL2*2H2O
COCL2*6W	COCL2*6H2O
COCL2*NH3	COCL2*NH3
COCL2*W	COCL2*H2O
COCL2C4H12O2	COCL2*2C2H5OH
COCL2C6H18O3	COCL2*3C2H5OH
COCL2C6H18O6	COCL2*3C2H4(OH)2
COCL2O8*6W	CO(CLO4)2*6H2O
COH2C2O4	CO(HCO2)2
COHPO4	COHPO4
COI2*2NH3	COI2*2NH3-BLUE
COI2O6*2W	CO(IO3)2*2H2O
CON12H9	(CO(NH3)3(N3)3)
CON13H12-C	(CO(NH3)4(N3)2)N3-CIS
CON13H12-T	(CO(NH3)4(N3)2)N3-TRANS
CON14H15	(CO(NH3)5N3)(N3)2
CON15H18	(CO(NH3)6)(N3)3
CON2H8C2CL2	(CO(C2H4(NH2)2))CL2
CON2O6*2W	CO(NO3)2*2H2O
CON2O6*3W	CO(NO3)2*3H2O
CON2O6*4W	CO(NO3)2*4H2O
CON2O6*6W	CO(NO3)2*6H2O
CON3H12C3CL2	COCL2*1.5C2H4(NH2)2
CON4H12CL3	(CO(NH3)4CL2)CL-CIS
CON4H16C4CL3	(CO(C2H4(NH2)2)2CL2)CL
CON4H16O2CL3	(CO(NH3)4(H2O)2)CL3
CON5H10C2O8	NH4(CO(NH3)2(NO2)2C2O4)
CON5H15BR3	(CO(NH3)5BR)BR2
CON5H15CL3	(CO(NH3)5CL)CL2
CON5H15CLBR2	(CO(NH3)5CL)BR2

Alias	Name
CON5H15CLC2O	(CO(NH3)5CL)C2O4
CON5H15CLI2	(CO(NH3)5CL)I2
CON5H15I3	(CO(NH3)5I)I2
CON5H15ICL2	(CO(NH3)5I)CL2
CON5H15SO4I	(CO(NH3)5SO4)I
CON5H16CO2I2	(CO(NH3)5HCO2)I2
CON5H17OBR3	(CO(NH3)5H2O)BR3
CON5H17OCL3	(CO(NH3)5H2O)CL3
CON5H17OF3	(CO(NH3)5H2O)F3
CON5H17OI3	(CO(NH3)5H2O)I3
CON5H19C4CL3	(CO(C2H4(NH2)2)2CL2)CL*NH3
CON6H11C2O6	(CO(C2H4(NH2)2)(NH3)(NO2)3
CON6H12O4CL	(CO(NH3)4(NO2)2)CL
CON6H12O4I-C	(CO(NH3)4(NO2)2)I-CIS
CON6H12O4I-T	(CO(NH3)4(NO2)2)I-TRANS
CON6H12O8S	(CO(NH3)4(NO2)2)SO4-CIS
CON6H15C2O6	(CO(NH3)5NO2)C2O4
CON6H15O2BR2	(CO(NH3)5NO2)BR2
CON6H15O2CL2	(CO(NH3)5NO2)CL2
CON6H15O2I2	(CO(NH3)5NO2)I2
CON6H15O3CL2	(CO(NH3)5NO3)CL2
CON6H15O3I2	(CO(NH3)5NO3)I2
CON6H15O7S	(CO(NH3)5SO4)NO3
CON6H17CO7	(CO(NH3)5CO3)NO3*H2O
CON6H18BR2	(CO(NH3)6)BR2
CON6H18BR3	(CO(NH3)6)BR3
CON6H18CL2	(CO(NH3)6)CL2
CON6H18CL3	(CO(NH3)6)CL3
CON6H18I2	(CO(NH3)6)I2
CON6H18I3	(CO(NH3)6)I3
CON6H24C6BR2	(CO(C2H4(NH2)2)3)BR2
CON6H24C6CL2	(CO(C2H4(NH2)2)3)CL2
CON6H24C6I2	(CO(C2H4(NH2)2)3)I2
CON6H24C6I3	(CO(C2H4(NH2)2)3)I3
CON6H9O6	(CO(NH3)3(NO2)3)
CON7H10O8	NH4(CO(NH3)2(NO2)4)
CON7H12O7	(CO(NH3)4(NO2)2)NO3
CON7H14O10	(CO(NH3)4(NO3)H2O)(NO3)2
CON7H15IO6	(CO(NH3)5I)(NO3)2
CON7H16C4O7	(CO(C2H4(NH2)2)2(NO2)2)NO3-CIS
CON7H16CO8	(CO(NH3)5HCO2)(NO3)2
CON8H15CSO6	(CO(NH3)5CNS)(NO3)2
CON8H15O8	(CO(NH3)5NO2)(NO3)2
CON8H15O9	(CO(NH3)5NO3)(NO3)2
CON8H17O10	(CO(NH3)5H2O)(NO3)3
CON9H18O9	(CO(NH3)6)(NO3)3
CON9H24C6O9	(CO(C2H4(NH2)2)3)(NO3)3

Alias	Name
CONH2COOK	CONH2COOK
COO2H2-B	CO(OH)2-BLUE,PRECIPITATED
COO2H2-P1	CO(OH)2-PINK,PRECIPITATED
COO2H2-P2	CO(OH)2-PINK,PRECIPITATED,AGED
COO3H3	CO(OH)3-PRECIPITATED
COSB	COSB
COSE	COSE
COSEO3*2W	COSEO3*2H2O
COSI	COSI
COSI2	COSI2
COSI3	COSI3
COSO4*6W	COSO4*6H2O
COSO4*7W	COSO4*7H2O
COTE2	COTE2

SOLIDS Component Databank: Cr

Alias	Name
CR	CHROMIUM
CR2H16O20S3	(CR2(H2O)6(SO4)3)*2H2O-GREEN
CR2H28O26S3	(CR(H2O)6)2(SO4)3*2H2O
CR2H30O27S3	(CR(H2O)6)2(SO4)3*3H2O
CR2H32O28S3	(CR(H2O)6)2(SO4)3*4H2O
CR2H34O29S3	(CR(H2O)6)2(SO4)3*5H2O
CR2O3	ESKOLAITE
CR2S3O12*18W	CR2(SO4)3*18H2O
CR2TE3	CR2TE3
CR3TE4	CR3TE4
CR5TE6	CR5TE6
CR7H2	CR7H2
CRCL2*2W	CRCL2*2H2O-LIGHT-GREEN
CRCL2*3W	CRCL2*3H2O-PALE-BLUE
CRCL2*4W	CRCL2*4H2O-DARK-BLUE
CRCL2N3H9	CRCL2*3NH3
CRCL2N6H18	CRCL2*6NH3
CRH11O7	(CR(H2O)4(OH)2)OH
CRH12O6BR3	(CR(H2O)6)BR3-PURPLE
CRH12O6BR3-G	(CR(H2O)4BR2)BR*2H2O-GREEN
CRH12O6CL3	(CR(H2O)4CL2)CL*2H2O-GREEN
CRH12O6CL3-V	(CR(H2O)6)CL3-VIOLET
CRH13O8	(CR(H2O)5OH)(OH)2
CRH20O10CL3	(CR(H2O)4CL2)CL*6H2O-GREEN
CRH8O4CL3	(CR(H2O)4CL2)CL-GREEN
CRIBR2	CRIBR2
CRICL2	CRICL2
CRN3O18H18	CR(NO3)3*9H2O
CRO3H3	CR(OH)3-PRECIPITATED
CRSB	CRSB
CRSB2	CRSB2

SOLIDS Component Databank: Cs

Alias	Name
CS	CESIUM
CS(UO2)2F5	CS(UO2)2F5
CS12H22C7O31	5CS2CO3*2CSHCO3*10H2O
CS2BAN4O8	BA(NO2)2*2CSNO2
CS2C2O4	CS2C2O4
CS2CO3	CESIUM-CARBONATE
CS2CO3*3W	CS2CO3*3H2O
CS2COCL4	CS2COCL4
CS2CR2O7	CS2CR2O7
CS2CRO4	CS2CRO4
CS2CUCL4	CS2CUCL4
CS2CUCL4*2W	CS2CUCL4*2H2O
CS2FECL4	CS2FECL4
CS2GECL6	CS2GECL6
CS2HFCL6	CS2HFCL6
CS2I8	CS2I8
CS2MNCL4	CS2MNCL4
CS2MO2O7	CS2MO2O7
CS2MOO4	CS2MOO4
CS2NACECL6	CS2NACECL6
CS2NADYCL6	CS2NADYCL6
CS2NAERCL6	CS2NAERCL6
CS2NAGDCL6	CS2NAGDCL6
CS2NALACL6	CS2NALACL6
CS2NALUCL6	CS2NALUCL6
CS2NANDCL6	CS2NANDCL6
CS2NAPUCL6	CS2NAPUCL6
CS2NAYCL6	CS2NAYCL6
CS2NBOCL5	CS2NBOCL5
CS2NPBR6	CS2NPBR6
CS2NPCL6	CS2NPCL6
CS2PACL6	CS2PACL6
CS2PTCL4	CS2PTCL4
CS2PUCL6	CS2PUCL6
CS2RECL6	CS2RECL6
CS2S	CS2S
CS2S2O5	CS2S2O5
CS2SEO3*W	CS2SEO3*H2O
CS2SEO4	CS2SEO4
CS2SNCL6	CS2SNCL6
CS2SO3	CS2SO3
CS2TEBR6	CS2TEBR6
CS2TEO3	CS2TEO3
CS2TEO3*5W	CS2TEO3*5H2O
CS2THCL6	CS2THCL6
CS2THCL6*8W	CS2THCL6*8H2O
CS2TIBR6	CS2TIBR6

Alias	Name
CS2TICL4	CS2TICL4
CS2TICL6	CS2TICL6
CS2U2O7	CS2U2O7
CS2UBR6	CS2UBR6
CS2UCL6	CS2UCL6
CS2UO4	CS2UO4
CS2ZNBR4	CS2ZNBR4
CS2ZNCL4	CS2ZNCL4
CS2ZNI4	CS2ZNI4
CS2ZRBR6	CS2ZRBR6
CS2ZRCL6	CS2ZRCL6
CS3COCL5	CS3COCL5
CS3CR2CL9	CS3CR2CL9
CS3CRCL6	CS3CRCL6
CS3CUCL5	CS3CUCL5
CS3FECL5	CS3FECL5
CS3MNCL5	CS3MNCL5
CS3NICL5	CS3NICL5
CS3TI2BR9	CS3TI2BR9
CS3TIBR6	CS3TIBR6
CS3UO2F5	CS3UO2F5
CS3V2CL9	CS3V2CL9
CS3VCL6	CS3VCL6
CS4THCL8	CS4THCL8
CS5U2O4F9	CS5(UO2)2F9
CSALH4	CSALH4
CSALS2O8*12W	CSAL(SO4)2*12H2O
CSB(CLO4)4	CSB(CLO4)4
CSBA2N5O10	CSNO2*2BA(NO2)2
CSBCL4	CSBCL4
CSBF4	CSBF4
CSBO2	CSBO2
CSBR2CL	CSBR2CL
CSBR3	CSBR3
CSBRCL2	CSBRCL2
CSBRO3	CSBRO3
CSC10	CSC10
CSC24	CSC24
CSC36	CSC36
CSC48	CSC48
CSC60	CSC60
CSC72	CSC72
CSC8	CSC8
CSCACL3	CSCACL3
CSCL*ZNSO4	CSCL*ZNSO4
CSCLO3	CSCLO3
CSCLO4	CSCLO4

Alias	Name
CSCN	CSCN
CSCOCL3	CSCOCL3
CSCUCL3	CSCUCL3
CSF*1.5W	CSF*1.5H2O
CSFECL3	CSFECL3
CSGDFEC6N6	CSGD(FE(CN)6)
CSH	CSH
CSH2PO4	CSH2PO4
CSHC2	CSHC2
CSHCO3	CSHCO3
CSHF2	CSHF2
CSHS	CSHS
CSHSE	CSHSE
CSHSO4	CSHSO4
CSI*3SO2	CSI*3SO2
CSI2BR	CSI2BR
CSI3	CSI3
CSI4	CSI4
CSIBR2	CSIBR2
CSIBRCL	CSIBRCL
CSIBRF	CSIBRF
CSICL2	CSICL2
CSICL4	CSICL4
CSIO3	CSIO3
CSIO4	CSIO4
CSKCLI	CSKCLI
CSMNCL3	CSMNCL3
CSMOF6	CSMOF6
CSN3	CSN3
CSNACLI	CSNACLI
CSNB2OCL9	CSNB2OCL9
CSNBCL6	CSNBCL6
CSNBO3	CSNBO3
CSNH2	CSNH2-TETRAGONAL
CSNICL3	CSNICL3
CSNO3	CSNO3
CSOH*W	CSOH*H2O
CSPF6	CSPF6
CSPO3	CSPO3
CSPTNH3CL3	CSPTNH3CL3
CSREO4	CSREO4
CSSO2F	CSSO2F
CSTACL6	CSTACL6
CSTIBR3	CSTIBR3
CSTICL3	CSTICL3
CSU2CL9	CSU2CL9
CSUCL5	CSUCL5

Alias	Name
CSUCL6	CSUCL6
CSUF6	CSUF6
CSWF6	CSWF6
CSYFEC6N6*2W	CSY(FE(CN)6)*2H2O

SOLIDS Component Databank: Cu

Alias	Name
CU	COPPER
CU2AL	CU2AL
CU2AL2O4	CU2AL2O4
CU2CD3	CU2CD3
CU2CL2*C2H2	(CUCL)2*C2H2
CU2CL2*CO*2W	(CUCL)2*CO*2H2O
CU2CO5H2	CUCO3*CU(OH)2
CU2FEC6N6	CU2FE(CN)6
CU2O	DICOPPER-OXIDE
CU2OCL2	CU2OCL2
CU2S	DICOPPER-SULFIDE
CU3AL	CU3AL
CU3AL2	CU3AL2
CU3C2O8H2	(CUCO3)2*CU(OH)2
CU3CL3*C2H2	(CUCL)3*C2H2
CU3N	CU3N
CU3P2O8	CU3(PO4)2
CU3SB	CU3SB
CU3SN	CU3SN
CU3SO8H4	CUSO4*2CU(OH)2
CU4BR2O12H6	CU(BRO3)2*3CU(OH)2
CU4BR2O6H6	CUBR2*3CU(OH)2
CU4CL2O3	CUCL2*3CUO
CU4CL2O3*4W	CUCL2*3CUO*4H2O
CU4CL2O6H6	CUCL2*3CU(OH)2
CU4I2O12H6	CU(IO3)2*3CU(OH)2
CU4N2O12H6	CU(NO3)2*3CU(OH)2
CU4SO10H6	CUSO4*3CU(OH)2
CU4SO10H6*W	CUSO4*3CU(OH)2*H2O
CUAL	CUAL
CUAL2	CUAL2
CUAL2O4	CUAL2O4
CUBR*1.5NH3	CUBR*1.5NH3
CUBR*2PH3	CUBR*2PH3
CUBR*3NH3	CUBR*3NH3
CUBR*NH3	CUBR*NH3
CUBR*PH3	CUBR*PH3
CUBR2*10NH3	CUBR2*10NH3
CUBR2*2NH3	CUBR2*2NH3
CUBR2*4W	CUBR2*4H2O
CUBR2*5NH3	CUBR2*5NH3

Alias	Name
CUBR2*6NH3	CUBR2*6NH3
CUC2H2O4	CU(CHO2)2
CUC2H2O4*4W	CU(CHO2)2*4H2O
CUC2O4	COPPER-OXALATE
CUC4H12O4N2	CU(CH3COO)2*2NH3
CUC4H12O6N2	CU(CH2OHCOO)2*2NH3
CUC4H14N4O4	CU(CH2NH2COO)2*2NH3
CUC4H24O4N6	CU(CH3COO)2*6NH3
CUC4H24O6N6	CU(CH2OHCOO)2*6NH3
CUC4H6O4	CU(CH3COO)2
CUC4H6O4*W	CU(CH3COO)2*H2O
CUC4H6O6	CU(CH2OHCOO)2
CUCL*1.5NH3	CUCL*1.5NH3
CUCL*2PH3	CUCL*2PH3
CUCL*3NH3	CUCL*3NH3
CUCL*NH3	CUCL*NH3
CUCL*PH3	CUCL*PH3
CUCL2*10NH3	CUCL2*10NH3
CUCL2*2NH3	CUCL2*2NH3
CUCL2*2W	CUCL2*2H2O
CUCL2*4NH3W2	CUCL2*4NH3*2H2O
CUCL2*5NH3	CUCL2*5NH3
CUCL2*6NH3	CUCL2*6NH3
CUCL2C2H8O2	CUCL2*2CH3OH
CUCL2C4H12O2	CUCL2*2C2H5OH
CUCL2O8*6W	CU(CLO4)2*6H2O
CUCL4N2H8	CUCL2*2NH4CL
CUCL4N2H8*2W	CUCL2*2NH4CL*2H2O
CUCNS	CUCNS
CUH	CUH
CUH14C2O4N4	CU(HCOO)2*4NH3
CUH20C2O4N6	CU(HCOO)2*6NH3
CUH8C2O4N2	CU(HCOO)2*2NH3
CUI*0.5NH3	CUI*0.5NH3
CUI*2NH3	CUI*2NH3
CUI*2PH3	CUI*2PH3
CUI*3NH3	CUI*3NH3
CUI*NH3	CUI*NH3
CUI*PH3	CUI*PH3
CUI2O6*W	CU(IO3)2*H2O
CUN2H8C4O4*W	CU(NH2CH2COO)2*H2O
CUN2H8C4O4-A	CU(NH2CH2COO)2-ALPHA
CUN2H8C4O4-B	CU(NH2CH2COO)2-BETA
CUN2O6	CU(NO3)2
CUN2O6*3W	CU(NO3)2*3H2O
CUN2O6*6W	CU(NO3)2*6H2O
CUN3	CUN3

Alias	Name
CUN4H12SO4	(CU(NH3)4)SO4
CUN4H15SO5.5	(CU(NH3)4)SO4*1.5H2O
CUN4H18C4O4	CU(NH3)4(CH3COO)2
CUN4H18C4O6	CU(NH3)4(CH2OHCOO)2
CUN6	CU(N3)2
CUN6H12O6	CU(NH3)4(NO3)2
CUN6H20C4O4	CU(NH3)4(CH2NH2COO)2
CUO	COPPER-MONOXIDE
CUO*CUSO4	CUO*CUSO4
CUONC	CUONC
CURB2CL4	CUCL2*2RBCL
CURB2CL4*4W	CUCL2*2RBCL*4H2O
CUS2O10N2H12	CUSO4*(NH4)2SO4*2H2O
CUS2O14N2H20	CUSO4*(NH4)2SO4*6H2O
CUS2O6*5W	CUS2O6*5H2O
CUS2O8N2H8	CUSO4*(NH4)2SO4
CUSE2	CUSE2
CUSEO4	CUSEO4
CUSEO4*5W	CUSEO4*5H2O
CUSO4	COPPER-SULFATE
CUSO4*2CH3OH	CUSO4*2CH3OH
CUSO4*2NH3	CUSO4*2NH3
CUSO4*5NH3	CUSO4*5NH3
CUSO4*NH3	CUSO4*NH3
CUWO4	CUWO4
CUWO4*2H2O	CUWO4*2H2O

SOLIDS Component Databank: Dy

Alias	Name
DY2C6O12*10W	DY2(C2O4)3*10H2O
DY2O3*CO2	DY2O3*CO2
DYAS	DYAS
DYBR3O9*9W	DY(BRO3)3*9H2O
DYC6H9O6	DY(CH3CO2)3
DYCO5	DYCO5
DYI3O9	DY(IO3)3
DYOCL	DYOCL

SOLIDS Component Databank: Er

Alias	Name
ER2C6O12*6W	ER2(C2O4)3*6H2O
ERBR3O9*9W	ER(BRO3)3*9H2O
ERH2	ERH2
ERH3	ERH3
ERI3O9	ER(IO3)3
EROCL	EROCL

SOLIDS Component Databank: Eu

Alias	Name
EU2S3O12*8W	EU2(SO4)3*8H2O
EUBR3O9*9W	EU(BRO3)3*9H2O
EUC2	EUC2
EUCL2	EUCL2
EUF3*H2O	EUF3*H2O
EUI3O9	EU(IO3)3
EUN3O9*6W	EU(NO3)3*6H2O
EUO3H3	EU(OH)3

SOLIDS Component Databank: Fe

Alias	Name
FE	IRON
FE1.042SE	FE1.042SE
FE1.111TE	FE1.111TE
FE2(WO4)3*8W	FE2(WO4)3*8H2O
FE2CDO4	CDFE2O4
FE2I6PB	(FEI2)2*PBI2
FE2MO3O12	FE2(MOO4)3
FE2O3	HEMATITE
FE2OC6N5	FE2CO(CN)5
FE2P	FE2P
FE2ZNO4	DIIRON-ZINC-TETRAOXIDE
FE3C	TRIIRON-CARBIDE
FE3O4	MAGNETITE
FE3P	FE3P
FE3SE4	FE3SE4
FE3SI	FE3SI
FE5SI3	FE5SI3
FE7C18N18	FE4(FE(CN)6)3
FE7S8	FE7S8-SULFUR-RICH-PYRRHOTITE
FE7SE8	FE7SE8
FE7W6	FE7W6
FEAL	FEAL
FEAL2	FEAL2
FEAL3	FEAL3
FEASS	FEASS
FEBR2*2NH3	FEBR2*2NH3
FEBR2*6NH3	FEBR2*6NH3
FEBR2*NH3	FEBR2*NH3
FEBR3*6NH3	FEBR3*6NH3
FEBRCL2	FEBRCL2
FEC2O4*2W	FEC2O4*2H2O
FEC4O4BR2	FE(CO)4BR2
FEC4O4I2	FE(CO)4I2
FEC6N5H5O2	H3FECO(CN)5*H2O
FECD2C6N6*7W	CD2FE(CN)6*7H2O
FECL2	FERROUS-CHLORIDE
FECL2*10NH3	FECL2*10NH3

Alias	Name
FECL2*2NH3	FECL2*2NH3
FECL2*2W	FECL2*2H2O
FECL2*4W	FECL2*4H2O
FECL2*6NH3	FECL2*6NH3
FECL2*NH3	FECL2*NH3
FECL2O8*6W	FE(CLO4)2*6H2O
FECL3	FERRIC-CHLORIDE
FECL3*6NH3	FECL3*6NH3
FECL3*6W	FECL3*6H2O
FECO2O4	FECO2O4
FECO3	IRON-CARBONATE
FECR2O4	FECR2O4
FEH4C6N6	H4FE(CN)6
FEI2*2NH3	FEI2*2NH3
FEI2*6NH3	FEI2*6NH3
FEN10H28C6O6	(NH4)4FE(CN)6*6H2O
FEN3O9*9W	FE(NO3)3*9H2O
FEO	FERROUS-OXIDE
FEO2H	FEO(OH)
FEP	FEP
FEP2	FEP2
FEPB2C6N6*3W	PB2FE(CN)6*3H2O
FEPO4*2W	FEPO4*2H2O
FES	IRON-MONOSULFIDE
FES2	IRON-DISULFIDE-PYRITE
FES2-2	IRON-DISULFIDE-MARCASITE
FESB	FESB
FESB2	FESB2
FESE	FESE
FESE2	FESE2
FESIO3	IRON-METASILICATE
FESO4*2NH3	FESO4*2NH3
FESO4*3NH3	FESO4*3NH3
FESO4*4NH3	FESO4*4NH3
FESO4*4W	FESO4*4H2O
FESO4*6NH3	FESO4*6NH3
FESO4*7W	FESO4*7H2O
FESO4*NH3	FESO4*NH3
FESO4*W	FESO4*H2O
FETE	FETE
FETL4C6N6*2W	TL4FE(CN)6*2H2O
FEWO4*3H2O	FEWO4*3H2O
FEZN2C6N6*2W	ZN2FE(CN)6*2H2O

SOLIDS Component Databank: Ga

Alias	Name
GA2BR6*CH3BR	(GABR3)2*CH3BR
GA2CL6*CH3CL	(GACL3)2*CH3CL
GA2CL7C2H5	(GACL3)2*C2H5CL
GA2S3O12	GALLIUM-SULFATE
GABR3*14NH3	GABR3*14NH3
GABR3*5NH3	GABR3*5NH3
GABR3*6NH3	GABR3*6NH3
GABR3*7NH3	GABR3*7NH3
GABR3*9NH3	GABR3*9NH3
GABR3*CH3BR	GABR3*CH3BR
GABR3*NH3	GABR3*NH3
GACH3I2	GACH3I2
GACL3*14NH3	GACL3*14NH3
GACL3*3NH3	GACL3*3NH3
GACL3*5NH3	GACL3*5NH3
GACL3*6NH3	GACL3*6NH3
GACL3*7NH3	GACL3*7NH3
GACL3*CH3CL	GACL3*CH3CL
GACL3*NH3	GACL3*NH3
GACL3*PCL3	GACL3*PCL3
GACL3*POCL3	GACL3*POCL3
GACL3C3H6O	GACL3*(CH3)2CO
GACL3C4H10O	GACL3*(C2H5)2O
GACL3C8H20O	GACL3*2(C2H5)2O
GACL4C2H3O	GACL3*CH3COCL
GAF3*3LIF	GAF3*3LIF
GAI3*13NH3	GAI3*13NH3
GAI3*20NH3	GAI3*20NH3
GAI3*5NH3	GAI3*5NH3
GAI3*6NH3	GAI3*6NH3
GAI3*7NH3	GAI3*7NH3
GAI3*9NH3	GAI3*9NH3
GAI3*NH3	GAI3*NH3
GAN	GALLIUM-NITRIDE
GAO3H3	GALLIUM-HYDROXIDE
GAPO4	GALLIUM-PHOSPHATE

SOLIDS Component Databank: Gd

Alias	Name
GD2C6O12*10W	GD2(C2O4)3*10H2O
GD2S3O12*8W	GD2(SO4)3*8H2O
GDAL2	GDAL2
GDAS	GDAS
GDBR3O9*9W	GD(BRO3)3*9H2O
GDC2	GDC2
GDCL3*6W	GDCL3*6H2O
GDF3*W	GDF3*H2O
GDH2	GDH2

Alias	Name
GDI3O9	GD(IO3)3
GDN3O9*6W	GD(NO3)3*6H2O
GDPO4*W	GDPO4*H2O

SOLIDS Component Databank: H

Alias	Name
H2MOO4	H2MOO4-WHITE
H2MOO4*W	H2MOO4*H2O-YELLOW
H2O	WATER
H2O(S)	ICE
H2PTBR6*9W	H2PTBR6*9H2O
H2PTCL6*6W	H2PTCL6*6H2O
H2RECL4	H2RECL4
H2S2O7	H2S2O7
H2SEO3	SELENIOUS-ACID
H2SEO4	SELENIC-ACID
H2SEO4*W	SELENIC-ACID-HYDRATE
H2SI2O5	DISILICIC-ACID
H2SIO3	METASILICIC-ACID
H3BO3	HYDROGEN-ORTHOBORATE
H3PO2	HYPOPHOSPHOROUS-ACID
H3PO3	PHOSPHOROUS-ACID
H3PO4	ORTHOPHOSPHORIC-ACID
H3PO4*0.5W	H3PO4*0.5H2O
H3PO4*HCLO4	H3PO4*HCLO4
H3PO4*W	ORTHOPHOSPHORIC-ACID-HYDRATE
H4P2O7	PYROPHOSPHORIC-ACID
H4P2O7*1.5W	H4P2O7*1.5H2O
H4SIO4	H4SIO4
H6SI2O7	H6SI2O7
H6TEO6	H6TEO6
HAUBR4*5W	HAUBR4*5H2O
HAUCL4*3W	HAUCL4*3H2O
HAUCL4*4W	HAUCL4*4H2O
HBO2-C	METABORIC-ACID-CUBIC
HBO2-M	METABORIC-ACID-MONOCLINIC
HCLO4*W	PERCHLORIC-ACID-HYDRATE
HCO2NH4	AMMONIUM-FORMATE
HCOOK	HCOOK
HCOONA	HCOONA
HCOONA*2W	HCOONA*2H2O
HCOONA*3W	HCOONA*3H2O
HIO3	IODIC-ACID
HPO3	METAPHOSPHORIC-ACID
HPTCL5*2W	HPTCL5*2H2O

SOLIDS Component Databank: Hg

Alias	Name
HG	MERCURY
HG2BR2N2H4	NHG2BR*NH4BR
HG2BR2O	HGBR2*HGO
HG2BR4N4H12	NHG2BR*3NH4BR
HG2C2N2O	HG(CN)2*HGO
HG2C2N2S2	HG2(CNS)2
HG2C2O4	HG2C2O4
HG2C4H6O4	HG2(CH3COO)2
HG2CL2*2NH3	HG2CL2*2NH3
HG2CL2N2H4	NHG2CL*NH4CL
HG2CL4N4H12	NHG2CL*3NH4CL
HG2CO3	HG2CO3
HG2N2O6*2W	HG2(NO3)2*2H2O
HG2N6	HG2(N3)2
HG2SEO3	HG2SEO3
HG3BR2O2	HGBR2*2HGO
HG3N2O8*W	HG(NO3)2*2HGO*H2O
HG3SO6	HGSO4*2HGO
HG4BR2O3	HGBR2*3HGO
HG4C6N6O	(HG(CN)2)3*HGO
HG4CL2N2*2W	(NHG2CL)2*2H2O
HG4CL2N2*W	(NHG2CL)2*H2O
HG4CL2N3H3	(NHG2CL)2*NH3
HG4CL2N4H6	(NHG2CL)2*2NH3
HG4N2O	(HG2N)2O
HG4N2O*4W	(HG2N)2O*4H2O
HG4N2O*W	(HG2N)2O*H2O
HG5BR2O4	HGBR2*4HGO
HG5BR4N2	(NHG2BR)2*HGBR2
HG5CL4N2	(NHG2CL)2*HGCL2
HG5TL2	HG5TL2
HG9BR6N4	(NHG2BR)4*HGBR2
HGBR2*2NH3	HGBR2*2NH3
HGBR2*8NH3	HGBR2*8NH3
HGBR2C2N2H8	HGBR2*C2H4(NH2)2
HGC2H2CL2	HGCLCHCHCL
HGC2H5BR	HGC2H5BR
HGC2H5CL	HGC2H5CL
HGC2H5I	HGC2H5I
HGC2N2	HG(CN)2
HGC2N3H4BR*W	HG(CN)2*NH4BR*H2O
HGC2O4	HGC2O4
HGC4H6O4	HG(CH3COO)2
HGCH3BR	HGCH3BR
HGCH3CL	HGCH3CL
HGCH3I	HGCH3I
HGCL2*2:3NH3	HGCL2*2:3NH3

Alias	Name
HGCL2*2NH3	HGCL2*2NH3
HGCL2*8NH3	HGCL2*8NH3
HGCL2*9.5NH3	HGCL2*9.5NH3
HGCL2C2N2H8	HGCL2*C2H4(NH2)2
HGCL2CH3OH	HGCL2CH3OH
HGCL3NO	HGCL2*NOCL
HGI2*2NH3	HGI2*2NH3
HGI2*4:3NH3	HGI2*4:3NH3
HGI2*6NH3	HGI2*6NH3
HGI2*C2H8N2	HGI2*C2H4(NH2)2
HGINO3	HGINO3
HGN2O6*0.5W	HG(NO3)2*0.5H2O
HGO2N2C2	HG(ONC)2

SOLIDS Component Databank: Ho

Alias	Name
HO2C3	HO2C3
HOAS	HOAS
HOBR3O9*9W	HO(BRO3)3*9H2O
HOC2	HOC2
HOI3	HOI3
HOI3O9	HO(IO3)3
HOOCL	HOOCL

SOLIDS Component Databank: In

Alias	Name
IN3S4	IN3S4
IN4S5	IN4S5
INBR3*15NH3	INBR3*15NH3
INBR3*3NH3	INBR3*3NH3
INBR3*5NH3	INBR3*5NH3
INBR3*7NH3	INBR3*7NH3
INBR3C4H12S	INBR3*2(CH3)2S
INCL3*15NH3	INCL3*15NH3
INCL3*2NH3	INCL3*2NH3
INCL3*3NH3	INCL3*3NH3
INCL3*5NH3	INCL3*5NH3
INCL3*7NH3	INCL3*7NH3
INCL3*NH3	INCL3*NH3
INCL3C4H12S	INCL3*2(CH3)2S
INI3*13NH3	INI3*13NH3
INI3*21NH3	INI3*21NH3
INI3*2NH3	INI3*2NH3
INI3*5NH3	INI3*5NH3
INI3*7NH3	INI3*7NH3
INI3*9NH3	INI3*9NH3
INI3C4H12S	INI3*2(CH3)2S

SOLIDS Component Databank: K

Alias	Name
K	POTASSIUM
K(UO2)2F5	K(UO2)2F5
K2AL(NO3)5	K2AL(NO3)5
K2B3F4O3OH	K2B3F4O3OH
K2B4O7*4W	K2B4O7*4H2O
K2BA(CO3)2	K2CO3*BACO3-AGED
K2BA(NO2)4	2KNO2*BA(NO2)2
K2BA(NO3)4	2KNO3*BA(NO3)2
K2BA(SO4)2-A	K2SO4*BASO4-AGED
K2BA(SO4)2-F	K2SO4*BASO4-FUSE
K2BACL4	K2BACL4-FUSE
K2BECL4	K2BECL4
K2BEF4	K2BEF4
K2C2O4	K2C2O4
K2C2O4*W	K2C2O4*H2O
K2CA(SO4)2*W	K2SO4*CASO4*H2O
K2CA5S6O24*W	K2SO4*5CASO4*H2O
K2CAP2O7	K2CAP2O7
K2CDFEC6N6	K2CDFE(CN)6
K2CDI4*2W	K2CDI4*2H2O
K2CDS2O9.5H3	K2CD(SO4)2*1.5H2O
K2CO3	POTASSIUM-CARBONATE
K2CO3*1.5W	K2CO3*1.5H2O
K2CO3*COCO3	K2CO3*COCO3
K2COC2O6*4W	K2CO3*COCO3*4H2O
K2CR2O7	K2CR2O7
K2CR3O10	K2CR3O10
K2CRCL4	K2CRCL4
K2CU(CO3)2	K2CU(CO3)2
K2CU(HCO3)4	K2CU(HCO3)4
K2CU(SO4)2	K2CU(SO4)2-BLUE
K2CU2FEC6N6	K2CU2FE(CN)6
K2CUCL3	K2CUCL3
K2CUCL4	K2CUCL4
K2CUCL4*2W	K2CUCL4*2H2O
K2CUS2O8*.5W	K2CU(SO4)2*0.5H2O
K2CUS2O8*2W	K2CU(SO4)2*2H2O
K2CUS2O8*6W	K2CU(SO4)2*6H2O
K2GEF6	K2GEF6
K2H2P2O7	K2H2P2O7
K2HFCL6	K2HFCL6
K2HG(CN)4	K2HG(CN)4
K2HGBR4	K2HGBR4
K2HGCL4	K2HGCL4
K2HGCL4*W	K2HGCL4*H2O
K2HGI4	K2HGI4
K2IRCL6	K2IRCL6

Alias	Name
K2LACL5	K2LACL5
K2LI2(SO4)2	K2SO4*LI2SO4
K2LI2B12O20	K2O*LI2O*6B2O3
K2LI2B16O26	K2O*LI2O*8B2O3
K2LI2B8O14	K2O*LI2O*4B2O3
K2LI6B16O28	K2O*3LI2O*8B2O3
K2LI6B24O40	K2O*3LI2O*12B2O3
K2LI6B32O52	K2O*3LI2O*16B2O3
K2MG(SEO4)2	K2MG(SEO4)2
K2MG2(SO4)3	K2SO4*2MGSO4
K2MGCL4*2KCL	K2MGCL4*2KCL
K2MGCL4-A	K2MGCL4-AGED-2-MONTHS
K2MGCL4-F	K2MGCL4-FUSED
K2MGS2O8	K2MG(SO4)2-AGED
K2MGS2O8*2W	K2MG(SO4)2*2H2O
K2MGS2O8*4W	K2MG(SO4)2*4H2O
K2MGS2O8*6W	K2MG(SO4)2*6H2O
K2MNS2O8	K2MN(SO4)2
K2MNS2O8*2W	K2MN(SO4)2*2H2O
K2MNS2O8*4W	K2MN(SO4)2*4H2O
K2MO2O7	K2MO2O7
K2MO3O10	K2MO3O10
K2MO4O13	K2MO4O13
K2MOCL6	K2MOCL6
K2MOO4	K2MOO4
K2NA2B12O20	K2O*NA2O*6B2O3
K2NA2B16O26	K2O*NA2O*8B2O3
K2NA2B8O14	K2O*NA2O*4B2O3
K2NA6B16O28	K2O*3NA2O*8B2O3
K2NA6B24O40	K2O*3NA2O*12B2O3
K2NA6B32O52	K2O*3NA2O*16B2O3
K2NBOBR5	K2NBOBR5
K2NBOCL5	K2NBOCL5
K2O	POTASSIUM-OXIDE
K2O*3B2O3	K2O*3B2O3
K2O*4B2O3	K2O*4B2O3
K2O*B2O3	K2O*B2O3
K2OSCL6	K2OSCL6
K2PB(SO4)2	K2PB(SO4)2
K2PBI4	K2PBI4
K2PBI4*2W	K2PBI4*2H2O
K2PDBR4	K2PDBR4
K2PDCL4	K2PDCL4
K2PDCL6	K2PDCL6
K2PRCL5	K2PRCL5
K2PT(NO2)4	K2PT(NO2)4
K2PTBR4	K2PTBR4

Alias	Name
K2PTBR6	K2PTBR6
K2PTCL4	K2PTCL4
K2PTCL6	K2PTCL6
K2PTI6	K2PTI6
K2PTN2O4CL2	K2PT(NO2)2CL2
K2PTN3O6CL	K2PT(NO2)3CL
K2PTNO2CL3	K2PT(NO2)CL3
K2REBR6	K2REBR6
K2RECL6	K2RECL6
K2S*2W	K2S*2H2O
K2S*5W	K2S*5H2O
K2S2	K2S2
K2S2O3	K2S2O3
K2S2O3*W	K2S2O3*H2O
K2S2O5	K2S2O5
K2S2O5*0.5W	K2S2O5*0.5H2O
K2S2O6	K2S2O6
K2S2O7	K2S2O7
K2S2O8	K2S2O8
K2S3	K2S3
K2S3O6	K2S3O6
K2S4	K2S4
K2S4*0.5W	K2S4*0.5H2O
K2S4*2W	K2S4*2H2O
K2S4O6	K2S4O6
K2S5	K2S5
K2S5O6*1.5W	K2S5O6*1.5H2O
K2S6	K2S6
K2SE	K2SE
K2SE*14W	K2SE*14H2O
K2SE*19W	K2SE*19H2O
K2SE*9W	K2SE*9H2O
K2SEO3	K2SEO3
K2SEO4	K2SEO4
K2SIF6	K2SIF6
K2SMCL5	K2SMCL5
K2SNBR6	K2SNBR6
K2SNCL6	K2SNCL6
K2SNCL6*W	K2SNCL6*H2O
K2SNOCL4	K2SNOCL4
K2SO4	POTASSIUM-SULFATE
K2SR(SO4)2	K2SO4*SRSO4-FUSED
K2SRCL4	K2SRCL4-FUSED
K2TACL6	K2TACL6
K2TE2O5	K2TE2O5
K2TE4O9	K2TE4O9
K2TE4O9*4W	K2TE4O9*4H2O

Alias	Name
K2TEBR6	K2TEBR6
K2TEO3	K2TEO3
K2TEO3*3W	K2TEO3*3H2O
K2THCL6	K2THCL6
K2TICL6	K2TICL6
K2TIO3	K2TIO3
K2UCL6	K2UCL6
K2UO4	K2UO4
K2WCL7	K2WCL7
K2WO4	K2WO4
K2ZN(CN)4	K2ZN(CN)4
K2ZN(SO4)2	K2ZN(SO4)2
K2ZNS2O8*2W	K2ZN(SO4)2*2H2O
K2ZNS2O8*6W	K2ZN(SO4)2*6H2O
K2ZRBR6	K2ZRBR6
K2ZRCL6	K2ZRCL6
K3AG2I5*W	K3AG2I5*H2O
K3AGBR4*0.5W	K3AGBR4*0.5H2O
K3AGI4	K3AGI4
K3AGI4*0.5W	K3AGI4*0.5H2O
K3AL(NO3)6	K3AL(NO3)6
K3AL2CL9	K3AL2CL9
K3ALF6*3.5W	K3ALF6*3.5H2O
K3AS	K3AS
K3BI	K3BI
K3CE2CL9	K3CE2CL9
K3CECL6	K3CECL6
K3CO(C2O4)3	K3(CO(C2O4)3)
K3CO(CN)6	K3CO(CN)6
K3COC6O12*3W	K3(CO(C2O4)3)*3H2O
K3CR2CL9	K3CR2CL9
K3CRC6O12	K3CR(C2O4)3
K3CRC6O12*3W	K3CR(C2O4)3*3H2O
K3CRCL6	K3CRCL6
K3CRO4F	K3CRO4F
K3FE(CN)6	K3FE(CN)6
K3FEC6N5O	K3FECO(CN)5
K3IRCL6	K3IRCL6
K3ND2CL9	K3ND2CL9
K3NDCL6	K3NDCL6
K3OSCL6	K3OSCL6
K3PR2CL9	K3PR2CL9
K3PRCL6	K3PRCL6
K3SB	K3SB
K3SMCL6	K3SMCL6
K3TICL6	K3TICL6
K3UO2F5	K3UO2F5

Alias	Name
K3V2CL9	K3V2CL9
K3VCL6	K3VCL6
K4BA(SO4)3	2K2SO4*BASO4-FUSED
K4CA(NO3)6	4KNO3*CA(NO3)2
K4CDCL6	K4CDCL6
K4FE(CN)6	K4FE(CN)6
K4FEC6N6*3W	K4FE(CN)6*3H2O
K4PB3I10	4KI*3PBI2
K4PB3I10*6W	4KI*3PBI2*6H2O
K4SR(SO4)3	2K2SO4*SRSO4-FUSED
K5AS4	K5AS4
K5SB4	K5SB4
K6EU4S9O36	3K2SO4*2EU2(SO4)3
K6EU4S9O36W8	3K2SO4*2EU2(SO4)3*8H2O
K6NA2B16O28	3K2O*NA2O*8B2O3
K6NA2B24O40	3K2O*NA2O*12B2O3
K6NA2B32O52	3K2O*NA2O*16B2O3
KAG(CN)2	KAG(CN)2
KAGBR2	KAGBR2
KAGCL2	KAGCL2
KAGI2	KAGI2
KAL(SEO4)2	KAL(SEO4)2
KAL(SO4)2	POTASSIUM-ALUMINIUM-SULFATE
KAL(SO4)2*3W	KAL(SO4)2*3H2O
KAL2BR7	KAL2BR7
KAL2H5P2O11	KAL2(PO4)2OH*2H2O
KALBR4	KALBR4
KALCL4*6NH3	KALCL4*6NH3
KALH4	KALH4
KALS2O8*12W	KAL(SO4)2*12H2O
KALSE2O8*12W	KAL(SEO4)2*12H2O
KAOLINITE	AL2SI2O7*2H2O
KAS	KAS
KAS2	KAS2
KB5O8*4W	KB5O8*4H2O
KBA2(NO2)5	KNO2*2BA(NO2)2
KBCL4	KBCL4
KBF3OH	KBF3OH
KBF4	KBF4
KBH4	KBH4
KBR	POTASSIUM-BROMIDE
KBR*ALCL3	KBR*ALCL3
KBR*ZNSO4	KBR*ZNSO4
3KBR*2SBBR3	3KBR*2SBBR3
KBRO3	KBRO3
KBRO4	KBRO4
KC10	KC10

Alias	Name
KC24	KC24
KC36	KC36
KC4	KC4
KC48	KC48
KC60	KC60
KC8	KC8
KCACL3	KCACL3
KCAFEC6N6*5W	KCAFE(CN)6*5H2O
KCD3BR7*4W	KBR*3CDBR2*4H2O
KCD3CL7*4W	KCL*3CDCL2*4H2O
KCDBR3*W	KCDBR3*H2O
KCDCL3	KCDCL3
KCDCL3*W	KCDCL3*H2O
KCDI3*W	KCDI3*H2O
KCE3CL10	KCE3CL10
KCECL4	KCECL4
KCEFEC6N6*2W	KCEFE(CN)6*2H2O
KCL	POTASSIUM-CHLORIDE
KCL*2ALBR3	KCL*2ALBR3
KCL*2PBCL2	KCL*2PBCL2
KCL*ALBR3	KCL*ALBR3
KCL*MGSO4*3W	KCL*MGSO4*3H2O
KCL*ZNSO4	KCL*ZNSO4
KCLBRI	KCLBRI
KCLO3	POTASSIUM-CHLORATE
KCNO	KCNO
KCNS	KCNS
KCNS*0.5SO2	KCNS*0.5SO2
KCNS*2SO2	KCNS*2SO2
KCOF3	KCOF3
KCON4C2O8H6	K(CO(NH3)2(NO2)2C2O4)
KCOO8N6H6	K(CO(NH3)2(NO2)4)
KCRCL3	KCRCL3
KCRO3CL	KOCRO2CL
KCRS2O8*1.5W	KCR(SO4)2*1.5H2O
KCRS2O8*12W	KCR(SO4)2*12H2O
KCRS2O8*6W	KCR(SO4)2*6H2O
KCUCL3	KCUCL3
KCUF3	KCUF3
KERCL4	KERCL4
KEUS2O8	KEU(SO4)2
KEUS2O8*W	KEU(SO4)2*H2O
KF*2HF	KF*2HF
KF*2W	KF*2H2O
KF*3HF	KF*3HF
KF*BRF3	KF*BRF3
KFECL4	KFECL4

Alias	Name
KGDFEC6N6	KGDFE(CN)6
KH2ASO4	KH2ASO4
KH3C2O3	CH2OHCOOK
KH3C2O3*0.5W	CH2OHCOOK*0.5H2O
KH3C4O8	KHC2O4*H2C2O4
KH3C4O8*2W	KHC2O4*H2C2O4*2H2O
KHCO3	POTASSIUM-BICARBONATE
KHF2	KHF2
KHG(CN)2BR	KBR*HG(CN)2
KHG(CN)2CL	KCL*HG(CN)2
KHG(CN)2CL*W	KCL*HG(CN)2*H2O
KHG(CN)2I	KI*HG(CN)2
KHGBR3	KHGBR3
KHGBR3*W	KHGBR3*H2O
KHGCL3	KHGCL3
KHGCL3*W	KHGCL3*H2O
KHGI3	KHGI3
KHGI3*W	KHGI3*H2O
KHS	KHS
KHS*0.25W	KHS*0.25H2O
KHSE	KHSE
KHSO4	KHSO4
KI*4SO2	KI*4SO2
KI*ZNSO4	KI*ZNSO4
KI3	KI3
KIBR2	KIBR2
KIBR2*W	KIBR2*H2O
KIO2F2	KIO2F2
KIO3	KIO3
KIO4	KIO4
KLA3CL10	KLA3CL10
KLACL4	KLACL4
KLAFE(CN)6	KLAFE(CN)6
KLICLI	KLICLI
KMGCL3	KMGCL3
KMGCL3*2W	KMGCL3*2H2O
KMGCL3*6W	KMGCL3*6H2O
KMGPO4*6W	KMGPO4*6H2O
KMNCL3	KMNCL3
KMNF3	KMNF3
KMNO4	KMNO4
KMOF6	KMOF6
KNABR2	KNABR2
KNACL2	KNACL2
KNACLI	KNACLI
KNAI2	KNAI2
KNAUCL6	KNAUCL6

Alias	Name
KNB2OCL9	KNB2OCL9
KNBCL6	KNBCL6
KNBO3	KNBO3
KNBOCL4	KNBOCL4
KNDCL4	KNDCL4
KNH2	KNH2
KNH3	KNH3
KNH4CRO4	KNH4CRO4
KNICL3	KNICL3
KNIF3	KNIF3
KNO2	KNO2
KNO2*KOH	KNO2*KOH
KNO3	POTASSIUM-NITRATE
KNO3*KOH	KNO3*KOH
KOH	POTASSIUM-HYDROXIDE
KOH*2W	KOH*2H2O
KOH*W	KOH*H2O
KPBCL3*1:3W	KPBCL3*1:3H2O
KPF6	KPF6
KPO3	KPO3
KPRCL4	KPRCL4
KPTNH3CL3	KPT(NH3)CL3
KPTNH3CL5	KPTNH3CL5
KREO4	KREO4
KSB	KSB
KSB2	KSB2
KSO2F	KSO2F
KSO3F	KSO3F
KSR2CL5	KSR2CL5
KTACL6	KTACL6
LTAO2CL2	KTAO2CL2
KTBS2O8	KTB(SO4)2
KTBS2O8*W	KTB(SO4)2*H2O
KTCO4	KTCO4
KTHCL5*9W	KTHCL5*9H2O
KTICL3	KTICL3
KUCL5	KUCL5
KUCL6	KUCL6
KUF6	KUF6
KVCL3	KVCL3
KVO3	KVO3
KVO4	KVO4
KWCL6	KWCL6
KWF6	KWF6
KYCL4	KYCL4
KZNF3	KZNF3

SOLIDS Component Databank: La

Alias	Name
LA2C3N6	LA2(CN2)3
LA2C3O9	LA2(CO3)3
LA2C6O12*10W	LA2(C2O4)3*10H2O
LA2S3O12	LA2(SO4)3
LA2S3O12*9W	LA2(SO4)3*9H2O
LA2SE3O9	LA2(SEO3)3
LAAL2	LAAL2
LAB6	LAB6
LABI	LABI
LABR3O9*9W	LA(BRO3)3*9H2O
LABSALT	NA4CA(SO4)3*2H2O
LAC2	LAC2
LACL3*7W	LACL3*7H2O
LAF3*W	LAF3*H2O
LAH3C3O6	LA(HCO2)3
LAI3O9	LA(IO3)3
LAINTE3	LAINTE3
LAN3O9	LA(NO3)3
LAN3O9*3W	LA(NO3)3*3H2O
LAN3O9*4W	LA(NO3)3*4H2O
LAN3O9*6W	LA(NO3)3*6H2O
LASB	LASB

SOLIDS Component Databank: Li

Alias	Name
LI	LITHIUM
LI.05ZN.9F-A	LI0.05ZN0.9FE2.05O4-ANNEALED
LI.05ZN.9F-Q	LI0.05ZN0.9FE2.05O4-QUENCHED
LI0.5FE2.5O4	LI0.5FE2.5O4
LI22SN5	LI22SN5
LI2AL2SI8O20	LI2AL2SI8O20
LI2B2C4H18O	(LIBH4)2*(C2H5)2O
LI2BECL4	LI2BECL4
LI2C2	LI2C2
LI2CRO4	LI2CRO4
LI2CRO4*2W	LI2CRO4*2H2O
LI2HFO3	LI2HFO3
LI2K6B16O28	LI2O*3K2O*8B2O3
LI2K6B24O40	LI2O*3K2O*12B2O3
LI2K6B32O52	LI2O*3K2O*16B2O3
LI2MOO4	LI2MOO4
LI2NH	LI2NH
LI2O*2BEO	LI2O*2BEO
LI2PBI4*4W	LI2PBI4*4H2O
LI2PTCL6	LI2PTCL6
LI2S2	LI2S2
LI2SE*9W	LI2SE*9H2O
LI2SEO3*W	LI2SEO3*H2O

Alias	Name
LI2SEO4	LI2SEO4
LI2SEO4*W	LI2SEO4*H2O
LI2SIF6	LI2SIF6
LI2SO3	LI2SO3
LI2SO4*W	LI2SO4*H2O
LI2THCL6	LI2THCL6
LI2UCL6	LI2UCL6
LI2UO4	LI2UO4
LI2WO4	LI2WO4
LI3ALH6	LI3ALH6
LI3BI	LI3BI
LI3PO4	LI3PO4
LI3SB	LI3SB
LI3SB2	LI3SB2
LI4P2O7	LI4P2O7
LI4PUF8	LI4PUF8
LI4ZRO4	LI4ZRO4
LI5I2O12	LI5(IO6)2
LI7PB2	LI7PB2
LI7SN2	LI7SN2
LI8ZRO6	LI8ZRO6
LIAL	LIAL
LIAL5O8	LIAL5O8
LIALBR4	LIALBR4
LIALCL4	LIALCL4
LIALH4	LIALH4
LIALO2	LITHIUM-ALUMINATE
LIBC4H16O2	LIBH4*2((CH3)2O)
LIBC6H22N2	LIBH4*2N(CH3)3
LIBF4	LIBF4
LIBH4	LIBH4
LIBH4*2NH3	LIBH4*2NH3
LIBH4*3NH3	LIBH4*3NH3
LIBH4*4NH3	LIBH4*4NH3
LIBH4*C2H6O	LIBH4*(CH3)2O
LIBH4*C4H8O	LIBH4*(CH2)4O
LIBH4*C6H14O	LIBH4*(CH(CH3)2)2O
LIBH4*NC3H9	LIBH4*N(CH3)3
LIBH4*NH3	LIBH4*NH3
2LIBH4*C2H6O	(LIBH4)2*(CH3)2O
LIBR*2NH3	LIBR*2NH3
LIBR*2W	LIBR*2H2O
LIBR*3NH3	LIBR*3NH3
LIBR*5NH3	LIBR*5NH3
LIBR*NH3	LIBR*NH3
LIBR*W	LIBR*H2O
LIBRO3	LIBRO3

Alias	Name
LICL*2W	LICL*2H2O
LICL*3NH3	LICL*3NH3
LICL*3W	LICL*3H2O
LICL*4NH3	LICL*4NH3
LICL*NH3	LICL*NH3
LICL*W	LICL*H2O
LICLO3	LICLO3
LICLO3*0.25W	LICLO3*0.25H2O
LICLO4*2N2H4	LICLO4*2N2H4
LICLO4*3W	LICLO4*3H2O
LICLO4*W	LICLO4*H2O
LICSCLI	LICSCLI
LIH	LITHIUM-HYDRIDE
LIH2PO4	LIH2PO4
LIHF2	LIHF2
LIHG	LIHG
LIHG2	LIHG2
LIHG3	LIHG3
LIHS	LIHS
LII*2NH3	LII*2NH3
LII*2SO2	LII*2SO2
LII*2W	LII*2H2O
LII*3NH3	LII*3NH3
LII*3W	LII*3H2O
LII*4NH3	LII*4NH3
LII*NH3	LII*NH3
LII*SO2	LII*SO2
LII*W	LII*H2O
LIIO3	LIIO3
LIN3	LIN3
LINBO3	LINBO3
LINH2	LINH2
LINO2	LINO2
LINO2*0.5W	LINO2*0.5H2O
LINO2*W	LINO2*H2O
LINO3	LITHIUM-NITRATE
LINO3*3W	LINO3*3H2O
LIOC2H5	LIOC2H5
LIOH	LITHIUM-HYDROXIDE
LIOH*W	LIOH*H2O
LIPB	LIPB
LIPO3	LIPO3
LIREO4	LIREO4
LIREO4*2W	LIREO4*2H2O
LIREO4*W	LIREO4*H2O
LISN	LISN
LITHCL5*8W	LITHCL5*8H2O

Alias	Name
LITL	LITL
LIUO2ASO4	LIUO2ASO4
LIUO5	LI4UO5
LIWF6	LIWF6

SOLIDS Component Databank: Lu

Alias	Name
LUAS	LUAS
LUBR3O9*9W	LU(BRO3)3*9H2O
LUCL3	LUCL3
LUCL3*6W	LUCL3*6H2O
LUI3	LUI3
LUI3O9	LU(IO3)3
LUN3O9*5W	LU(NO3)3*5H2O
LUOCL	LUOCL

SOLIDS Component Databank: Mg

Alias	Name
MG	MAGNESIUM
MG(OH)2	MAGNESIUM-HYDROXIDE
MG17Y3	MG17Y3
MG2AL4SI5O18	MG2AL4SI5O18-CORDIERITE
MG2CU-G	MG2CU-GAMMA
MG2GE	MG2GE
MG2NI	MG2NI
MG2OCL2*16W	MGO*MGCL2*16H2O
MG2OCL2*6W	MGO*MGCL2*6H2O
MG2P2O7-A	MG2P2O7-ALPHA
MG2PB	2-MAGNESIUM-LEAD
MG2SN	MG2SN
MG2TIO4	DIMAGNESIUM-TITANIUM-TETRAOXIDE
MG2ZN11	MG2ZN11
MG3AS2	MG3AS2
MG3AS2O8	MG3(ASO4)2
MG3BI2-B	MG3BI2-BETA
MG3CD	MG3CD
MG3CE	MG3CE
MG3LA	MG3LA
MG3P2O8	MG3(PO4)2
MG3PR	MG3PR
MG3SB2-A	MG3SB2-ALPHA
MG4C3O14H8	(MGCO3)3*MG(OH)2*3H2O
MG4O10H14CL2	(MG(OH)2)3*MGCL2*4H2O
MG4O13H20CL2	(MG(OH)2)3*MGCL2*7H2O
MG4O14H22CL2	(MG(OH)2)3*MGCL2*8H2O
MG4O18H22S	(MG(OH)2)3*MGSO4*8H2O
MG4O6H6CL2	(MG(OH)2)3*MGCL2
MG5Y2	MG5Y2
MG6O18H26CL2	(MG(OH)2)5*MGCL2*8H2O

Alias	Name
MGAS4	MGAS4
MGB12	MGB12
MGBR2*2NH3	MGBR2*2NH3
MGBR2*6W	MGBR2*6H2O
MGBR2*NH3	MGBR2*NH3
MGC2O4	MGC2O4
MGC2O4*2W	MGC2O4*2H2O
MGC4H6O6	MG(CH2OHCO2)2
MGC4H6O6*2W	MG(CH2OHCO2)2*2H2O
MGCD	MGCD
MGCD3	MGCD3
MGCE	MGCE
MGCL2	MAGNESIUM-CHLORIDE
MGCL2*2NH3	MGCL2*2NH3
MGCL2*2W	MGCL2*2H2O
MGCL2*4W	MGCL2*4H2O
MGCL2*6C2OH6	MGCL2*6C2H5OH
MGCL2*6COH4	MGCL2*6CH3OH
MGCL2*6W	MGCL2*6H2O
MGCL2*NH3	MGCL2*NH3
MGCL2*W	MGCL2*H2O
MGCL2O8	MG(CLO4)2
MGCL2O8*2W	MG(CLO4)2*2H2O
MGCL2O8*4W	MG(CLO4)2*4H2O
MGCL2O8*6NH3	MG(CLO4)2*6NH3
MGCL2O8*6W	MG(CLO4)2*6H2O
MGCN2	MGCN2
MGCO3	MAGNESIUM-CARBONATE
MGCO3*5W	MGCO3*5H2O
MGCR2O4	MGCR2O4
MGCRO4	MGCRO4
MGCU2-B	MGCU2-BETA
MGFE2O4	MGFE2O4
MGH2C2O4	MG(HCO2)2
MGI2*2NH3	MGI2*2NH3
MGLA	MGLA
MGN2O6*2W	MG(NO3)2*2H2O
MGN2O6*6COH4	MG(NO3)2*6CH3OH
MGN2O6*6W	MG(NO3)2*6H2O
MGNH4ASO4*6W	MGNH4ASO4*6H2O
MGO	MAGNESIUM-OXIDE
MGO*AL2O3-S	MGO*AL2O3-SPINEL
MGO*MGCL2	MGO*MGCL2
MGOHCL	MGOHCL
MGPR	MGPR
MGS2O3*3W	MGS2O3*3H2O

Alias	Name
MGS2O3*6W	MGS2O3*6H2O
MGSEO3	MAGNESIUM-SELENITE
MGSEO3*6W	MGSEO3*6H2O
MGSEO4	MGSEO4
MGSEO4*4W	MGSEO4*4H2O
MGSEO4*6W	MGSEO4*6H2O
MGSEO4*W	MGSEO4*H2O
MGSO3	MGSO3
MGSO3*3W	MGSO3*3H2O
MGSO3*6W	MGSO3*6H2O
MGSO4*2W	MGSO4*2H2O
MGSO4*4W	MGSO4*4H2O
MGSO4*6W	MGSO4*6H2O
MGSO4*7W	MGSO4*7H2O
MGSO4*W	MGSO4*H2O
MGTIO3	MAGNESIUM-TITANIUM-TRIOXIDE
MGTL	MGTL
MGU3O10	MGU3O10
MGUO4	MGUO4
MGV2O6	MGV2O6
MGWO4	MAGNESIUM-TUNGSTATE
MGY	MGY
MGZN	MGZN
MGZN2	MGZN2

SOLIDS Component Databank: Mn

Alias	Name
MN	MANGANESE
MN2C10O10	MN2(CO)10
MN2FEC6N6	MN2FE(CN)6
MN2O11PB4	PB(MNO4)2*3PBO
MN2O3-B	DIMANGANESE-TRIOXIDE-BRAUNITE
MN3O4-H	MANGANESE-OXIDE-HAUSMANNITE
MN3P2O8	MN3(PO4)2
MN8N2	MN8N2
MNBI	MNBI
MNBR2	MANGANESE-DIBROMIDE
MNBR2*2NH3	MNBR2*2NH3
MNBR2*4W	MNBR2*4H2O
MNBR2*6NH3	MNBR2*6NH3
MNBR2*C2H5OH	MNBR2*C2H5OH
MNBR2*NH3	MNBR2*NH3
MNBR2*W	MNBR2*H2O
MNC2H2O4	MN(CHO2)2
MNC2H2O4*2W	MN(CHO2)2*2H2O
MNC2O4	MANGANESE-OXALATE
MNC2O4*2W	MNC2O4*2H2O
MNC2O4*3W	MNC2O4*3H2O

Alias	Name
MNC4H6O4	MN(CH3CO2)2
MNC4H6O4*4W	MN(CH3CO2)2*4H2O
MNCL2	MANGANESE-DICHLORIDE
MNCL2*2CH3OH	MNCL2*2CH3OH
MNCL2*2W	MNCL2*2H2O
MNCL2*3CH3OH	MNCL2*3CH3OH
MNCL2*4W	MNCL2*4H2O
MNCL2*CH3OH	MNCL2*CH3OH
MNCL2*W	MNCL2*H2O
MNCL4N2H12O2	MNCL2*2NH4CL*2H2O
MNCO3	MANGANESE-CARBONATE
MNCO3-N	MNCO3-NATURAL
MNCO3-P	MNCO3-PRECIPITATED
MNFE2O4	MNFE2O4
MNHASO4	MNHASO4
MNHPO4	MNHPO4
MNI2*2W	MNI2*2H2O
MNI2*4W	MNI2*4H2O
MNI2O6	MN(IO3)2
MNN2O6	MN(NO3)2
MNN6	MN(N3)2-MANGANESE-AZIDE
MNO-M	MANGENESE-OXIDE-MANGANOSITE
MNO2-P	MANGANESE-DIOXIDE-PYROLUSITE
MNO2H2	MN(OH)2-PRECIPITATED
MNS-P	MNS-PRECIPITATED-PINK
MNS2O14H20N2	(NH4)2MN(SO4)2*6H2O
MNS2O6*2W	MNS2O6*2H2O
MNS2O6*6W	MNS2O6*6H2O
MNSO4*4W	MNSO4*4H2O
MNSO4*5W	MNSO4*5H2O
MNSO4*7W	MNSO4*7H2O
MNSO4*W-A	MNSO4*H2O-ALPHA
MNSO4*W-B	MNSO4*H2O-BETA
MNV2O6	MN(VO3)2

SOLIDS Component Databank: Mo

Alias	Name
MO	MOLYBDENUM
MO2B	MO2B
MO3GE	MO3GE
MOB	MOB
MOBR2	MOBR2
MOBR4	MOBR4
MOCL2	MOCL2
MOCL3	MOCL3
MOCL4	MOCL4
MOCL5	MOCL5
MOO2BR2	MOO2BR2

Alias	Name
MOO2CL2*W	MOO2CL2*H2O
MOOCL4	MOOCL4

SOLIDS Component Databank: N

Alias	Name
N2H6*B2H6	(NH3)2*B2H6
N2H6U3O9*4W	(NH3)2(UO3)3*4H2O
N2H7PTCL3	NH4(PT(NH3)CL3)
N2H8CD2S3O12	(NH4)2CD2(SO4)3
N2H8CR2O7	(NH4)2CR2O7
N2H8CR3O10	(NH4)2CR3O10
N2H8CRO4	(NH4)2CRO4
N2H8PTCL4	(NH4)2PTCL4
N3H12UO2F5	(NH4)3UO2F5
NH28ALS2O20	NH4AL(SO4)2*12H2O
NH28CRS2O20	NH4CR(SO4)2*12H2O
NH2COONA	NH2COONA
NH2COONH4	AMMONIUM-CARBAMATE
NH3*B3H7	AMMONIATRIBORANE,TETRAGONAL-BETA
NH3*BF3	NH3*BF3
NH3U2O6*3W	NH3(UO3)2*3H2O
NH3U3O9*5W	NH3(UO3)3*5H2O
NH4ALS2O8	AMMONIUM-ALUMINUM-SULFATE
NH4B5O8*4W	NH4B5O8*4H2O
NH4BO3*0.5W	NH4BO3*0.5H2O
NH4BR	AMMONIUM-BROMIDE
NH4BR*1.5NH3	NH4BR*1.5NH3
NH4BR3	NH4BR3
NH4CL	AMMONIUM-CHLORIDE
NH4CN	AMMONIUM-CYANIDE
NH4CNS*SO2	NH4CNS*SO2
NH4F	AMMONIUM-FLUORIDE
NH4H2ASO4	AMMONIUM-DIHYDROGEN-ARSENATE
NH4H2PO2	NH4H2PO2
NH4H2PO4	AMMONIUM-DIHYDROGEN-PHOSPHATE
NH4HCO3	AMMONIUM-HYDROGEN-CARBONATE
NH4HF2	AMMONIUM-HYDROGEN-FLUORIDE
NH4HS	AMMONIUM-HYDROGEN-SULFIDE
NH4HSE	AMMONIUM-HYDROGEN-SELENIDE
NH4HSO3	AMMONIUM-HYDROGEN-SULFITE
NH4HSO4	AMMONIUM-BISULFATE
NH4HTE	AMMONIUM-HYDROGEN-TELLURIDE
NH4I*2NH3	NH4I*2NH3
NH4I*3SO2	NH4I*3SO2
NH4I*NH3	NH4I*NH3
NH4I3	NH4I3
NH4IBR2	NH4IBR2

Alias	Name
NH4IBRCL	NH4IBRCL
NH4ICL2	NH4ICL2
NH4ICL4	NH4ICL4
NH4IO3	AMMONIUM-IODATE
NH4N3	AMMONIUM-AZIDE
NH4NO2	AMMONIUM-NITRITE
NH4NO3	AMMONIUM-NITRATE
NH4OCN	AMMONIUM-CYANATE
NH4PF6	NH4PF6
NH4REO4	NH4REO4
NH4SCN	AMMONIUM-THIOCYANATE
NH4TACL6	NH4TACL6
NH4U2O4F5	NH4(UO2)2F5
NH4U2O4F5*3W	NH4(UO2)2F5*3H2O
NH4U2O4F5*4W	NH4(UO2)2F5*4H2O
NH4VO3	NH4VO3
(NH4)2HASO4	DIAMMONIUM-HYDROGEN-ARSENATE
(NH4)2HPO4	DIAMMONIUM-PHOSPHATE
(NH4)2S2O8	(NH4)2S2O8
(NH4)2S4	(NH4)2S4
(NH4)2S5	(NH4)2S5
(NH4)2S8	(NH4)2S8
(NH4)2SEO4	AMMONIUM-SELENATE
(NH4)2SIF6-C	(NH4)2SIF6-CUBIC
(NH4)2SIF6-H	(NH4)2SIF6-HEXAGONAL
(NH4)2SNBR6	(NH4)2SNBR6
(NH4)2SNCL6	(NH4)2SNCL6
(NH4)2SO3	AMMONIUM-SULFITE
(NH4)2SO3*W	AMMONIUM-SULFITE-HYDRATE
(NH4)2SO4	AMMONIUM-SULFATE
(NH4)2SO4*3N	(NH4)2SO4*3NH3
(NH4)3ASO4	AMMONIUM-ARSENATE
(NH4)3ASO4*3	AMMONIUM-ARSENATE-TRIHYDRATE
(NH4)3PO4	AMMONIUM-PHOSPHATE
(NH4)3PO4*3W	AMMONIUM-PHOSPHATE-TRIHYDRATE
2NH4NASO4*W	NA2SO4*(NH4)2SO4*H2O
NHG2BR	NHG2BR
NOVF6	NOVF6

SOLIDS Component Databank: Na

Alias	Name
NA	SODIUM
NA(UO2)2F5	NA(UO2)2F5
NA2AG2O3	NA2AG2O3
NA2B4O7*10W	NA2B4O7*10H2O
NA2B4O7*4W	NA2B4O7*4H2O
NA2B4O7*5W	NA2B4O7*5H2O
NA2BA(CO3)2	NA2CO3*BACO3

Alias	Name
NA2BA(SO4)2	NA2SO4*BASO4
NA2BECL4	NA2BECL4
NA2C2	SODIUM-CARBIDE
NA2C2H2O3	DISODIUM-HYDROXYACERATE
NA2C2H2O3*2W	NAOCH2CO2NA*2H2O
NA2C2O4	NA2C2O4
NA2CA(SO4)2	NA2CA(SO4)2
NA2CACL4	NA2CACL4
NA2CO3	SODIUM-CARBONATE
NA2CO3.10H2O	SODIUM-CARBONATE-DECAHYDRATE
NA2CO3.3NAHC	WEGSCHEIDER
NA2CO3.7H2O	SODIUM-CARBONATE-HEPTAHYDRATE
NA2CO3.H2O	SODIUM-CARBONATE-MONOHYDRATE
NA2CO3.NAHCO	TRONA
NA2COO3	NA2COO3
NA2CR2O7	SODIUM-DICHROMATE
NA2CR2O7*2W	NA2CR2O7*2H2O
NA2CRO4*10W	NA2CRO4*10H2O
NA2CRO4*4NAO	NA2CRO4*4NAOH
NA2CRO4*4W	NA2CRO4*4H2O
NA2CUC2O6	NA2CU(CO3)2
NA2CUC2O6*3W	NA2CU(CO3)2*3H2O
NA2CUO3	NA2CUO3
NA2H2P2O5	NA2H2P2O5
NA2H2P2O7	NA2H2P2O7
NA2H2P2O7*6W	NA2H2P2O7*6H2O
NA2HFCL6	NA2HFCL6
NA2HPO4	DISODIUM-PHOSPHATE
NA2HPO4*12W	NA2HPO4*12H2O
NA2HPO4*2W	NA2HPO4*2H2O
NA2HPO4*7W	NA2HPO4*7H2O
NA2HSEO3	NAHSEO3
NA2HSEO4	NAHSEO4
NA2IRCL6	NA2IRCL6
NA2K2(CO3)2	NA2CO3*K2CO3-AGED
NA2K2(SO4)2	NA2SO4*K2SO4-AGED
NA2K4(CO3)3	NA2CO3*2K2CO3-AGED
NA2K4(SO4)3	NA2SO4*2K2SO4-AGED
NA2K6(CO3)4	NA2CO3*3K2CO3-AGED
NA2K6(SO4)4	NA2SO4*3K2SO4-GLASERITE
NA2K8(CO3)5	NA2CO3*4K2CO3-AGED
NA2MG(SO4)2	NA2MG(SO4)2
NA2MGS2O8*2W	NA2MG(SO4)2*2H2O
NA2MN(SO4)2	NA2MN(SO4)2
NA2MNO4	NA2MNO4
NA2MNS2O8*2W	NA2MN(SO4)2*2H2O
NA2MO2O7	NA2MO2O7

Alias	Name
NA2MOCL6	NA2MOCL6
NA2MOF8	NA2MOF8
NA2MOO4*2W	NA2MOO4*2H2O
NA2MOO6*W	NA2MOO6*H2O
NA2MOO8*2W	NA2MOO8*2H2O
NA2MOO8*4W	NA2MOO8*4H2O
NA2N2O3	NA2N2O3
NA2NBF7	NA2NBF7
NA2O	SODIUM-OXIDE
NA2O*3B2O3	NA2O*3B2O3
NA2O*4B2O3	NA2O*4B2O3
3NA2O*NB2O5	3NA2O*NB2O5
NA2OSCL6	NA2OSCL6
NA2PBI4*4W	(NAI)2PBI2*4H2O
NA2PBI4*6W	(NAI)2PBI2*6H2O
NA2PBO3	NA2PBO3
NA2PTCL6	NA2PTCL6
NA2PTCL6*2W	NA2PTCL6*2H2O
NA2PTCL6*6W	NA2PTCL6*6H2O
NA2S*4.5W	NA2S*4.5H2O
NA2S*5W	NA2S*5H2O
NA2S*9W	NA2S*9H2O
NA2S2O3	SODIUM-THIOSULFATE
NA2S2O3*5W	NA2S2O3*5H2O
NA2S2O4	SODIUM-HYDROSULFITE
NA2S2O5	NA2S2O5
NA2S2O6	NA2S2O6
NA2S2O6*2W	NA2S2O6*2H20
NA2S2O7	NA2S2O7
NA2S3O6*3W	NA2S3O6*3H2O
NA2S4O6*2W	NA2S4O6*2H2O
NA2S5	NA2S5
NA2SE	NA2SE
NA2SE*16W	NA2SE*16H2O
NA2SE*4.5W	NA2SE*4.5H2O
NA2SE*9W	NA2SE*9H2O
NA2SE2	NA2SE2
NA2SEO3	NA2SEO3
NA2SEO3*5W	NA2SEO3*5H2O
NA2SEO4	NA2SEO4
NA2SEO4*10W	NA2SEO4*10H2O
NA2SIF6	NA2SIF6
NA2SIO3*5W	NA2SIO3*5H2O
NA2SIO3*9W	NA2SIO3*9H2O
NA2SNO3	NA2SNO3
NA2SO3*7W	NA2SO3*7H2O
NA2SO4	SODIUM-SULFATE

Alias	Name
NA2SO4*SRSO4	NA2SO4*SRSO4
NA2SO4.10H2O	GLAUBER
NA2SO4.NAOH	DOUBLE
NA2TAF7	NA2TAF7
NA2TE2	NA2TE2
NA2TEO3	NA2TEO3
NA2TEO3*5W	NA2TEO3*5H2O
NA2THCL6	NA2THCL6
NA2U2O7	NA2U2O7
NA2U2O7*1.5W	NA2U2O7*1.5H2O
NA2UCL6	NA2UCL6
NA2UO4-A	NA2UO4-ALHPA
NA2UO4-B	NA2UO4-BETA
NA2V3F11	NA2V3F11
NA2W2O7	NA2W2O7
NA2W4O13	NA2W4O13
NA2WF8	NA2WF8
NA2WO4*2W	NA2WO4*2H2O
NA2WO6*W	NA2WO6*H2O
NA2WO8*2W	NA2WO8*2H2O
NA2ZN(SO4)2	NA2ZN(SO4)2
NA2ZNO2	NA2ZNO2
NA2ZNS2O8*2W	NA2ZN(SO4)2*2H2O
NA2ZNS2O8*4W	NA2ZN(SO4)2*4H2O
NA2ZRCL6	NA2ZRCL6
NA3ALF6	CRYOLITE
NA3ALF6*3.5W	NA3ALF6*3.5H2O
NA3ASO4*12W	NA3ASO4*12H2O
NA3BI	NA3BI
NA3BIO4	NA3BIO4
NA3CON6O12	NA3(CO(NO2)6)
NA3CRCL6	NA3CRCL6
NA3FECO(CN)5	NA3FECO(CN)5
NA3HG	NA3HG
NA3HG2	NA3HG2
NA3HP2O7	NA3HP2O7
NA3HP2O7*6W	NA3HP2O7*6H2O
NA3HP2O7*W	NA3HP2O7*H2O
NA3IRCL6	NA3IRCL6
NA3P	NA3P
NA3PW3O13*4W	NA3PW3O13*4H2O
NA3RHCL6	NA3RHCL6
NA3RHCL6*12W	NA3RHCL6*12H2O
NA3SB	NA3SB
NA3SCF6	NA3SCF6
NA3TICL6	NA3TICL6
NA3UO2F5	NA3UO2F5

Alias	Name
NA3UO4	NA3UO4
NA3VCL6	NA3VCL6
NA3VF6	NA3VF6
NA3VO4*.5W-O	NA3VO4*0.5H2O-ORTHO
NA3VO4*.5W-P	NA3VO4*0.5H2O-PSEUDOSALT
NA3VO4*10W-O	NA3VO4*10H2O-ORTHO
NA3VO4*10W-P	NA3VO4*10H2O-PSEUDOSALT
NA3VO4*12W	NA3VO4*12H2O-ORTHO
NA3VO4*2W	NA3VO4*2H2O-ORTHO
NA3VO4*3.5W	NA3VO4*3.5H2O-PSEUDOSALT
NA3VO4*7W	NA3VO4*7H2O-ORTHO
NA3VO4*8W	NA3VO4*8H2O-PSEUDOSALT
NA4BA(SO4)3	2NA2SO4*BASO4
NA4CA(SO4)3	NA4CA(SO4)3
NA4CEO4	NA4CEO4
NA4K2(CO3)3	2NA2CO3*K2CO3-AGED
NA4K2(SO4)3	2NA2SO4*K2SO4-AGED
NA4O4UO4	NA4O4UO4
NA4O4UO4*9W	NA4O4UO4*9H2O
NA4P2O7	TETRASODIUM-PYROPHOSPHATE
NA4P2O7*10W	NA4P2O7*10H2O
NA4P4O12	NA4P4O12
NA4SN	NA4SN
NA4SO4CLOH	TRIPLE
NA4SR(SO4)3	2NA2SO4*SRSO4
NA4UO2(CO3)3	NA4UO2(CO3)3
NA4UO5	NA4UO5
NA4V2O7*10W	NA4V2O7*10H2O
NA4V2O7*12W	NA4V2O7*12H2O
NA4V2O7*18W	NA4V2O7*18H2O
NA4V2O7*2W	NA4V2O7*2H2O
NA5H3(CO3)4	3NAHCO3*NA2CO3
NA5HG2	NA5HG2
NA5P3O10*6W	NA5P3O10*6H2O
NA5P3O10-1	NA5P3O10-FORM-1-QUENCHED
NA5P3O10-2	NA5P3O10-FORM-2
NA5PB2	NA5PB2
NA5V3F14	NA5V3F14
NA6K2(CO3)4	3NA2CO3*K2CO3-AGED
NA6U7O24	NA6U7O24
NA6ZR2SI4O15	NA6ZR2SI4O15
NA7HG8	NA7HG8
NA8K2(CO3)5	4NA2CO3*K2CO3-AGED
NAALH4	NAALH4
NAALS2O8*12W	NAAL(SO4)2*12H2O
NAALS2O8*2W	NAAL(SO4)2*2H2O
NAALS2O8*5W	NAAL(SO4)2*5H2O

Alias	Name
NAALS2O8*6W	NAAL(SO4)2*6H2O
NAAS	NAAS
NAAS2	NAAS2
NAASO2	NAASO2
NAB(OCH3)4	NAB(OCH3)4
NAB5O8*5W	NAB5O8*5H2O
NABF4	NABF4
NABH4	NABH4
NABH4*2W	NABH4*2H2O
NABH4*3NH3	NABH4*3NH3
NABH4*4.5NH3	NABH4*4.5NH3
NABO2*2W	NABO2*2H2O
NABO2*4W	NABO2*4H2O
NABO3*4W	NABO3*4H2O
NABR*2W	NABR*2H2O
NABR*5.25NH3	NABR*5.25NH3
NABR*5.75NH3	NABR*5.75NH3
NABRF4	NABRF4
NABRO3	NABRO3
NAC2H5O2	SODIUM-ETHLYLENE-GLYCOLATE
NAC3H9O3	NAC2H5O2*CH3OH
NAC4H11O3	NAC2H5O2*C2H5OH
NAC4H11O4	NAC2H5O2*(CH2OH)2
NAC4H7O6	CH2OHCOONA*CH2OHCOOH
NAC6H17O3	NAOC2H5*2C2H5OH
NACH3CO2	NACH3CO2
NACH3CO2*3W	NACH3CO2*3H2O
NACL	SODIUM-CHLORIDE
NACL*5NH3	NACL*5NH3
NACLO2	NACLO2
NACLO2*3W	NACLO2*3H2O
NACLO3	SODIUM-CHLORATE
NACLO4*W	NACLO4*H2O
2NACL*BACL2	2NACL*BACL2
2NACL*MGCL2	2NACL*MGCL2
2NACL*SRCL2	2NACL*SRCL2
NACN*0.5W	NACN*0.5H2O
NACN*2W	NACN*2H2O
NACN-c	NACN-CUBIC
NACN-o	NACN-ORTHORHOMBIC
NACNO	NACNO
NACNS	NACNS
NACNS*2SO2	NACNS*2SO2
NACOO8N4C2H6	NA(CO(NH3)2(NO2)2C2O4)
NACRO2	NACRO2
NACS2CRCL6	NACS2CRCL6
NAF	SODIUM-FLUORIDE

Alias	Name
NAFECL4	NAFECL4
NAFEF3	NAFEF3
NAFEO2	NAFEO2
NAH2F3	NAH2F3
NAH2PO2	NAH2PO2
NAH2PO3	NAH2PO3
NAH2PO3*2.5W	NAH2PO3*2.5H2O
NAH2PO4	MONOSODIUM-PHOSPHATE
NAH2PO4*2W	NAH2PO4*2H2O
NAH2PO4*W	NAH2PO4*H2O
NAH3(SEO3)2	NAH3(SEO3)2
NAH3P2O7	NAH3P2O7
NAHC2	SODIUM-ACETYLIDE
NAHC2O4	NAHC2O4
NAHC2O4*W	NAHC2O4*H2O
NAHCO3	SODIUM-BICARBONATE
NAHF2	NAHF2
NAHG	NAHG
NAHG2	NAHG2
NAHG4	NAHG4
NAHGC2N2I*2W	NAHG(CN)2I*2H2O
NAHPO3	NA2HPO3
NAHPO3*5W	NA2HPO3*5H2O
NAHS	NAHS
NAHS*2W	NAHS*2H2O
NAHSE	NAHSE
NAHSO4	SODIUM-BISULFATE
NAHSO4*W	NAHSO4*H2O
2NAHSO3CHO*W	(CHO)2*2NAHSO3*H2O
NAI*2W	NAI*2H2O
NAI*3CH3OH	NAI*3CH3OH
NAI*4SO2	NAI*4SO2
NAI3	NAI3
3NAI*8SO2	3NAI*8SO2
NAIBR2	NAIBR2
NAICL2	NAICL2
NAICL4	NAICL4
NAIO2F2	NAIO2F2
NAIO3	NAIO3
NAIO3*5W	NAIO3*5H2O
NAIO3*W	NAIO3*H2O
NAIO4	NAIO4
NAIO4*3W	NAIO4*3H2O
NAK(CNS)2	NACNS*KCNS
NAK3(CNS)4	NACNS*3KCNS
NALIB4O7	0.5NA2O*0.5LI2O*2B2O3

Alias	Name
NALIB6O10	0.5NA2O*0.5LI2O*3B2O3
NALIB8O13	0.5NA2O*0.5LI2O*4B2O3
NALIICL	NALIICL
NAMGF3	NAMGF3
NAMNCL3	NAMNCL3
NAMNO4*3W	NAMNO4*3H2O
NAMNO4*W	NAMNO4*H2O
NAMOF7	NAMOF7
NAN3	NAN3
NANBCL6	NANBCL6
NANBO3	NANBO3
NANBO3*3.5W	NANBO3*3.5H2O
NANBOCL4	NANBOCL4
NANH2	SODIUM-AMIDE
NANH3	NANH3
NANH4HPO4*4W	NANH4HPO4*4H2O
NANO2*NAOH	NANO2*NAOH
NANO3	SODIUM-NITRATE
NANO3*2NAOH	NANO3*2NAOH
NANO3*NAOH	NANO3*NAOH
NAOC2H5	NAOC2H5
NAOCH3	NAOCH3
NAOH	SODIUM-HYDROXIDE
NAOH*BF3	NAOH*BF3
NAOH*W	NAOH*H2O
(NAPO3)3	(NAPO3)3
NAPB	NAPB
NAPTBR6	NA2PTBR6
NAPTBR6*6W	NA2PTBR6*6H2O
NARB2CRCL6	NARB2CRCL6
NAREO4	NAREO4
NASB	NASB
NASN	NASN
NASO3F	NASO3F
NATACL6	NATACL6
NATEO4	NA2TEO4
NATHCL5*10W	NATHCL5*10H2O
NATICL3	NATICL3
NATL	NATL
NAUCL6-A	NAUCL6-ALPHA
NAUCL6-B	NAUCL6-BETA
NAUF6	NAUF6
NAUO3	NAUO3
NAWF6	NAWF6
NAWF7	NAWF7
NAZRF5	NAZRF5
NAZRSI2O7	NA2ZRSI2O7

	Alias	Name
	NAZRSIO5	NA2ZRSIO5

SOLIDS Component Databank: Nb

Alias	Name
NB1.136S2	NB1.136S2
NBB1.875	NBB1.875
NBB1.963	NBB1.963
NBCO2	NBCO2
NBCO3	NBCO3
NBCR2	NBCR2
NBGE0.15	NBGE0.15
NBGE0.54	NBGE0.54
NBGE0.67	NBGE0.67
NBGE2	NBGE2
NBOBR3	NBOBR3

SOLIDS Component Databank: Nd

Alias	Name
ND2C3O9	ND2(CO3)3
ND2C6O12*10W	ND2(C2O4)3*10H2O
ND2S3O12*8W	ND2(SO4)3*8H2O
ND2SE3O12*5W	ND2(SEO4)3*5H2O
NDAL2	NDAL2
NDBR3O9*9W	ND(BRO3)3*9H2O
NDCL2	NDCL2
NDCL3*6W	NDCL3*6H2O
NDF3*W	NDF3*H2O
NDI3O9	ND(IO3)3
NDN3O9	ND(NO3)3
NDN3O9*3W	ND(NO3)3*3H2O
NDN3O9*4W	ND(NO3)3*4H2O
NDN3O9*6W	ND(NO3)3*6H2O

SOLIDS Component Databank: Ni

Alias	Name
NI	NICKEL
NI2I6PB	(NII2)2*PBI2
NI2I6PB*3W	(NII2)2*PBI2*3H2O
NI2P2O7	NI2P2O7
NI2SI	NI2SI
NI2TE3	NI2TE3
NI3N	NI3N
NI4SO10H6	NISO4*3NI(OH)2
NI4W	NI4W
NI6S5	NI6S5
NI7S3O20H8	(NISO4)3*4NI(OH)2
NI7S6	NI7S6
NIAL	NIAL
NIB2O4	NI(BO2)2
NIBR2*3W	NIBR2*3H2O
NIBR2*6CH3OH	NIBR2*6CH3OH

Alias	Name
NIBR2N2H6	NIBR2*2NH3
NIBR2NH3	NIBR2*NH3
NIC2N2	NI(CN)2-PRECIPITATED
NIC2N2O2	NI(CNO)2
NIC2N2S2	NI(CNS)2
NIC2O4	NICKEL-OXALATE
NIC4H6O4N4	NI(C2H3O2N2)2
NICL2	NICKEL-CHLORIDE
NICL2*2W	NICL2*2H2O
NICL2*4W	NICL2*4H2O
NICL2*6W	NICL2*6H2O
NICL2N2H6	NICL2*2NH3
NICL2NH3	NICL2*NH3
NICL2O8*6W	NI(CLO4)2*6H2O
NIF2*4W	NIF2*4H2O
NIFE2O4	NIFE2O4
NIH2C2O4	NI(HCO2)2
NII2N2H6	NII2*2NH3
NII2O6	NI(IO3)2
NIN2H8C4O4	NI(NH2CH2COO)2
NIN2O6	NI(NO3)2
NIN2O6*3W	NI(NO3)2*3H2O
NIN2O6*6W	NI(NO3)2*6H2O
NIN6*W	NI(N3)2*H2O
NIN6H12SO4	NI(N2H4)3SO4
NIN6H18BR2	NI(NH3)6BR2
NIN6H18CL2	NI(NH3)6CL2
NIN6H18I2	NI(NH3)6I2
NIN6H24C6CL2	NI(N2H8C2)3CL2
NIN8H18O6	NI(NH3)6(NO3)2
NIO-B	NICKEL-OXIDE-BUNSENITE
NIO2H2	NI(OH)2
NIO8H8B2	NI(OH)2*2H3BO3
NIS-P	NIS-PRECIPITATED
NIS2O6*6W	NIS2O6*6H2O
NISE	NISE
NISEO3*2W	NISEO3*2H2O
NISEO3*2W-P	NISEO3*2H2O-PRECIPITATED
NISO4*4W	NISO4*4H2O
NISO4*6W	NISO4*6H2O-ALPHA,GREEN
NISO4*7W	NISO4*7H2O
NITE	NITE
NITE2	NITE2

SOLIDS Component Databank: P

Alias	Name
P-W	PHOSPHORUS-WHITE
P2H6*B2H6	(PH3)2*B2H6
P2O5	DIPHOSPHORUS-PENTAOXIDE
P2S3	P2S3
P3N5	P3N5
P4O10	TETRAPHOSPHORUS-DECAOXIDE
PH3*BCL3	PH3*BCL3
PH4BR	PH4BR
PH4CL	PH4CL
PH4I	PH4I
POCL3*BCL3	POCL3*BCL3

SOLIDS Component Databank: Pa

Alias	Name
PABR4	PABR4
PABR5	PABR5
PACL4	PACL4
PACL5	PACL5
PAI4	PAI4
PAOBR2	PAOBR2

SOLIDS Component Databank: Pb

Alias	Name
PB	LEAD
PB(N3)2-M	PB(N3)2-MONOCLINIC
PB(N3)2-O	PB(N3)2-ORTHORHOMBIC
PB(NO3)2	PB(NO3)2
PB(OH)2	PB(OH)2
PB(OH)2-P	PB(OH)2-PPTD
PB2CL4*NH4CL	(PBCL2)2*NH4CL
PB2N6O	PB(N3)2*PBO
PB2O2*PBCL2	(PBO)2*PBCL2
PB2SIO4	DILEAD-ORTHOSILICATE
PB2V2O7	PB2V2O7
PB3AM4I10*6W	(PBI2)3*4NH4I*6H2O
PB3ASI9*12W	(PBI2)3*ASI3*12H2O
PB3C2N2O3H2	PB(CN)2*2PBO*H2O
PB3I6*4NH4I	(PBI2)3*4NH4I
PB3I6*ASI3	(PBI2)3*ASI3
PB3I6*PI3	(PBI2)3*PI3
PB3I6*SBI3	(PBI2)3*SBI3
PB3I9P*12W	(PBI2)3*PI3*12H2O
PB3O2BR2	(PBO)2*PBBR2
PB3O3*PBCL2	(PBO)3*PBCL2
PB3P2O8	PB3(PO4)2
PB3SBI9*12W	(PBI2)3*SBI3*12H2O
PB3V2O8	PB3(VO4)2
PB4O3BR2	(PBO)3*PBBR2
PB4O6H6CL2	(PB(OH)2)3*PBCL2

Alias	Name
PBBR2*2NH3	PBBR2*2NH3
PBBR2*3NH3	PBBR2*3NH3
PBBR2*5.5NH3	PBBR2*5.5NH3
PBBR2*8NH3	PBBR2*8NH3
PBBR2*NH3	PBBR2*NH3
PBBR2O6	PB(BRO3)2
PBBRF	PBBRF
PBC2H2O4	PB(HCO2)2
PBC2O4	PBC2O4
PBC4H6O4	PB(CH3CO2)2
PBC4H6O4*3W	PB(CH3CO2)2*3H2O
PBCL2	LEAD-DICHLORIDE
PBCL2*1.5NH3	PBCL2*1.5NH3
PBCL2*2NH3	PBCL2*2NH3
PBCL2*3.25NH	PBCL2*3.25NH3
PBCL2*8NH3	PBCL2*8NH3
PBCL2*NH3	PBCL2*NH3
PBCL2*PBCO3	PBCL2*PBCO3
PBCLOH	PBCLOH
PBFCL	PBFCL
PBH2PO4	RBH2PO4
PBHPO3	PBHPO3
PBI2*0.5NH3	PBI2*0.5NH3
PBI2*2MGI2	PBI2*2MGI2
PBI2*2NH3	PBI2*2NH3
PBI2*2RBI	PBI2*2RBI
PBI2*2RBI*4W	PBI2*2RBI*4H2O
PBI2*2ZNI2	PBI2*2ZNI2
PBI2*5NH3	PBI2*5NH3
PBI2*8NH3	PBI2*8NH3
PBI2*HI*5W	PBI2*HI*5H2O
PBI2*NH3	PBI2*NH3
PBI2*SNI2	PBI2*SNI2
PBI2*SNI2*8W	PBI2*SNI2*8H2O
PBI2O6	PB(IO3)2
PBI8CR2	PBI2*2CRI3
PBI8CR2H6O3	PBI2*2CRI3*3H2O
PBN2O6*3NH3	PB(NO3)2*3NH3
PBN2O6*6NH3	PB(NO3)2*6NH3
PBN2O6*NH3	PB(NO3)2*NH3
PBNA4S6O9	PBS2O3*2NA2S2O3
PBO*PBBR2	PBO*PBBR2
PBO*PBCL2	PBO*PBCL2
PBO*PBCO3	DILEAD-OXIDE-CARBONATE
PBR5	PHOSPHORUS-PENTABROMIDE
PBRE2O8*2W	PB(REO4)2*2H2O
PBS	LEAD-SULFIDE

Alias	Name
PBS2C2N2	PB(SCN)2
PBS2O3	PBS2O3
PBS2O6*4W	PBS2O6*4H2O
PBS3O6	PBS3O6
PBSO3	PBSO3
PBSO4	LEAD-SULFATE
PBSO4*2NH3	PBSO4*2NH3
PBSO4*2PBO	PBSO4*2PBO
PBSO4*3PBO	PBSO4*3PBO
PBSO4*4NH3	PBSO4*4NH3
PBSO4*PBO	PBSO4*PBO
PBTEO4	PBTEO4

SOLIDS Component Databank: Pd

Alias	Name
PD2H	PD2H
PD3SB	PD3SB
PDBR2	PDBR2
PDC2N2	PD(CN)2
PDC2N2S2	PD(CNS)2
PDCL2*2NH3	PDCL2*2NH3
PDCL2*4NH3	PDCL2*4NH3
PDI2*2NH3	PDI2*2NH3
PDI2*4NH3	PDI2*4NH3
PDO2H2	PD(OH)2-PRECIPITATED
PDO4H4	PD(OH)4-PRECIPITATED
PDSB	PDSB
PDSB2	PDSB2
PDTE2	PDTE2

SOLIDS Component Databank: Pr

Alias	Name
PR2C3O9	PR2(CO3)3
PR2C6O12*10W	PR2(C2O4)3*10H2O
PR2SE3O12*5W	PR2(SEO4)3*5H2O
PR2SE4O12H2	PR2(SEO3)3*H2SEO3
PR2SE4O17H12	PR2(SEO3)3*H2SEO3*5H2O
PRAL2	PRAL2
PRAL4	PRAL4
PRAS	PRAS
PRBI	PRBI
PRBR3O9*9W	PR(BRO3)3*9H2O
PRC	PRC
PRCL3*6W	PRCL3*6H2O
PRCL3*7W	PRCL3*7H2O
PRF3*W	PRF3*H2O
PRI3O9	PR(IO3)3
PRN3O9	PR(NO3)3
PRN3O9*6W	PR(NO3)3*6H2O

	Alias	Name
	PRO3H3	PR(OH)3
	PROCL	PROCL
	PRSB	PRSB

SOLIDS Component Databank: Pt

Alias	Name
PT	PLATINUM
PT3N6H18CL6	(PT(NH3)4)(PT(NH3)CL3)2
PTBR	PTBR
PTCL	PTCL
PTCL2*5NH3	PTCL2*5NH3
PTCL4*5W	PTCL4*5H2O
PTF6	PTF6
PTN2H6CL2-C	PT(NH3)2CL2-CIS
PTN2H6CL2-T	PT(NH3)2CL2-TRANS
PTN3H9CL2	(PT(NH3)3CL)CL
PTN3H9CL2O4	(PT(NH3)3CL)CLO4
PTN4H12CL2	(PT(NH3)4)CL2
PTN4H12CL2*W	(PT(NH3)4)CL2*H2O
PTN4H12I2	(PT(NH3)4)I2
PTN6H12O6	PT(NH3)4(NO3)2
PTO2H2	PT(OH)2
PTTE	PTTE
PTTE2	PTTE2

SOLIDS Component Databank: Ra

Alias	Name
RA	RA
RA(IO3)2	RA(IO3)2
RA(NO3)2	RA(NO3)2
RACL2	RACL2
RACL2*2W	RACL2*2H2O
RASO4	RASO4

SOLIDS Component Databank: Rb

Alias	Name
RB	RUBIDIUM
RB(UO2)2F5	RB(UO2)2F5
RB2BA(NO2)4	2RBNO2*BA(NO2)2
RB2CO3	RUBIDIUM-CARBONATE
RB2CO3*1.5W	RB2CO3*1.5H2O
RB2CO3*3W	RB2CO3*3H2O
RB2CO3*W	RB2CO3*H2O
RB2COCL4	RB2COCL4
RB2CRO4	RB2CRO4
RB2FECL4	RB2FECL4
RB2GECL6	RB2GECL6
RB2H2P2O7	RB2H2P2O7
RB2IRCL6	RB2IRCL6
RB2NBOCL5	RB2NBOCL5
RB2PTCL4	RB2PTCL4

Alias	Name
RB2PTCL6	RB2PTCL6
RB2S	RB2S
RB2SEO3	RB2SEO3
RB2SEO4	RB2SEO4
RB2SIF6	RB2SIF6
RB2SNBR6	RB2SNBR6
RB2SNCL6	RB2SNCL6
RB2TEBR6	RB2TEBR6
RB2TEO3	RB2TEO3
RB2TEO3*3W	RB2TEO3*3H2O
RB2TEO3*W	RB2TEO3*H2O
RB2THCL6	RB2THCL6
RB2THCL6*9W	RB2THCL6*9H2O
RB2TIBR6	RB2TIBR6
RB2TICL4	RB2TICL4
RB2TICL6	RB2TICL6
RB2UBR6	RB2UBR6
RB2UCL6	RB2UCL6
RB2ZNBR4	RB2ZNBR4
RB2ZNCL4	RB2ZNCL4
RB3AGI3	RB2AGI3
RB3COCL5	RB3COCL5
RB3CR2CL9	RB3CR2CL9
RB3CRCL6	RB3CRCL6
RB3CRO4F	RB3CRO4F
RB3SB	RB3SB
RB3SB7	RB3SB7
RB3TI2BR9	RB3TI2BR9
RB3TIBR6	RB3TIBR6
RB3UO2F5	RB3UO2F5
RB3V2CL9	RB3V2CL9
RB3VCL6	RB3VCL6
RB4THCL8	RB4THCL8
RB4UCL8	RB4UCL8
RB5(UO2)2F9	RB5(UO2)2F9
RB5SB4	RB5SB4
RBAG4I5	RBAG4I5
RBB(CLO4)4	RBB(CLO4)4
RBBA2(NO2)5	RBNO2*2BA(NO2)2
RBBCL4	RBBCL4
RBBF4	RBBF4
RBBO2	RBBO2
RBBR2CL	RBBR2CL
RBBR3	RBBR3
7RBBR*3SBBR3	7RBBR*3SBBR3
RBBRCL2	RBBRCL2
RBBRO3	RBBRO3

Alias	Name
RBC10	RBC10
RBC24	RBC24
RBC36	RBC36
RBC48	RBC48
RBC4H11O2	C2H5ORB*C2H5OH
RBC60	RBC60
RBC72	RBC72
RBC8	RBC8
RBCACL3	RBCACL3
RBCEFEC6N6W2	RBCE(FE(CN)6)*2H2O
RBCL*ZNSO4	RBCL*ZNSO4
RBCLO3	RBCLO3
RBCLO4	RBCLO4
RBCN	RBCN
RBCOCL3	RBCOCL3
RBF*1.5W	RBF*1.5H2O
RBFECL3	RBFECL3
RBGDFEC6N6	RBGD(FE(CN)6)
RBH	RBH
RBHCO3	RBHCO3
RBHF2	RBHF2
RBHS	RBHS
RBHSE	RBHSE
RBHSO4	RBHSO4
RBI*3SO2	RBI*3SO2
RBI3	RBI3
RBIBR2	RBIBR2
RBIBRCL	RBIBRCL
RBICL2	RBICL2
RBICL4	RBICL4
RBIO3	RBIO3
RBKCL2	RBKCL2
RBMNCL3	RBMNCL3
RBMOF6	RBMOF6
RBN3	RBN3
RBNBCL6	RBNBCL6
RBNBO3	RBNBO3
RBNH2	RBNH2
RBNICL3	RBNICL3
RBNO2	RBNO2
RBNO3	RBNO3
RBOH	RBOH
RBOH*2W	RBOH*2H2O
RBOH*W	RBOH*H2O
RBPF6	RBPF6
RBPO3	RBPO3
RBPTNH3CL3	RBPTNH3CL3

	Alias	Name
	RBREO4	RBREO4
	RBSB	RBSB
	RBSB2	RBSB2
	RBSO2F	RBSO2F
	RBTACL6	RBTACL6
	RBTICL3	RBTICL3
	RBUCL5	RBUCL5
	RBUCL6	RBUCL6
	RBUF6	RBUF6
	RBWF6	RBWF6

SOLIDS Component Databank: Sb

Alias	Name
SB(OH)3	ANTIMONY-TRIHYDROXIDE
SB4O5CL2	SB4O5CL2
SBCL3*3RBCL	SBCL3*3RBCL
SBF3*2NH3	SBF3*2NH3
SBF3*3NH3	SBF3*3NH3
SBF3*4NH3	SBF3*4NH3
SBF3*6NH3	SBF3*6NH3
SBF3*NH3	SBF3*NH3
SBOCL	ANTIMONY-CHLORIDE-OXIDE

SOLIDS Component Databank: Sc

Alias	Name
SC2C6O12	SC2(C2O4)3
SC2O5H5CL	SC2(OH)5CL
SC2S3O12	SC2(SO4)3
SC2SE3O9*10W	SC2(SEO3)3*10H2O
SCAS	SCAS
SCCL3*6W	SCCL3*6H2O
SCH1.97	SCH1.97
SCH2	SCH2
SCH3C3O6	SC(HCO2)3
SCO2H2CL	SC(OH)2CL
SCO3H3	SC(OH)3

SOLIDS Component Databank: Si

Alias	Name
SI	SILICON
SIC-A	SILICON-CARBIDE-HEXAGONAL-ALPHA
SIC-B	SILICON-CARBIDE-CUBIC-BETA
SIF4*2NC3H9	SIF4*2N(CH3)3
SIF4*2NH3	SIF4*2NH3
SIF4*NC3H9	SIF4*N(CH3)3
SIO2	SILICON-DIOXIDE
SISE2	SILICON-DISELENIDE

SOLIDS Component Databank: Sm

Alias	Name
SM2C3O9	SM2(CO3)3
SM2C6O12*10W	SM2(C2O4)3*10H2O

Alias	Name
SM2S3O12	SM2(SO4)3
SM2S3O12*8W	SM2(SO4)3*8H2O
SM2S3O9	SM2(SO3)3
SM2SE3O12*8W	SM2(SEO4)3*8H2O
SMAS	SMAS
SMBR3O9*9W	SM(BRO3)3*9H2O
SMC2	SAMARIUM-DICARBIDE
SMCL3*6W	SMCL3*6H2O
SMF3	SMF3
SMF3*W	SMF3*H2O
SMI3	SMI3
SMI3O9	SM(IO3)3
SMN3O9	SM(NO3)3
SMN3O9*6W	SM(NO3)3*6H2O
SMOCL	SMOCL

SOLIDS Component Databank: Sn

Alias	Name
SN(OH)2-P	SN(OH)2-PPTD
SN(OH)4-P	SN(OH)4-PPTD
SNBR2	TIN-DIBROMIDE
SNBR2*2NH3	SNBR2*2NH3
SNBR2*3NH3	SNBR2*3NH3
SNBR2*5NH3	SNBR2*5NH3
SNBR2*9NH3	SNBR2*9NH3
SNBR2*NH3	SNBR2*NH3
SNBR4*8W	SNBR4*8H2O
SNC2H6CL2	SN(CH3)2CL2
SNCL2*2.5NH3	SNCL2*2.5NH3
SNCL2*2W	SNCL2*2H2O
SNCL2*4NH3	SNCL2*4NH3
SNCL2*9NH3	SNCL2*9NH3
SNCL4*1.5PH3	SNCL4*1.5PH3
SNI2*2NH3	SNI2*2NH3
SNI2*3NH3	SNI2*3NH3
SNI2*5NH3	SNI2*5NH3
SNI2*9NH3	SNI2*9NH3
SNI2*NH3	SNI2*NH3
SNOHCL*W	SNOHCL*H2O

SOLIDS Component Databank: Sr

Alias	Name
SR2AL2SIO7	(SRO)2*AL2O3*SIO2
SR2BI	SR2BI
SR2GE	SR2GE
SR2O2*FE2O3	(SRO)2*FE2O3
SR2PB	SR2PB
SR2SB	SR2SB
SR2SIO4	STRONTIUM-ORTHOSILICATE

Alias	Name
SR2SN	SR2SN
SR2U3O11	SR2U3O11
SR2UO5	SR2UO5
SR3AL4CL18	(SRCL2)3*4ALCL3
SR3AS2	SR3AS2
SR3BI2	SR3BI2
SR3O3*AL2O3	(SRO)3*AL2O3
SR3O3*FE2O3	(SRO)3*FE2O3
SR3P2	SR3P2
SR3P2O8	SR3(PO4)2
SR3SB2	SR3SB2
SR3UO6	SR3UO6
SR4AL2O7-A	(SRO)4*AL2O3-ALPHA
SR4AL2O7-B	(SRO)4*AL2O3-BETA
SR7FE10O22	(SRO)7*5FE2O3
SRB2F8	SR(BF4)2
SRBI	SRBI
SRBR2	STRONTIUM-BROMIDE
SRBR2*2NH3	SRBR2*2NH3
SRBR2*6W	SRBR2*6H2O
SRBR2*8NH3	SRBR2*8NH3
SRBR2*NH3	SRBR2*NH3
SRBR2*SRO*3W	SRBR2*SRO*3H2O
SRBR2*SRO*9W	SRBR2*SRO*9H2O
SRBR2*W	SRBR2*H2O
SRBR2CO0.5H3	SRBR2*0.5C2H5OH
SRBR2O6*W	SR(BRO3)2*H2O
SRBRH	SRBRH
SRC2N2*4W	SR(CN)2*4H2O
SRC2O4	SRC2O4
SRC4H6O4	SR(CH3CO2)2
SRC4H6O4.5H	SR(CH3CO2)2*0.5H2O
SRC4H6O6	SR(CH2OHCO2)2
SRCL2*2W	SRCL2*2H2O
SRCL2*6W	SRCL2*6H2O
SRCL2*SRO*9W	SRCL2*SRO*9H2O
SRCL2*W	SRCL2*H2O
SRCL2-A	SRCL2-ALPHA
SRCL2N8H24	SRCL2*8NH3
SRCL2NH3	SRCL2*NH3
SRCL2O8	SR(CLO4)2
SRCL2O8*2W	SR(CLO4)2*2H2O
SRCL2O8*4W	SR(CLO4)2*4H2O
SRCL2O8N2H6	SR(CLO4)2*2NH3
SRCL2O8N6H18	SR(CLO4)2*6NH3
SRCL2O8N7H21	SR(CLO4)2*7NH3
SRCLH	SRCLH

Alias	Name
SRCN2	SRCN2
SRCO3	STRONTIUM-CARBONATE
SRF2	STRONTIUM-FLUORIDE
SRFCL	SRFCL
SRH2C2O4	SR(HCO2)2
SRH2C2O4*2W	SR(HCO2)2*2H2O
SRH4P2O8	SR(H2PO4)2
SRHFO3	SRHFO3
SRHPO4	SRHPO4
SRI2*2NH3	SRI2*2NH3
SRI2*2PBI2	SRI2*2PBI2
SRI2*2W	SRI2*2H2O
SRI2*6NH3	SRI2*6NH3
SRI2*6W	SRI2*6H2O
SRI2*8NH3	SRI2*8NH3
SRI2*NH3	SRI2*NH3
SRI2*W	SRI2*H2O
SRI2O6	SR(IO3)2
SRI2O6*6W	SR(IO3)2*6H2O
SRI2O6*W	SR(IO3)2*H2O
SRI6PB2*7W	SRI2*2PBI2*7H2O
SRIH	SRIH
SRMG2-B	SRMG2-BETA
SRMOO3	SRMOO3
SRN2H4	SR(NH2)2
SRN2H8S2O8	SR(NH4)2(SO4)2
SRN2O2*5W	SRN2O2*5H2O
SRN2O4	SR(NO2)2
SRN2O4*W	SR(NO2)2*H2O
SRN2O6	SR(NO3)2
SRN2O6*4W	SR(NO3)2*4H2O
SRN6	SR(N3)2
SRN6H18	SR(NH3)6
SRO*AL2O3	SRO*AL2O3
SRO2H2*8W	SR(OH)2*8H2O
SRO2H2*W	SR(OH)2*H2O
SRS	STRONTIUM-SULFIDE
SRS2I2O4	SRI2*2SO2
SRS2O6*4W	SRS2O6*4H2O
SRS4I2O8	SRI2*4SO2
SRSB	SRSB
SRSE	SRSE
SRSEO3	SRSEO3
SRSEO4	SRSEO4
SRSO3	SRSO3
SRUO4-A	SRUO4-ALPHA,RHOMBOHEDRAL
SRUO4-B	SRUO4-BETA,ORTHORHOMBIC

SOLIDS Component Databank: Tb

Alias	Name
TB2C3O9	TB2(CO3)3
TB2C6O12*10W	TB2(C2O4)3*10H2O
TBAS	TBAS
TBBR3O9*9W	TB(BRO3)3*9H2O
TBCL3*6W	TBCL3*6H2O
TBI3O9	TB(IO3)3
TBOCL	TBOCL

SOLIDS Component Databank: Th

Alias	Name
TH2CO17	TH2CO17
TH2CO7	TH2CO7
TH2FE17	TH2FE17
TH2FE7	TH2FE7
TH2N2O	DITHORIUM-DINITRIDE-MONOXIDE
TH2NI17	TH2NI17
TH3GE	TH3GE
TH3GE2	TH3GE2
TH3GE5	TH3GE5
TH3S7	TH3S7
TH3SI2	TH3SI2
TH3SI5	TH3SI5
TH7CO3	TH7CO3
TH7FE3	TH7FE3
TH7S12	TH7S12
THBR4*10W	THBR4*10H2O
THBR4*12W	THBR4*12H2O
THBR4*7W	THBR4*7H2O
THC	THC
THC4O8*6W	TH(C2O4)2*6H2O
THCL4*12NH3	THCL4*12NH3
THCL4*18NH3	THCL4*18NH3
THCL4*2W	THCL4*2H2O
THCL4*4NH3	THCL4*4NH3
THCL4*4W	THCL4*4H2O
THCL4*6NH3	THCL4*6NH3
THCL4*7NH3	THCL4*7NH3
THCL4*7W	THCL4*7H2O
THCL4*8W	THCL4*8H2O
THCL4*NH4CL	THCL4*NH4CL
THCO	THCO
THCO5	THCO5
THF4*2.5W	THF4*2.5H2O
THFE3	THFE3
THFE5	THFE5
THGE	THGE
THGE2	THGE2
THGE3	THGE3

Alias	Name
THH3.75	THH3.75
THIN3	THIN3
THN4O12	TH(NO3)4
THN4O12*4W	TH(NO3)4*4H2O
THN4O12*5W	TH(NO3)4*5H2O
THNI2	THNI2
THNI5	THNI5
THOF2	THORIUM-DIFLUORIDE-OXIDE
THOHI3*10W	TH(OH)I3*10H2O
THOI2*3.5W	THOI2*3.5H2O
THPB3	THPB3
THSI	THSI
THSI2	THSI2
THSN3	THSN3
THTL3	THTL3

SOLIDS Component Databank: Ti

Alias	Name
TI	TITANIUM
TI3AL	TI3AL
TI5SI3-E	TI5SI3-EPSILON
TIAL	TIAL
TIAL3	TIAL3
TIAS	TIAS
TIBR4*2CH3CN	TIBR4*2CH3CN
TIBR4*2H2S	TIBR4*2H2S
TIBR4*2PH3	TIBR4*2PH3
TIBR4*H2S	TIBR4*H2S
TIBR4*PH3	TIBR4*PH3
TICL4*2CH3CN	TICL4*2CH3CN
TICL4*2H2S	TICL4*2H2S
TICL4*2PH3	TICL4*2PH3
TICL4*2POCL3	TICL4*2POCL3
TICL4*H2S	TICL4*H2S
TICL4*PH3	TICL4*PH3
TICL4*POCL3	TICL4*POCL3
TIF4*CH3CN	TIF4*CH3CN
TIO2	TITANIUM-DIOXIDE-RUTILE
TIP	TIP
TISB	TISB
TISI-G	TISI-GAMMA
TISI2-B	TISI2-BETA

SOLIDS Component Databank: Tl

Alias	Name
TL2CO3	TL2CO3
TL2CRO4	TL2CRO4
TL2S	THALLIUM-SULFIDE
TL2SE	DITHALLIUM-SELENIDE

Alias	Name
TL2SE3O9	TL2(SEO3)3
TL2SEO4	TL2SEO4
TL2SO4	THALLIUM-SULFATE
TL2TE	THALLIUM-TELLURIDE
TL2TICL6	TL2TICL6
TL4V2O7	TL4V2O7
TLBR*3NH3	TLBR*3NH3
TLBR3*4W	TLBR3*4H2O
TLBRO3	TLBRO3
TLCH3CO2	TLCH3CO2
TLCL*3NH3	TLCL*3NH3
TLCL2BR*4W	TLCL2BR*4H2O
TLCL3*3NH3	TLCL3*3NH3
TLCL3*4W	TLCL3*4H2O
TLCLBR2*4W	TLCLBR2*4H2O
TLHF2	TLHF2
TLI*3NH3	TLI*3NH3
TLIO3	TLIO3
TLN3	TLN3
TLNO3	THALLIUM-NITRATE
TLO3H3	TL(OH)3
TLOCH3	TLOCH3
TLOH	THALLIUM-HYDROXIDE
TLONC	THALLOUS-FULMINATE
TLSCN	TLCNS
TLVO3	TLVO3

SOLIDS Component Databank: U

Alias	Name
U(OH)2SO4	U(OH)2SO4
U2O4CL3	(UO2)2CL3
U3AS4	U3AS4
U3BI4	U3BI4
U3O7-A	U3O7-ALPHA,TETRAGONAL
U3O7-B	U3O7-BETA,TETRAGONAL
U3O8-A	U3O8-ALPHA,ORTHORHOMBIC
U3P4	U3P4
U3SB4	U3SB4
U3SI	U3SI
U3SI2	U3SI2
U4O9	TETRAURANIUM-NONAOXIDE
UAL2	UAL2
UAL3	UAL3
UAL4	UAL4
UAS	UAS
UAS2	UAS2
UB1.98	UB1.98
UBI	UBI

Alias	Name
UBI2	UBI2
UCL2BR	UCL2BR
UCL2BR2	UCL2BR2
UCL3BR	UCL3BR
UCLBR2	UCLBR2
UCLBR3	UCLBR3
UF2CL2	UF2CL2
UF3CL	UF3CL
UF4*2.5W-O	UF4*2.5H2O-ORTHORHOMBIC
UF4-M	UF4-MONOCLINIC
UFCL3	UFCL3
UFE2	UFE2
UGA	UGA
UGA2	UGA2
UGA3	UGA3
UIN3	UIN3
UN0.997	UN0.997
UN1.466-B	UN1.466-BETA,SESQUINITRIDE
UN1.5	UN1.5
UN1.51-A	UN1.51-ALPHA,SESQUINITRIDE
UN1.59-A	UN1.59-ALPHA,SESQUINITRIDE
UN1.606-A	UN1.606-ALPHA,SESQUINITRIDE
UN1.674-A	UN1.674-ALPHA,SESQUINITRIDE
UN1.73-A	UN1.73-ALPHA,SESQUINITRIDE
UO2.86*0.5W	UO2.86*0.5H2O
UO2.86*1.5W	UO2.86*1.5H2O
UO2BR2*3W	UO2BR2*3H2O
UO2BR2*W	UO2BR2*H2O
UO2C2O4	UO2C2O4
UO2C2O4*3W	UO2C2O4*3H2O
UO2C2O4*W	UO2C2O4*H2O
UO2CL2*3W	UO2CL2*3H2O
UO2CL2*W	UO2CL2*H2O
UO2CO3	UO2CO3
UO2F2*3W	UO2F2*3H2O
UO2H2C2O4	UO2(HCO2)2
UO2H2C2O4*W	UO2(HCO2)2*H2O
UO2KASO	UO2KASO4
UO2KPO4	UO2KPO4
UO2OHCL*2W	UO2(OH)CL*2H2O
UO2OHF*2W	UO2(OH)F*2H2O
UO2OHF*W	UO2(OH)F*H2O
UO2SEO3	UO2SEO3
UO2SEO4-A	UO2SEO4-ALPHA
UO2SO3	UO2SO3
UO2SO3*4.5W	UO2SO3*4.5H2O
UO2SO4*2.5W	UO2SO4*2.5H2O

Alias	Name
UO2SO4*3.5W	UO2SO4*3.5H2O
UO2SO4*3W	UO2SO4*3H2O
UO2SO4*W	UO2SO4*H2O
UO2SO4-B	UO2SO4-BETA
UO2TEO3	UO2TEO3
UO3HBR*2W	UO2(OH)BR*2H2O
UO4*2W	UO4*2H2O
UO4*4W	UO4*4H2O
UO6C4H6	UO2(CH3CO2)2
UO6C4H6*2W	UO2(CH3CO2)2*2H2O
UO6CR*5.5W	UO2CRO4*5.5H2O
UO8N2*2W	UO2(NO3)2*2H2O
UO8N2*3W	UO2(NO3)2*3H2O
UO8N2*6W	UO2(NO3)2*6H2O
UO8N2*W	UO2(NO3)2*H2O
UOF2	UOF2
UOF2*W	UOF2*H2O
UOFOH	UOF(OH)
UOFOH*0.5W	UOF(OH)*0.5H2O
UP	UP
UP2	UP2
UPB3	UPB3
US1.5	US1.5
US1.9-A	US1.9-ALPHA,HYPOSTOICHIOMETRIC
US2-B	US2-BETA
US2O8*4W	U(SO4)2*4H2O
US2O8*8W	U(SO4)2*8H2O
US3	US3
USB	USB
USB2	USB2
USE1.33	USE1.33
USE1.5	USE1.5
USE2-A	USE2-ALPHA
USI	USI
USI2	USI2
USI3	USI3
USN3	USN3
USO6.2.5H2O	USO6.2.5H2O
USO6.3.5H2O	USO6.3.5H2O
UTE	UTE
UTE1.33	UTE1.33
UTE3	UTE3
UTL3	UTL3

SOLIDS Component Databank: V

Alias	Name
V2SI	V2SI
V3O11P2	(VO)3(PO4)2

	Alias	Name
	V3SI	V3SI
	V5AL8	V5AL8
	V5SI3	V5SI3
	VAL3	VAL3
	VO2CL	VO2CL
	VOCL	VOCL
	VOCL2	VOCL2
	VOSO4	VOSO4
	VSI2	VSI2

SOLIDS Component Databank: W

Alias	Name
W	TUNGSTEN
WO2	TUNGSTEN-DIOXIDE
WO2BR2	WO2BR2
WO3	TUNGSTEN-TRIOXIDE
WOBR4	WOBR4
WSI2	WSI2

SOLIDS Component Databank: Y

Alias	Name
Y2C3O9	Y2(CO3)3
Y2C6O12*9W	Y2(C2O4)3*9H2O
Y2O5H5CL	Y2(OH)5CL
Y2S3O12	Y2(SO4)3
Y2S3O12*8W	Y2(SO4)3*8H2O
Y2SE3O9	Y2(SEO3)3
Y2ZN17	Y2ZN17
YAS	YAS
YC2	YC2
YCL3*2CH3NH2	YCL3*2CH3NH2
YCL3*3CH3NH2	YCL3*3CH3NH2
YCL3*4CH3NH2	YCL3*4CH3NH2
YCL3*6W	YCL3*6H2O
YCL3*CH3NH2	YCL3*CH3NH2
YH2	YH2
YH2.6	YH2.6
YH3	YH3
YI3	YTTRIUM-TRIIODIDE
YI3O9	Y(IO3)3
YNBO4	YNBO4
YO2H2CL	Y(OH)2CL
YO3H3	Y(OH)3
YRE3O12	Y(REO4)3
YZN	YZN
YZN11	YZN11
YZN2-A	YZN2-ALPHA
YZN3	YZN3
YZN4	YZN4

	Alias	Name
	YZN5	YZN5

SOLIDS Component Databank: Yb

Alias	Name
YB2C6O12*5W	YB2(C2O4)3*5H2O
YB2OC	YB2OC
YBBR3O9*9W	YB(BRO3)3*9H2O
YBC2	YBC2
YBCL3*6W	YBCL3*6H2O
YBH2	YBH2
YBI3O9	YB(IO3)3
YBOCL	YBOCL

SOLIDS Component Databank: Zn

Alias	Name
ZN	ZINC
ZN(OH)2	ZINC-HYDROXIDE
ZN(OH)2-B	ZINC-HYDROXIDE-BETA
ZN(OH)2-E	ZINC-HYDROXIDE-EPSILON
ZN2O3H3CL	ZN2(OH)3CL
ZN2P2O7	ZN2(P2O7)
ZN3AS2O8	ZINC-ARSENATE
ZN4C6N6O	(ZN(CN)2)3*ZNO
ZN4CL2O3*5W	ZNCL2*3ZNO*5H2O
ZN5BR2O4*13W	ZNBR2*4ZNO*13H2O
ZN5CL2O4*11W	ZNCL2*4ZNO*11H2O
ZN5N2O14H8	ZN(NO3)2*4ZN(OH)2
ZN6CL2O5*8W	ZNCL2*5ZNO*8H2O
ZN6I2O5*11W	ZNI2*5ZNO*11H2O
ZN9CL2O8*10W	ZNCL2*8ZNO*10H2O
ZNAL2O4	ZNAL2O4
ZNAS2	ZNAS2
ZNB2O4	ZN(BO2)2
ZNBR2*2N2H4	ZNBR2*2N2H4
ZNBR2*2NH3	ZNBR2*2NH3
ZNBR2*2W	ZNBR2*2H2O
ZNBR2*4NH3	ZNBR2*4NH3
ZNBR2*6NH3	ZNBR2*6NH3
ZNBR2*6NH3*W	ZNBR2*6NH3*H2O
ZNBR2*NH3	ZNBR2*NH3
ZNC2H2O4	ZINC-FORMATE
ZNC2H6O6	ZINC-FORMATE-DIHYDRATE
ZNC2N2	ZINC-CYANIDE
ZNC2O4*2W	ZINC-OXALATE-DIHYDRATE
ZNC4H10O6	ZINC-ACETATE-DIHYDRATE
ZNC4H12O4N2	ZN(CH3CO2)2*2NH3
ZNC4H12O6N2	ZN(CH2OHCOO)2*2NH3
ZNC4H18O4N4	ZN(CH3CO2)2*4NH3
ZNC4H18O6N4	ZN(CH2OHCOO)2*4NH3

Alias	Name
ZNC4H24O4N6	ZN(CH3CO2)2*6NH3
ZNC4H24O6N6	ZN(CH2OHCOO)2*6NH3
ZNC4H30O4N8	ZN(CH3CO2)2*8NH3
ZNC4H6O4	ZINC-ACETATE
ZNC4H6O6	ZINC-GLYCOLATE
ZNC4H8O5	ZINC-ACETATE-HYDRATE
ZNC4H8O7	ZINC-GLYCOLATE-HYDRATE
ZNC4H9O4N	ZN(CH3CO2)2*NH3
ZNCL2*2N2H4	ZNCL2*2N2H4
ZNCL2*2NH3	ZNCL2*2NH3
ZNCL2*4NH3	ZNCL2*4NH3
ZNCL2*5NH3*W	ZNCL2*5NH3*H2O
ZNCL2*6NH3	ZNCL2*6NH3
ZNCL2*NH3	ZNCL2*NH3
ZNCL2AM4W0.5	ZNCL2*4NH3*0.5H2O
ZNCL2O8*6W	ZN(CLO4)2*6H2O
ZNCO3*W	ZINC-CARBONATE-HYDRATE
ZNI2*2N2H4	ZNI2*2N2H4
ZNI2*2NH3	ZNI2*2NH3
ZNI2*4NH3	ZNI2*4NH3
ZNI2*6NH3	ZNI2*6NH3
ZNI2*NH3	ZNI2*NH3
ZNI2O6	ZINC-IODATE
ZNN2H4	ZINC-AMIDE
ZNN2H6CS3	ZN(NH3)2CS3
ZNN2O6	ZINC-NITRATE
ZNN2O6*2W	ZINC-NITRATE-DIHYDRATE
ZNN2O6*4W	ZINC-NITRATE-TETRAHYDRATE
ZNN2O6*6W	ZINC-NITRATE-HEXAHYDRATE
ZNN2O6*W	ZINC-NITRATE-HYDRATE
ZNN6	ZINC-AZIDE
ZNO	ZINC-OXIDE
ZNO*2ZNSO4	ZNO*2ZNSO4
ZNO2H2-G	ZN(OH)2-GAMMA
ZNO2H2-P	ZN(OH)2-PPTD
ZNP2O6	ZN(PO3)2
ZNS-1	ZINC-SULFIDE(SPHALENITE)
ZNS-2	ZINC-SULFIDE(WURTZITE)
ZNS2O6*6W	ZINC-SULFATE-HEXAHYDRATE
ZNSB	ZNSB
ZNSEO3*W	ZNSEO3*H2O
ZNSEO4	ZINC-SELENATE
ZNSEO4*6W	ZINC-SELENATE-HEXAHYDRATE
ZNSEO4*W	ZINC-SELENATE-HYDRATE
ZNSO4	ZINC-SULFATE
ZNSO4*ZNO2H2	ZNSO4*ZN(OH)2
ZNTIO3	ZNTIO3

SOLIDS Component Databank: Zr

Alias	Name
ZR2SI	ZR2SI
ZR3SI	ZR3SI
ZR3SI2	ZR3SI2
ZR5SI3	ZR5SI3
ZR6SI5	ZR6SI5
ZRBR4*2CH3CN	ZRBR4*2CH3CN
ZRCL4*2CH3CN	ZRCL4*2CH3CN
ZRF4*2NH4F	ZRF4*2NH4F
ZRF4*3NH4F	ZRF4*3NH4F
ZRF4*3W	ZRF4*3H2O
ZRF4*NH4F	ZRF4*NH4F
ZRF4*NH4F*W	ZRF4*NH4F*H2O
ZRF4*W	ZRF4*H2O
ZRH2	ZRH2
ZRO2	ZIRCONIUM-DIOXIDE
ZROBR2*3.5W	ZROBR2*3.5H2O
ZROBR2*8W	ZROBR2*8H2O
ZROCL2*2W	ZROCL2*2H2O
ZROCL2*3.5W	ZROCL2*3.5H2O
ZROCL2*6W	ZROCL2*6H2O
ZROCL2*8W	ZROCL2*8H2O
ZRS2O8	ZR(SO4)2
ZRS2O8*4W	ZR(SO4)2*4H2O
ZRS2O8*W	ZR(SO4)2*H2O
ZRSI	ZRSI
ZRSI2	ZRSI2

SOLIDS Component Databank: Other Elements

Alias	Name
ANALCITE	NAALSI2O6*H2O
AS	ARSENIC
(AS2O5)3*5W	(AS2O5)3*5H2O
AS2O3*SO3	AS2O3*SO3
CHRYSOTILE	MG3SI2O5(OH)4
GE3N4	GERMANIUM-TETRANITRIDE
GEI2	GERMANIUM-DIIODIDE
HFB	HFB
I2	IODINE
I2O5*HIO3	I2O5*HIO3
ICL-A	ICL-ALPHA
ICL3	ICL3
IRCL	IRCL
IRCL3C12H30S	IRCL3*3(C2H5)2S
NESQUEHONITE	MGCO3*3H2O
OSCL3	OSCL3
OSCL4	OSCL4
PO(OH)4	PO(OH)4
POS	POLONIUM-SULFIDE

Alias	Name
PYROPHYLLITE	AL2SI4O10(OH)2
RE3SI	RE3SI
REAS2	REAS2
RECL5	RECL5
RHCL3C12H30S	RHCL3*3(C2H5)2S
RUBR3	RUBR3
RUCL3C12H30S	RUCL3*3(C2H5)2S
RUI3	RUI3
SE(OH)3CLO4	SE(OH)3CLO4
SEO2SO3	SEO2SO3
S	SULFUR
TA2H	TA2H
TA5SI3	TA5SI3
TASI2	TASI2
(TEO2)2SO3	(TEO2)2SO3
TMC2	TMC2
TMI3O9	TM(IO3)3
TMOCL	TMOCL

CHAPTER 2

Electrolytes Data

Overview

The Aspen Physical Property System provides extensive built-in parameters for the electrolyte NRTL model. These parameters were developed using data for over 30 industrially important electrolytic systems. This help describes each system including the:

- Solution chemistry
- Range of applications
- Sources of literature used

The solution chemistry includes:

- Equilibrium reaction indicated by a two way arrow ($\leftrightarrow$)
- Complete dissociation reaction indicated by an arrow ($\rightarrow$)
- Salt precipitation reaction indicated by a two way arrow ($\leftrightarrow$). A salt component is indicated by (s) in the formula.

The solution chemistry used for all the systems is internally consistent. The hydronium ion (H_3O^+) is used for all systems. A single set of model parameters is used to describe the interactions between a given pair of components that may appear in several systems.

For some systems, such as caustic systems, it is not possible to describe the data accurately over the entire range of concentration. In that case, a separate set of parameters and components has been developed and are available in the form of an insert file.

Table 2.1 Electrolytes Data Available in the Aspen Physical Property System

System	Apparent Components
2-Amino-2-Methyl-1-Propanol with acid gas	AMP, H_2S, CO_2, H_2O
Ammonia and carbon dioxide	NH_3, CO_2, H_2O
Ammonia and hydrogen cyanide	NH_3, HCN, H_2O
Ammonia and hydrogen sulfide	NH_3, H_2S, H_2O
Ammonia and phosphoric acid	NH_3, H_2S, H_3PO_4, H_2O
Ammonia and sulfur dioxide	NH_3, SO_2, H_2O
Ammonia and water	NH_3, H_2O
Brine solution with sour gases	NaCl, CO_2, H_2S, H_2O
Caustic solutions	NaCl, Na_2SO_4, NaOH, H_2O
Chlorine	Cl_2, H_2O
Chlorine, hydrogen chloride and sodium hydroxide	Cl_2, HCl, CO_2, NaOH, H_2O
Diethanolamine with acid gases	DEA, H_2S, CO_2, H_2O
Diglycolamine with acid gases	DGA, H_2S, CO_2, H_2O
Flue-gas and water	H_2O, SO_2, SO_3, CO_2, CO, NO_2, NO, N_2, O_2, HCl, HF, HNO_3, HNO_2, H_2SO_4, H_2SeO_3, $HgCl_2$, Hg_2Cl_2, Hg, C, Se, SeO_2, $Hg(OH)_2$, $CaSO_4 * 2H_2O$, CaF_2, CaO, $Ca(OH)_2$
Hot carbonate CO_2 absorption	K_2CO_3, CO_2, H_2O
Hot carbonate with diethanolamine	K_2CO_3, CO_2, DEA, H_2O
Hydrogen bromide	HBr, H_2O
Hydrogen chloride	HCl, H_2O
Hydrogen chloride and magnesium chloride	HCl, $MgCl_2$, H_2O
Hydrogen flouride	HF, H_2O

System	Apparent Components
Hydrogen iodide	HI, H_2O
Methyldiethanolamine with acid gases	MDEA, H_2S, CO_2, H_2O
Monoethanolamine with acid gases	MEA, H_2S, CO_2, H_2O
Nitric acid	HNO_3, H_2O
Potassium hydroxide	KOH, H_2O
Sodium hydroxide	NaOH, H_2O
Sodium hydroxide and sulfur dioxide	NaOH, SO_2, H_2O
Sour water	NH_3, CO_2, H_2S, H_2O
Sour water and caustic	NH_3, CO_2, H_2S, NaOH, H_2O
Sulfuric acid	H_2SO_4, H_2O
Sulfuric acid and hydrogen bromide	H_2SO_4, HB_r, H_2O
Sulfuric acid and hydrogen chloride	H_2SO_4, HCl, H_2O

2-Amino-2-Methyl-1-Propanol with Acid Gases

The components included in this system are: H_2O, CO_2, 2-Amino-2-Methyl-1-Propanol (AMP), and water. Henry's law is used for H_2S and CO_2. AMP is a hindered amine.

Application: H_2S, and CO_2, absorption/stripping with AMP solutions.

Solution Chemistry

The aqueous phase reactions considered for this system are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$H_2S + H_2O \leftrightarrow H_3O^+ + HS^-$$

$$HS^- + H_2O \leftrightarrow H_3O^+ + S^{-2}$$

$$CO_2 + 2H_2O \leftrightarrow H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{-2}$$

$$AMP^+ + H_2O \leftrightarrow H_3O^+ + AMP$$

Range of Applicability

Temperatures: 40 – 100°C

AMP Concentration: up to 28.5 weight percent.

Data Sources

Bruce E. Roberts and Alan E. Mather, *Chem. Eng. Comm.*, Vol. 65, pp. 105-111 (1988).

Tjoon T. Teng and Alan E. Mather, *J. Chem. Eng. Data*, Vol. 35, pp. 410-411 (1990).

Additional Data Packages

A special data package is also available for this amine system in the form of an insert file: KEAMP. This data package contains kinetic reactions and rate constants, allowing you to model the AMP system more accurately using RADFRAC or RATEFRAC.

Ammonia and Carbon Dioxide

The components included in this system are: ammonia (NH_3), carbon dioxide (CO_2), and water. Henry's law is used for NH_3 and CO_2.

Applications:

- Sour water stripping
- Absorption of CO_2 with ammonia

Solution Chemistry

The aqueous phase reactions that are considered are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$CO_2 + 2H_2O \leftrightarrow H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{-2}$$

$$NH_3 + H_2O \leftrightarrow NH_4^+ + OH^-$$

$$NH_3 + HCO_3^- \leftrightarrow NH_2CO_2^- + H_2O$$

Range of Applicability

Temperature	0 – 100ºC
Pressure	250 psia
NH_3 concentration	up to approximately 23 molal
CO_2 concentration	up to approximately 8 molal

Data Sources

D.H. Miles and G.M. Wilson, "Vapor-liquid Equilibrium Data for Design of Sour Water Strippers," Annual Report to the API for 1974, October 1975.

E. Otsaka, S. Yoshimura, M. Yokabe and S. Inque, Kogyo Kagaku Zasshi, 63, 1214 (1960).

Ammonia and Hydrogen Cyanide

The components included in this system are: water, ammonia (NH_3), and hydrogen cyanide (HCN). Henry's law is used for NH_3 and HCN.

Application: Absorption of HCN with NH_3

Solution Chemistry

The aqueous phase reactions considered in this system are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$H_2O + NH_3 \leftrightarrow NH_4^+ + OH^-$$

$$HCN + H_2O \leftrightarrow H_3O^+ + CN^-$$

Range of Applicability

Temperature	0 – 100ºC
NH_3 concentration	up to about 23 molal

Ammonia and Hydrogen Sulfide

The components included in this system are: ammonia (NH_3), hydrogen sulfide (H_2S), and water. Henry's law is used for NH_3 and H_2S.

Applications:

- Sour water stripping
- Absorption of H_2S with ammonia

Solution Chemistry

The aqueous phase reactions that are considered are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$NH_3 + H_2O \leftrightarrow NH_4^+ + OH^-$$

$$H_2S + H_2O \leftrightarrow H_3O^+ + HS^-$$

$$HS^- + H_2O \leftrightarrow H_3O^+ + S^{-2}$$

Range of Applicability

Temperature	80 – 120ºC
Pressure	250 psia
NH_3 concentration	up to approximately 23 molal
H_2S concentration	up to approximately 8 molal

Extrapolation for this system has been checked to produce reasonable results.

Data Sources

D.H. Miles and G.M. Wilson, "Vapor-liquid Equilibrium Data for Design of Sour Water Strippers," Annual Report to the API for 1974, October 1975.

Ammonia and Phosphoric Acid

The components included in this system are: ammonia (NH_3), phosphoric acid (H_3PO_4), H_2S, and water. Henry's law is used for, NH_3, H_3PO_4 and H_2S.

Application: Stripping NH_3, H_2S from phosphoric acid

Solution Chemistry

The aqueous phase reactions considered for this system are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$H_2O + NH_3 \leftrightarrow NH_4^+ + OH^-$$

$$H_2S + H_2O \leftrightarrow H_3O^+ + HS^-$$

$$HS^- + H_2O \leftrightarrow H_3O^+ + S^{-2}$$

$$H_3PO_4 + H_2O \leftrightarrow H_3O^+ + H_2PO_4^-$$

$$H_2PO_4^- + H_2O \leftrightarrow H_3O^+ + HPO_4^{-2}$$

$$HPO_4^{-2} + H_2O \leftrightarrow H_3O^+ + PO_4^{-3}$$

Range of Applicability

Temperature	up to 120ºC
H_3PO_4 concentration	up to 50 weight percent
NH_3: H_3PO_4 molar ratio	up to 2

Data Sources

F.A. Lenfesty and Brosheer, J.C., "Ammonia-Phosphoric Acid-Water System at 25°C," *J. Chem. and Eng. Data*, (1960).

N.G. Bunakov and Kharlampovich, G.D., "The pressure of Ammonia Vapor Above Solutions of Ammonium Orthophosphate," *Zhurnal Prokladnoi Khimii*, Vol. 37, pp. 36–41, (1964).

Ammonia and Sulfur Dioxide

The components included in this system are: water, ammonia (NH_3), and sulfur dioxide (SO_2). Henry's law is used for NH_3 and. SO_2.

Application: Absorption of SO_2 with ammonia

Solution Chemistry

The aqueous phase reactions considered in this system are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$H_2O + NH_3 \leftrightarrow NH_4^+ + OH^-$$

$$SO_2 + 2H_2O \leftrightarrow H_3O^+ + HSO_3^-$$

$$HSO_3^- + H_2O \leftrightarrow H_3O^+ + SO_3^{-2}$$

Range of Applicability

Temperature	0 – 100ºC
NH_3 concentration	to about 12 molal
SO_2 concentration	to about 10 molal

Data Sources

H.F. Johnstone and P.W. Leppla, "The Solubility of Sulfur Dioxide at Low Partial Pressures. The Ionization Constant and Heat of Ionization of Sulfurous Acid," *J. Am. Chem. Soc*, Vol. 56, p. 2233, (1934).

Ammonia and Water

The components included in this system are: water and ammonia (NH_3). Henry's law is used for NH_3.

Application: Absorption of NH_3 with water

Solution Chemistry

The aqueous phase reactions considered in this system are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$H_2O + NH_3 \leftrightarrow NH_4^+ + OH^-$$

Range of Applicability

Temperature	0 – 150ºC
NH_3 concentration	up to about 23 molal

Additional Data Packages

A special data package is also available for the ammonia system in the form of an insert file: NH3H2O. This data package assumes ammonia as a solvent and uses a special corresponding state method for enthalpy calculation, allowing you to model the ammonia system over the concentration range up to 100 weight percent of ammonia.

Brine Solution with Sour Gases

The components included in this system are H_2S, CO_2, NaCl and water. Henry's law is used for H_2S and CO_2.

Applications:

- Sea water desalting
- H_2S, CO_2 stripping
- Downstream processing of water decant in platform separation

Solution Chemistry

The aqueous phase reactions considered in this system are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$H_2S + H_2O \leftrightarrow H_3O^+ + HS^-$$

$$HS^- + H_2O \leftrightarrow H_3O^+ + S^{-2}$$

$$2H_2O + CO_2 \leftrightarrow H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{-2}$$

$$NaCL \leftrightarrow Na^+ + Cl^-$$

$$NaCL(s) \leftrightarrow Na^+ + Cl^-$$

Range of Applicability

Temperature	0 – 200ºC
Pressure	up to 1000 atm for CO_2
NaCl concentration	up to saturation

Data Sources

The main data source is: S.E. Drummond, Ph.D. thesis, Pennsylvania State University, (1981).

Additional Data Packages

A special data package is also available for this brine system in the form of an insert file: EBRINX. This data package uses special parameter values, allowing you to model the brine system over the temperature range up to 400ºC

Caustic Solutions

The components included in this system are: sodium hydroxide (NaOH), sodium chloride (NaCl), sodium sulfate (Na_2SO_4), and water. Salt precipitation is considered.

Application:

- Downstream processing of HCl or H_2SO_4 neutralization
- Multieffect evaporators in NaOH production

Solution Chemistry

The aqueous phase reactions considered for this system are:

$NaOH$	$\leftrightarrow$	$Na^+ + OH^-$
$NaCl$	$\leftrightarrow$	$Na^+ + Cl^-$
$NaCl(s)$	$\leftrightarrow$	$Na^+ + Cl^-$
Na_2SO_4	$\leftrightarrow$	$2Na^+ + SO_4^{-2}$
$Na_2SO_4(s)$	$\leftrightarrow$	$2Na^+ + SO_4^{-2}$
$GLAUBER(s)$	$\leftrightarrow$	$2Na^+ + SO_4^{-2} + 10H_2O$
$DOUBLE(s)$	$\leftrightarrow$	$3Na^+ + SO_4^{-2} + OH^-$
$TRIPLE(s)$	$\leftrightarrow$	$4Na^+ + SO_4^{-2} + Cl^- + OH^-$

Salt precipitation is considered for NaCl(s), Na2SO4(s), as well as for the Glauber, double, and triple salts.

Range of Applicability

Temperature	0 – 200ºC
Pressure	up to 10 atm
NaOH concentration	up to 50 weight percent
NaCl concentration	up to saturation
Na2SO4 concentration	up to saturation

Data Sources

H.L. Silcock, Solubilities of Inorganic and Organic Compounds, Volume 3: Ternary and Multicomponent Systems of Inorganic Substances, Part 2, (Pergamon Press, 1979).

W.F. Linke and A. Seidell, Solubilities: Inorganic and Metal-Organic Compounds, 4th ed., Vol. II, *Am. Chem. Soc*., (1965).

W. C. Schroeder, A. Gabriel, and E. P. Partridge, *J. Am. Chem. Soc*., Vol. 57, (1935), p. 1539.

Chlorine and Water

The components included in this system are chlorine (Cl_2) and water. Henry's law is used for Cl_2, HCl, and HClO.

Application: Absorption of Cl_2 with water

Solution Chemistry

The aqueous phase reactions considered in this system are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$2H_2O + Cl_2 \leftrightarrow H_3O^+ + Cl^- + HClO$$

$$HClO + H_2O \leftrightarrow H_3O^+ + ClO^-$$

$$HCl + H_2O \leftrightarrow H_3O^+ + Cl^-$$

Range of Applicability

Temperature 0 – 100°C

This system forms two liquid phases at high concentration.

Data Sources

Vapor-liquid equilibrium data used for this system:

W. F. Linke, *Solubilities, Inorganic and Metal-Organic Compounds*, 4th ed.,Vol. I, (Princeton, NJ: D. Van Nostrand Co., 1958), pp. 782-783.

Chlorine, Hydrogen Chloride, and Sodium Hydroxide

The components included in this system are: chlorine (Cl_2), carbon dioxide (CO_2), hydrogen chloride (HCl), sodium hydroxide (NaOH), and water. Henry's law is used for Cl_2, CO_2, HCl and HClO.

Application: Cl_2 - NaOH scrubber with the addition of HCl

Solution Chemistry

The aqueous phase reactions considered for this system are:

$2H_2O$	$\leftrightarrow$	$H_3O^+ + OH^-$
$CO_2 + 2H_2O$	$\leftrightarrow$	$H_3O^+ + HCO_3$
$HCO_3^- + H_2O$	$\leftrightarrow$	$H_3O^+ + CO_3^{-2}$
$Cl_2 + 2H_2O$	$\leftrightarrow$	$H_3O^+ + Cl^- + HClO$
$HClO + H_2O$	$\leftrightarrow$	$H_3O^+ + ClO^-$
$HCl + H_2O$	$\leftrightarrow$	$H_3O^+ + Cl^-$
$NaOH$	$\leftrightarrow$	$Na^+ + OH^-$
Na_2CO_3	$\leftrightarrow$	$Na^+ + CO_3^{-2}$
$NaHCO_3$	$\leftrightarrow$	$Na^+ + HCO_3^-$
$NaCl$	$\leftrightarrow$	$Na^+ + Cl^-$
$NaCLO$	$\leftrightarrow$	$Na^+ + ClO^-$

Range of Applicability

Temperature	0 – 100°C
HCl concentration	up to 40 weight percent
NaOH concentration	up to 40 weight percent

Data Sources

Jurgen Krey, "Dampfdruck und Dichte des Systems H_2O-NAOH," *Z. Phys. Chem. Neue Folge,* Bd. 81, (1972), p. 252.

I.A. Dibrov, G.Z. Maltsev, and V.P. Masovets, "Saturated Vapor Pressure of Caustic Soda and Sodium Aluminate Solution in the 25-350 C Temperature Range Over a Wide Range of Concentrations, *Zh. Prik. Khimii*," Vol. 37, (1964), No. 9, pp. 1920-1929.

J.W. Bertetti and W.L. McCabe, *Ind. Eng. Chem.,* 28, p. 247, (1936).

H.R. Wilson and W.L. McCabe, "Specific Heats and Heats of Dilution of Concentrated Sodium Hydroxide Solutions," *Ind. Eng. Chem.,* Vol. 34, p. 558, (1942).

Horvath, *Handbook of Aqueous Electrolyte Solutions,* 1986.

W. F. Linke, *Solubilities, Inorganic and Metal-Organic Compounds*, 4th ed., Vol. I, D. Van Nostrand Co., Priceton, NJ, (1958), pp. 782-783.

D.D. Wagman et al., *J. Phys. Chem. Ref.* Data, Vol. 11, (1982), Suppl 2.

R.H. Pery and C. H. Chilton, *Chemical Engineer's Handbook*, 5th ed., (1973) McGraw-Hill.

R. Vega and J. H. Vera, *Can. J. Chem. Eng.*, Vol.54, (1976), p. 245.

R. Hasse et al., *Coll. Czech. Chem. Comm. Engl. Edn.*, Vol. 37, p. 220, (1963).

Diethanolamine with Acid Gases

The components included in this system are: H_2S, CO_2, diethanolamine (DEA), and water. Henry's law is used for H_2S and CO_2. Enthalpy of solution data is used to develop this model.

Application: H_2S and CO_2 absorption/stripping with DEA solutions

Solution Chemistry

The aqueous phase reactions considered for this system are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$H_2S + H_2O \leftrightarrow H_3O^+ + HS^-$$

$$HS^- + H_2O \leftrightarrow H_3O^+ + S^{-2}$$

$$2H_2O + CO_2 \leftrightarrow H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{-2}$$

$$DEA^+ + H_2O \leftrightarrow DEA + H_3O^+$$

$$DEACOO^- + H_2O \leftrightarrow DEA + HCO_3^-$$

Range of Applicability

Temperature	up to 140ºC
DEA Concentration	up to 30 weight percent

Data Sources

The parameter values are obtained from:

D.M. Austgen, G.T. Rochelle, X. Peng and C.C. Chen, "A Model of Vapor-Liquid Equilibria in the Aqueous Acid Gas-

Alkanolamine System Using the Electrolyte-NRTL Equation," paper presented at the New Orleans AICHE meeting, March 1988.

Helton, R., J.J. Christensen and R.M. Izatt, Enthalpies of Solution of CO2 in Aqueous Diethanolamine Solutions," RR-108, Gas Processors Association, 1987.

Van Dam, R., J.J. Christensen, R.M. Izatt and J.L. Oscarson, "Enthalpies of Solution of H2S in Aqueous Diethanolamine Solutions, RR-114, Gas Processors Association, 1988.

Additional Data Packages

Two special data packages are also available for this amine system in the form of insert files: KDEA and KEDEA. Both data packages contain kinetic reactions and rate constants, allowing you to model the DEA system more accurately using RADFRAC or RATEFRAC. The main difference between KDEA and KEDEA is that KDEA uses option set of SYSOP15M and KEDEA uses option set of ELECNRTL.

Diglycolamine with Acid Gases

The components included in this system are: H_2S, CO_2, diglycolamine (DGA), and water. Henry's law is used for H_2S and CO_2.

Application: H_2S and CO_2 absorption/stripping with DGA solutions

Solution Chemistry

The aqueous phase reactions considered in this system are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$DGA + 2H_2O \leftrightarrow DGA^+ + OH^-$$

$$H_2S + H_2O \leftrightarrow H_3O^+ + HS^-$$

$$HS^- + H_2O \leftrightarrow H_3O^+ + S^{-2}$$

$$CO_2 + 2H_2O \leftrightarrow H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{-2}$$

$$HCO_3^- + DGA \leftrightarrow H_2O + DGACOO^-$$

Range of Applicability

Temperature	up to 100ºC
DGA concentration	up to 65 weight percent

Additional Data Packages

A special data package is also available for this amine system in the form of an insert file: KEDGA. This data package contains kinetic reactions and rate constants, allowing you to model the DGA system more accurately using RADFRAC or RATEFRAC.

Flue-Gas and Water

This is a special data package in the form of an insert file: FLUE_G. The components included in the flue-gas / water system are: water, SO2, SO3, CO, CO2, NO, NO2, N2, O2, HCl, HF, HNO3, HNO2, H2SO4, H2SeO3, HgCl2, Hg2Cl2, Hg, C, Se, SeO2, Hg(OH) 2, CaSO4*2H2O, CaF2, CaO and Ca(OH) 2. Henry's law is used for SO2, CO, CO2, NO, N2, O2, HCl and Hg. Salt precipitation is considered.

Application: flue-gas cleaning for fossil power plant and waste incineration plant

Solution Chemistry

The reactions that are considered in this system are shown as follows:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$CO_2 + 2H_2O \leftrightarrow H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{-2}$$

$$SO_3 + 2H_2O \leftrightarrow H_3O^+ + HSO_4^-$$

$$H_2O + H_2SO_4 \leftrightarrow H_3O^+ + HSO_4^-$$

$$H_2O + HSO_4^- \leftrightarrow H_3O^+ + SO_4^{-2}$$

$$HCl + H_2O \leftrightarrow H_3O^+ + Cl^-$$

$$H_2O + HF \leftrightarrow H_3O^+ + F^-$$

$$H_2O + HNO_3 \leftrightarrow H_3O^+ + NO_3^-$$

$$H_2O + HNO_2 \leftrightarrow H_3O^+ + NO_2^-$$

$$SO_2 + 2H_2O \leftrightarrow H_3O^+ + HSO_3^-$$

$$HSO_3^- + H_2O \leftrightarrow H_3O^+ + SO_3^{-2}$$

$$SeO_2 + 2H_2O \leftrightarrow H_3O^+ + HSeO_3^-$$

$$HSeO_3^- + H_2O \leftrightarrow H_3O^+ + SeO_3^{-2}$$

$$H_2SeO_3 + H_2O \leftrightarrow H_3O^+ + HSeO_3^-$$

$$Hg^{+2} + Hg \leftrightarrow Hg_2^{+2}$$

$$Hg^{+2} + 2H_2O \leftrightarrow H_3O^+ + Hg(OH)^+$$

$$Hg(OH)^+ + 2H_2O \leftrightarrow H_3O^+ + Hg(OH)_2$$

$$Hg^{+2} + Cl^- \leftrightarrow HgCl^+$$

$$HgCl^+ + Cl^- \leftrightarrow HgCl_2$$

$$HgCl_2 + Cl^- \leftrightarrow HgCl_3^-$$

$$NO + NO_2 + H_2O \leftrightarrow 2HNO_2$$

$$HgCl_2 + 3H_2O + 0.5C \leftrightarrow Hg + 2Cl^- + 2H_3O^+ + 0.5CO_2$$

$$SO_2 + 2H_2O + 0.5SeO_2 \leftrightarrow HSO_4^- + H_3O^+ + 0.5Se$$

$$SO_2 + NO_2 \leftrightarrow SO_3 + NO$$

$$SO_2 + 0.5O_2 \leftrightarrow SO_3$$

$$SO_2 + NO_2 \leftrightarrow SO_3 + NO$$

$$Ca(OH)^+ \leftrightarrow Ca^{+2} + OH^-$$

$$2NO_2 + 0.5O_2 + H_2O \leftrightarrow 2HNO_3$$

$$CaO + H_2O \leftrightarrow Ca(OH)^+ + OH^-$$

$$HgCl_2 + 5H_2O + SO_2 \leftrightarrow Hg + 2Cl^- + 3H_3O^+ + HSO_4^-$$

$$Hg_2Cl_2 \leftrightarrow Hg_2^{+2} + 2Cl^-$$

$$HgCl_2(s) \leftrightarrow HgCl^+ + Cl^-$$

$$CaSO_4*2H_2O(s) \leftrightarrow Ca^{+2} + SO_4^{-2} + 2H_2O$$

$$CaF_2(s) \leftrightarrow Ca^{+2} + 2F^-$$

$$Ca(OH)_2(s) \leftrightarrow Ca(OH)^+ + OH^-$$

Range of Applicability

Temperature	0 – 100°C

Data Sources

M. Luckas, K. Lucas and H. Roth, AIChE Journal, Vol. 40, pp 1892-1900, (1994).

H. L. Clever, S. A. Johnson and M. E. Derrick, J. Phys. Chem. Ref. Data, Vol. 14, pp 631-680, (1985).

L. D. Hansen, R. M. Izatt and J. J. Christensen, Inorg. Chem., Vol. 2, pp 1243-1245, (1963).

Hot Carbonate CO2 Absorption

The components included in the hot carbonate CO_2 absorption system are: water, CO_2, and potassium carbonate (K_2CO_3). Henry's law is used for CO_2. Salt precipitation is considered.

Application: CO_2 absorption/stripping with K_2CO_3 solutions

Solution Chemistry

The aqueous phase reactions that are considered in this system are shown as follows:

$$K_2CO_3 \leftrightarrow 2K^+ + CO_3^{-2}$$

$$KHCO_3 \leftrightarrow K^+ + HCO_3^-$$

$$CO_2 + 2H_2O \leftrightarrow H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{-2}$$

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$K_2CO_3(s) \leftrightarrow 2K^+ + HCO_3^-$$

$$KHCO_3(s) \leftrightarrow K^+ + HCO_3^-$$

Range of Applicability

Temperature	70 – 140ºC
Pressure	up to approximately 150 psia
K_2CO_3 oncentration	up to 40 weight percent

Extrapolation to higher temperature, pressure, and potassium carbonate concentration will also give reasonable results.

Data Sources

J. S. Tosh, J.H. Field, H.E. Benson, and W.P. Haynes, "Equilibrium Study of the System Potassium-Carbonate, Potassium Bicarbonate, Carbon Dioxide, and Water.", Report of Investigation 5484, U.S. Department of Interior, 1959.

Hot Carbonate with Diethanolamine

The components included in this system are: CO_2, potassium carbonate (K_2CO_3), diethanolamine (DEA), and water. Henry's law is used for CO_2.

Application: CO_2 absorption/stripping with K_2CO_3 and DEA solutions

Solution Chemistry

The aqueous phase reactions considered in this system are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$CO_2 + H_2O \leftrightarrow H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{-2}$$

$$DEA^+ + H_2O \leftrightarrow DEA + H_3O^+$$

$$DEACOO^- + H_2O \leftrightarrow DEA + HCO_3^-$$

$$K_2CO_3 \leftrightarrow 2K^+ + CO_3^{-2}$$

$$KHCO_3 \leftrightarrow K^+ + HCO_3^-$$

Range of Applicability

Temperature	70 – 140ºC
Pressure	up to approximately 150 psia
K_2CO_3 concentration	up to 40 weight percent
DEA concentration	up to 30 weight percent

Data Sources

J. S. Tosh, J.H. Field, H.E. Benson, and W.P. Haynes, "Equilibrium Study of the System Potassium-Carbonate, Potassium Bicarbonate, Carbon Dioxide, and Water.", Report of Investigation 5484, U.S. Department of Interior, 1959.

D.M. Austgen, G.T. Rochelle, X. Peng and C.C. Chen, "A Model of Vapor-Liquid Equilibria in the Aqueous Acid Gas-Alkanolamine System Using the Electrolyte-NRTL Equation," Paper presented at the New Orleans AICHE Meeting, March, 1988.

Hydrogen Bromide

The components included in this system are: water and hydrogen bromide (HBr).

Application: Absorption of HBr from gas or air using water

Solution Chemistry

The aqueous phase reaction considered in this system is:

$$HBr + H_2O \quad \leftrightarrow \quad HBr + H_2O$$

The H_2O dissociation reaction is not considered because the H_3O^+ concentration is determined primarily by HBr dissociation reaction.

Range of Applicability

Temperature	25 – 125ºC
Pressure	up to 780 torr
HBr concentration	up to 60 weight percent

Data Sources

D.D. Wagman et al., *J. Phys. Chem. Ref. Data*, Vol. 11, (1982), Suppl 2.

S.J. Bates, and H.D. Kirschman, *J. Am. Chem. Soc*, Vol. 41, (1991), p. 1919.

L. Chevaller and Gaston-Bonhomme Y.H., *J. Chem. Eng. Data*, (1980), Vol. 25, p. 271.

R. Hasse et al., *Collin Czech. Chem. Comm. Engl. Edn*., Vol. 37, (1963), p. 220.

G. Wuster, G. Wozny, and Z. Giazitzoglou, *Fluid Phase Eq*., Vol. 6, (1981), p. 93.

International Critical Tables, Vol. 3, p. 306.

Hydrogen Chloride

The components included in this system are: water and hydrogen chloride (HCl). Henry's law is used for HCl.

Application: Absorption of HCl from gas or air, using water

Solution Chemistry

The aqueous phase reaction considered in this system is:

$$HCl + H_2O \quad \leftrightarrow \quad H_3O^+ + Cl^-$$

The water dissociation reaction is not considered because the H_3O^+ concentration is determined primarily by HCl dissociation reaction.

Range of Applicability

Temperature	0 – 110ºC
Pressure	up to 2 bar
HCl concentration	up to 40 weight percent

Data Sources

D. D. Wagman, et al., *J. Phys. Chem. Ref. Data*, Vol. 11, (1982), Suppl 2.

R. H. Perry, and C.H. Chilton, *Chemical Engineer's Handbook*, 5th ed., McGraw-Hill, (1973).

R. Vega, and J.H. Vera, *Can. J. Chem. Eng.*, Vol. 54, (1976), p. 245.

Hasse, R. et al., *Collin Czech. Chem. Comm. Engl. Edn.*, Vol. 37, (1963), p. 220.

Additional Data Packages

Two special data package are also available for hydrogen chloride system in the form of insert files: EHCLLE and EHCLFF. EHCLLE is for liquid-liquid equilibrium applications. EHCLFF uses the vapor-liquid equilibria (VLE) data of Fritz and Fuget (*Ind. And Eng. Chem., 10, 1956*) instead of those from Perry and Chilton in parameter regression. It is believed that the VLE data of Fritz and Fuget is more accurate at low concentration range.

Hydrogen Chloride and Magnesium Chloride

The components included in this system are: water, hydrogen chloride (HCl), and magnesium chloride ($MgCl_2$). Henry's law is used for HCl.

Application:

- Extractive distillation of HCl
- Breaking the H_2O-HCl azeotrope

Solution Chemistry

The aqueous phase reaction considered in this system is:

$$H_2O + HCl \leftrightarrow H_3O^+ + Cl^-$$

$$MgCl_2 \leftrightarrow Mg^{+2} + 2Cl^-$$

Range of Applicability

Temperature	0 – 100°C
HCl concentration	up to 40 weight percent
$MgCl_2$ concentration	up to 6 m

Data Sources

T. Sako et al., *J. Chem. Eng. Data*, Vol. 30, (1985), pp. 224-228.

N. Pochtarev and Kozhemyakin, V.A., *Tsvetn. Met*., Vol. 4, (1977), pp. 47-49.

Hydrogen Fluoride

The components included in this system are: water and hydrogen fluoride (HF). Hydrogen fluoride is treated as a solvent, so Henry's law is not used.

Application: Absorption of HF from gas or air, using water

Solution Chemistry

The aqueous phase reaction considered in this system is:

$$H_2O + HF \leftrightarrow H_3O^+ + F^-$$

Range of Applicability

Temperature	25 – 100ºC
Pressure	up to 1.2 bar
HF concentration	up to 100 weight percent

Data Sources

D. D. Wagman et al., *J. Phys. Chem. Ref. Data*, (1982), 11, Suppl 2.

J. C. Brosheer, F.A. Lenfesty, and K.L. Elmore, *Ind. Eng. Chem*, Vol. 39, No. 3, (1947), p. 423.

P. A. Munter, Aepli, O.T., and Kossatz, R.A., *Ind. Eng. Chem*., Vol. 39, No. 3, (1947), p. 427.

Weast, *Handbook of Chemistry and Physics*, (CRC Press: 1987-88), p. D-122.

Additional Data Packages

A special data package is also available for the hydrogen fluoride system in the form of an insert file: MHF2. This data package uses option set of ENRTL-HF which considers HF association in the vapor phase.

Hydrogen Iodide and Water

The components included in this system are hydrogen iodide (HI) and water. Henry's Law is used for HI.

Application: Absorption of HI from gas or air, using water

Solution Chemistry

The aqueous phase reaction considered in this system is:

$$HI + H_2O \quad \leftrightarrow \quad H_3O^+ + I^-$$

Water dissociation is not considered because the H_3O^+ concentration is determined primarily by HI dissociation reaction.

Range of Applicability

Temperature	25 – 130ºC
Pressure	up to 1 bar
HI concentration	up to 70 weight percent

Data Sources

D. D. Wagman, et al., *J. Phys. Chem. Ref. Data*, Vol. 11, (1982), Suppl 2.

T. Sako, et al., *Kagaku Kogako Ronbunshu*, Vol. 7, No. 2, (1981), p. 191.

S. J. Bates, and H.D. Kirschman, *J. Am. Chem. Soc*., Vol. 41, (1991) p. 1919.

Methyldiethanolamine with Acid Gases

The components included in this system are: H_2S, CO_2, methyldiethanolamine (MDEA), and water. Henry's law is used for H_2S and CO_2. Enthalpy of solution data is used to develop this model.

Application: H_2S and CO_2 absorption/stripping with MDEA solutions

Solution Chemistry

The aqueous phase reactions considered for this system are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$H_2S + 2H_2O \leftrightarrow H_3O^+ + HS^-$$

$$HS^- + H_2O \leftrightarrow H_3O^+ + S^{-2}$$

$$CO_2 + 2H_2O \leftrightarrow H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{-2}$$

$$MDEA^+ + H_2O \leftrightarrow H_3O^+ + MDEA$$

Range of Applicability

Temperature	25 – 120°C
MDEA concentration	up to 51.4 weight percent

Data Sources

Jou Fang-Yuan et al., *Can. J. Chem. Eng*., Vol. 71, (1993), p. 264.

Jou Fang-Yuan, A. E. Mather and F. D. Otto, *Ind. Eng. Chem. Process Des. Dev*., Vol. 21, (1982), p. 539.

D. M. Austgen, G. T. Rochelle, and C. -C. Chen, *Ind. Eng. Chem. Res*., Vol. 30, (1991), p. 543.

Jou Fang-Yuan, J.J. Carroll, A.E. Mather, and F.D. Otto, *J. Chem. Eng. Data*, Vol. 38, (1993), p. 75.

Merkley, K.E., J.J. Christensen and R.M. Izatt, "Enthalpies of Solution of CO2 in Aqueous Methyldiethanolamine Solutions," RR-102, Gas Processors Association, 1986.

Oscarson, J.L., and R.M. Izatt, "Enthalpies of Solution of H2S in Aqueous Diethanolamine Solutions," RR-127, Gas Processors Association, 1990.

Additional Data Packages

Three special data packages are also available for this amine system in the form of insert files: KMDEA, KEMDEA and PMDEA. Both KMDEA and KEMDEA contain kinetic reactions and rate constants, allowing you to model the MDEA system more accurately using RADFRAC or RATEFRAC. The main difference between KMDEA and KEMDEA is that KMDEA uses option set of SYSOP15M and KEMDEA uses option set of ELECNRTL. PMDEA is based on the work of Posey and Rochelle (*Ind. Eng. Chem. Res*., Vol. 36, 1997, p. 3944-3953). PH and conductivity data are utilized to supplement vapor-liquid equilibria data in parameter regression. The result at low acid gas loading is improved.

Monoethanolamine with Acid Gases

The components included in this system are: H_2S, CO_2, monoethanolamine (MEA), and water. Henry's law is used for H_2S and CO_2.

Applications:

- Cleaning natural gas or flue gas
- H_2S, CO_2 absorption/stripping using aqueous MEA solutions

Solution Chemistry

The aqueous phase reactions considered in this system are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$H_2S + 2H_2O \leftrightarrow H_3O^+ + HS^-$$

$$HS^- + H_2O \leftrightarrow H_3O^+ + S^{-2}$$

$$CO_2 + 2H_2O \leftrightarrow H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{-2}$$

$$MEA^+ + H_2O \leftrightarrow H_3O^+ + MEA$$

$$MEACOO^- + H_2O \leftrightarrow HCO_3^- + MEA$$

Range of Applicability

Temperature	up to 120ºC
MEA concentration	up to 50 weight percent

Data Sources

The parameter values are obtained from:

D.M. Austgen, G.T. Rochelle, X. Peng, and C.C. Chen, "A Model of Vapor-Liquid Equilibria in the Aqueous Acid Gas-Alkanolamine System Using the Electrolyte-NRTL Equation," Paper presented at the New Orleans AICHE Meeting, March 1988.

Additional Data Packages

Two special data packages are also available for this amine system in the form of insert files: KMEA and KEMEA. Both data packages contain kinetic reactions and rate constants, allowing you to model the MEA system more accurately using RADFRAC or RATEFRAC. The main difference between KMEA and KEMEA is that KMEA uses option set of SYSOP15M and KEMEA uses option set of ELECNRTL.

Nitric Acid

The components included in this system are nitric acid (HNO_3) and water.

Application: Nitric acid distillation

Solution Chemistry

The aqueous phase reaction considered in this system is:

$$H_2O + HNO_3 \leftrightarrow H_3O^+ + NO_3^-$$

Water dissociation is not considered because the H_3O^+ concentration is determined primarily by HNO_3 dissociation reaction.

Range of Applicability

Temperature	0 – 100°C
HNO_3concentration	up to 100 weight percent

Data Sources

D. D. Wagman et al., *J. Phys. Chem. Ref. Data*, Vol. 11, (1982), Suppl 2.

R. H. Perry and C.H. Chilton, *Chemical Engineer's Handbook*, 6th ed., McGraw-Hill, (1984).

Kirk Othmer, *Encyclopedia of Chemical Technology*, Vol. 15, p. 855.

Potassium Hydroxide

The components included in this system are potassium hydroxide (KOH) and water.

Application: Upstream of neutralization

Solution Chemistry

The aqueous phase reaction considered in this system is:

$$KOH \leftrightarrow K^+ + OH^-$$

Range of Applicability

Temperature	0 – 80°C
KOH concentration	up to 36 weight percent

Data Sources

H. S. Harned and B. B. Owen, *The Physical Chemistry of Electrolytic Solutions*, 3rd ed., Reinhold Publishing Corporation, New York (1958).

D. D. Wagman et al., *J. Phys. Chem. Ref. Data,* Vol. 11, (1982), Suppl. 2.

Sodium Hydroxide

The components included in this system are sodium hydroxide (NaOH) and water.

Application: Upstream of neutralization

Solution Chemistry

The aqueous phase reaction considered in this system is:

$$NaOH \leftrightarrow Na^{+} + OH^{-}$$

Range of Applicability

Temperature	0 – 200ºC
NaOH concentration	up to 40 weight percent

Data Sources

Jurgen Krey, Dampfdruck und Dichte des Systems H2O-NAOH *Z. Phys. Chem. Neue Folge*, Bd. 81, (1972), p. 252.

I. A. Dibrov, G. Z. Maltsev, and V. P. Masovets, "Saturated Vapor Pressure of Caustic Soda and Sodium Aluminate Solution in the 25-350 C Temperature Range of Concentrations," *Zh. Prik. Khimii,* Vol. 37, No. 9, (1964), pp. 1920-1929.

J. W. Bertetti and W. L. McCabe, *Ind. Eng. Chem*., Vol. 28, (1936), p 247.

H. R. Wilson and W. L. McCabe, "Specific Heats and Heats of Dilution of Concentrated Sodium Hydroxide Solutions," *Ind. Eng. Chem*., Vol. 34, (1942), p. 558.

Horvath, *Handbook of Aqueous Electrolyte Solutions*, (1986).

Additional Data Packages

A special data package is also available for the sodium hydroxide system in the form of an insert file: MNAOH. This data package considers ion hydration effect, allowing you to model the sodium hydroxide system over the concentration range up to 60 weight percent.

Sodium Hydroxide and Sulfur Dioxide

The components included in this system are: water, sulfur dioxide (SO_2), and sodium hydroxide (NaOH). Henry's law is used for SO_2.

Application: Absorption of SO_2 in NaOH solution

Solution Chemistry

The aqueous phase reactions considered in this system are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$2H_2O + SO_2 \leftrightarrow H_3O^+ + HSO_3^-$$

$$HSO_3^- + H_2O \leftrightarrow H_3O^+ + SO_3^{-2}$$

$$NaOH \leftrightarrow Na^+ + OH^-$$

Range of Applicability

Temperature	35 – 90ºC
NaOH concentration	up to 8 molal
SO2 concentration	up to 7 molal

Data Sources

H.F. Johnstone et al., "Recovery of Sulfur Dioxide From Waste Gases," *Ind. Eng. Chem.*, Vol. 30, (1938), p. 101.

Jurgen Krey, Dampfdruck und Dichte des Systems H2O-NAOH *Z. Phys. Chem. Neue Folge*, Bd. 81, (1972), p. 252.

I. A. Dibrov, G. Z. Maltsev, and V. P. Masovets, "Saturated Vapor Pressure of Caustic Soda and Sodium Aluminate Solution in the 25-350 C Temperature Range of Concentrations," *Zh. Prik. Khimii*, Vol. 37, No. 9, (1964), pp. 1920-1929.

J. W. Bertetti and W. L. McCabe, *Ind. Eng. Chem.*, Vol. 28, (1936), p 247.

H. R. Wilson and W. L. McCabe, "Specific Heats and Heats of Dilution of Concentrated Sodium Hydroxide Solutions," *Ind. Eng. Chem.*, Vol. 34, (1942), p. 558.

Horvath, *Handbook of Aqueous Electrolyte Solutions*, (1986).

E. Otsaka, S. Yoshimura, M. Yokabe, and S. Inque, *Kogyo Kagaku Zasshi*, Vol. 63, (1960), p. 1214.

Sour Water

The components included in this sour water system are: ammonia (NH_3), hydrogen sulfide (H_2S), carbon dioxide (CO_2), and water. Henry's law is used for NH_3, CO_2, and H_2S.

Application: Sour water stripping

Solution Chemistry

The aqueous phase reactions that are considered in this system are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$H_2S + H_2O \leftrightarrow H_3O^+ + HS^-$$

$$HS^- + H_2O \leftrightarrow H_3O^+ + S^{-2}$$

$$CO_2 + 2H_2O \leftrightarrow H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{-2}$$

$$NH_3 + H_2O \leftrightarrow NH_4^+ + OH^-$$

$$NH_3 + HCO_3^- \leftrightarrow NH_2CO_2^- + H_2O$$

Range of Applicability

Temperature	0 – 120ºC
Maximum Pressure	250 psia
NH_3 concentration	up to about 23 molal
H_2S concentration	up to about 8 molal
CO_2 concentration	up to about 8 molal

Extrapolation of this system has been checked to produce reasonable results.

Data Sources

D.H. Miles and G.M. Wilson, "Vapor-liquid Equilibrium Data for Design of Sour Water Strippers," Annual Report to the API for 1974, October 1975.

Sour Water and Caustic

The components included in this system are: water, ammonia (NH_3), hydrogen sulfide (H_2S), carbon dioxide (CO_2), and caustic (NaOH). Henry's law is used for NH_3, CO_2, and H_2S.

Applications: Sour water with caustic

Solution Chemistry

The aqueous phase reactions considered in this system are:

$$2H_2O \leftrightarrow H_3O^+ + OH^-$$

$$H_2S + 2H_2O \leftrightarrow H_3O^+ + HS^-$$

$$HS^- + H_2O \leftrightarrow H_3O^+ + S^{-2}$$

$$CO_2 + 2H_2O \leftrightarrow H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{-2}$$

$$NH_3 + H_2O \leftrightarrow NH_4^+ + OH^-$$

$$NH_3 + HCO_3^- \leftrightarrow NH_2CO_2^- + H_2O$$

$$NaOH \leftrightarrow NA^+ + OH^-$$

Range of Applicability

Temperature	0 – 100ºC
Pressure	250 psi
NH_3 concentration	up to 23 molal
H_2S concentration	up to 8 molal
CO_2 concentration	up to 8 molal
NaOH concentration	up to 20 weight percent

Data Sources

D.H. Miles and G.M. Wilson, "Vapor-Liquid Equilibrium Data for Design of Sour Water Strippers," Annual Report to the API for 1974, October 1975.

Jurgen Krey, Dampfdruck und Dichte des Systems H2O-NAOH *Z. Phys. Chem. Neue Folge*, Bd. 81, (1972), p. 252.

E. Otsaka, S. Yoshimura, M. Yokabe, and S. Inque, *Kogyo Kagaku Zasshi*, Vol. 63, (1960), p. 1214.

I. A. Dibrov, G. Z. Maltsev, and V. P. Masovets, "Saturated Vapor Pressure of Caustic Soda and Sodium Aluminate Solution in the 25-350 C Temperature Range of Concentrations," *Zh. Prik. Khimii*, Vol. 37, No. 9, (1964), pp. 1920-1929.

J. W. Bertetti and W. L. McCabe, *Ind. Eng. Chem.*, Vol. 28, (1936), p. 247.

H. R. Wilson and W. L. McCabe, "Specific Heats and Heats of Dilution of Concentrated Sodium Hydroxide Solutions," *Ind. Eng. Chem.*, Vol. 34, (1942), p. 558.

Horvath, *Handbook of Aqueous Electrolyte Solutions*, (1986).

Sulfuric Acid

The components included in this system are: water and sulfuric acid (H_2SO_4).

Application: Sulfuric acid production

Solution Chemistry

The aqueous phase reactions considered in this system are:

$$H_2O + H_2SO_4 \leftrightarrow H_3O^+ + HSO_4^-$$

$$H_2O + HSO_4^- \leftrightarrow H_3O^+ + SO_4^{-2}$$

Range of Applicability

Temperature	0 – 200ºC
H_2SO_4 concentration	up to 98 weight percent

Data Sources

D. D. Wagman et al., *J. Phys. Chem. Ref. Data*, Vol. 11, (1982), Suppl 2.

R. H. Perry and C.H. Chilton, *Chemical Engineer's Handbook*, 6th ed., McGraw-Hill, (1984).

Sulfuric Acid and Hydrogen Bromide

The components included in this system are sulfuric acid (H_2SO_4), hydrogen bromide, and water.

Application: Simultaneous HBr + H_2SO_4 absorption

Break azeotrope H_2O + H2SO4

Solution Chemistry

The aqueous phase reactions considered in this system are:

$$H_2SO_4 + H_2O \leftrightarrow H_3O^+ + HSO_4^-$$

$$HSO_4^- + H_2O \leftrightarrow H_3O^+ + SO_4^{-2}$$

$$HBr + H_2O \leftrightarrow H_3O^+ + Br^-$$

Range of Application

Temperature	25 – 125°C
HBr concentration	up to 60 weight percent
H_2SO_4 concentration	up to 98 weight percent

Data Sources

D.D. Wagman et al., *J. Phys. Chem. Ref. Data*, Vol. 11, (1982), Suppl 2.

S.J. Bates, and H.D. Kirschman, *J. Am. Chem. Soc*, Vol. 41, (1991), p. 1919.

L. Chevaller and Gaston-Bonhomme Y.H., *J. Chem. Eng. Data*, (1980), Vol. 25, p. 271.

R. Hasse et al., *Collin Czech. Chem. Comm. Engl. Edn.*, Vol. 37, (1963), p. 220.

G. Wuster, G. Wozny, and Z. Giazitzoglou, *Fluid Phase Eq.*, Vol. 6, (1981), p. 93.

International Critical Tables, Vol. 3, p. 306.

R. H. Perry and C. H. Chilton, *Chemical Engineer's Handbook*, 6th ed., McGraw-Hill, (1984).

Sulfuric Acid and Hydrogen Chloride

The components included in this system are: water, hydrogen chloride (HCl), and sulfuric acid (H_2SO_4). Henry's law is used for HCl.

Applications:

- Simultaneous $HCl + H_2SO_4$
- Break azeotrope $H_2O + H_2SO_4$

Solution Chemistry

The aqueous phase reactions considered in this system are:

$$H_2O + H_2SO_4 \leftrightarrow H_3O^+ + HSO_4^-$$

$$HSO_4^- + H_2O \leftrightarrow H_3O^+ + SO_4^{-2}$$

$$H_2O + HCl \leftrightarrow H_3O^+ + Cl^-$$

Range of Applications

Temperature	0 – 110°C
HCl concentration	up to 16 molal
H_2SO_4 concentration	up to 100 weight percent

Data Sources

D. D. Wagman et al., *J. Phys. Chem. Ref. Data*, Vol. 11, (1982), Suppl 2.

R. H. Perry and C.H. Chilton, *Chemical Engineer's Handbook*, 6th ed., McGraw-Hill, (1984).

J-L. E. Chevalier and Y. H. Gaston-Bonhomme, *J. Chem. Eng. Data*, Vol. 25, (1980), p. 271.

CHAPTER 3

Group Contribution Method Functional Groups

Overview

The tables in this chapter list the groups for each of the group contribution methods available in the Aspen Physical Property System.

The tables are:

- PCES Functional Groups
- UNIFAC Functional Groups

PCES Functional Groups

Tables 3.1 through 3.11A list the functional groups for the methods used in the Property Constant Estimation System (PCES). There are two types of functional groups:

- Group increments, such as $-CH_3$ or *–COO–3*
- Corrections, such as the correction for the presence of a benzene ring

You must identify both kinds of functional groups for any method used. Identify group increments to account for all the atoms in a molecule. Then identify any corrections to be applied.

The group definitions for most methods are obtained from Reid et al., *The Properties of Gases and Liquids*, 3rd and 4th editions, McGraw-Hill, 1977 and 1987. Groups for the Bondi Method are adapted from A. Bondi, *Physical Properties of Molecular Liquids*, Wiley, 1968. Groups for the Ogata-Tsuchida method are from Reid and Sherwood, *The Properties of Gases and Liquids*, 2nd edition,

McGraw-Hill, 1966. Slight modifications have been made to the group definitions for the Fedors and Parachor methods.

Table 3.1 Ambrose Method Functional Groups

Functional Group [1]	Group Number
Carbon Atoms in Alkyl Groups	**100**
Corrections:	
>CH- (each)	101
>C<(each)	102
Double Bonds (nonaromatic)	103
Triple Bonds	104
Delta Platt Number [2]	105
Aliphatic Functional Groups	
-O-	106
>C=O	107
O=CH- (aldehyde)	108
-COOH (acid)	109
-CO-O-CO- (anhydride)	110
-COO- (ester)	111
-NO2	112
-NH2	113
>NH	114
>N-	115
-CN	116
-S-	117
-SH	118
-SIH3	119
-O-SI(CH3)2	120
-F	121
-CL	122
-BR	123
-I	124
Halogen Corrections in Aliphatic Compounds	
-F is present	125
-F is absent, but -CL, -BR, -I are present	126
Aliphatic alcohols[3], -OH3	127

Ring Compound Increments (listed only when different from aliphatic values)

>CH2	128
>CH- (in fused ring)	129
Double Bond	130
-O-	131
>NH	132
-S-	133

Aromatic Compounds

Benzene	134
Pyridine	135
C4H4 (fused as in Naphthalene)	136
-F	137
-CL	138
-BR	139
-I	140
-OH	141
Corrections for nonhalogenated substitutions	
First substitution	142
Each subsequent	143
Ortho pairs containing -OH	144
Ortho pairs with no -OH	145

Highly Fluorinated Aliphatic Compounds

-CF3, >CF2, >CF-	146
>CF2, >CF- (RING)	147
>CF- (in fused ring)	148
-H (monosubstitution)	149
Double bond (nonring)	150
Double bond (ring)	151

Compound Containing Only

Halogen	152

Silicon

>SI<	153
>SIH-	154
-SI-O-	155
-SI-O-(ring)	156

Table 3.2 Benson Method Functional Groups

Functional Group	Group Number
Hydrocarbon Groups	
C-(C)(H)3	100
C-(C)2(H)2	101
C-(C)3(H)	102
C-(C)4	103
CD-(H)2 [4]	104
CD-(C)(H)	105
CD-(C)2	106
CD-(CD)(H)	107
CD-(CD)(C)	108
CD-(CD)2	109
CD-(CB)(H)	110
CD-(CB)(C)	111
CD-(CB)2	112
CD-(CT)(H)	113
CD-(CT)(C)	114
C-(CD)(H)3	115
C-(CD)2(H)2	116
C-(CD)(C)(H)2	117
C-(CD)(C)3	118
C-(CD)(C)(H)2	119
C-(CD)(C)2(H)	120
C-(CD)2(C)(H)	121
C-(CT)(H)3	122
C-(CT)(C)(H)2	123
C-(CT)(C)2(H)	124
C-(CT)(C)3	402
C-(CB)(H)3	125
C-(CB)(C)(H)2	126
C-(CB)(C)2(H)	127
C-(CB)(C)3	128
C-(CB)2(C)(H)	129
C-(CB)2(C)2	130
C-(CB)(CD)(H)2	131
CT-(H) [5]	132
CT-(C)	133
CT-(CD)	134
CT-(CB)	135
CB-(H) [6]	136

Functional Group	Group Number
Hydrocarbon Groups	
CB-(C)	137
CB-(CD)	138
CB-(CT)	139
CB-(CB)	140
CA [7]	141
CBF-(CB)2(CBF) [8]	142
CBF-(CB)(CBF)2	143
CBF-(CBF)3	144
Next-Nearest-Neighbor Correction	
Alkane Gauche	145
Alkene Gauche	146
Cis	147
Ortho	148
Corrections for Ring Compounds	
Cyclopropane	149
Cyclopropene	150
Cyclobutane	151
Cyclobutene	152
Cyclopentane	153
Cyclopentene	154
Cyclopentadiene	155
Cyclohexane	156
Cyclohexene	157
Cycloheptane	158
Cyclooctane	159
Naphthalene	160
Oxygen-Containing Compounds	
CO-(CO)(H)	161
CO-(CO)(C)	162
CO-(O)(CD)	163
CO-(O)(CB)	164
CO-(O)(C)	165
CO-(O)(H)	166
CO-(CD)(H)	167
CO-(CB)2	168
CO-(CB)(C)	169
CO-(CB)(H)	170

Functional Group	Group Number
Oxygen-Containing Compounds	
CO-(C)2	171
CO-(C)(H)	172
CO-(H)2	173
O-(CB)(CO)	174
O-(CO)2	175
O-(CO)(O)	176
O-(CO)(CD)	177
O-(CO)(C)	178
O-(CO)(H)	179
O-(O)(C)	180
O-(O)2	181
O-(O)(H)	182
O-(CD)2	183
O-(CD)(C)	184
O-(CD)(H)	401
O-(CB)2	185
O-(CB)(C)	186
O-(CB)(H)	187
O-(C)2	188
O-(C)(H)	189
CD-(CO)(O)	190
CD-(CO)(C)	191
CD-(CO)(H)	192
CD-(O)(CD)	193
CD-(O)(C)	194
CD-(O)(H)	195
CB-(CO)	196
CB-(O)	197
C-(CO)2(H)2	198
C-(CO)(C)2(H)	199
C-(CO)(C)(H)2	200
C-(CO)(C)3	201
C-(CO)(H)3	202
C-(O)2(C)2	203
C-(O)2(C)(H)	204
C-(O)2(H)2	205
C-(O)(CB)(H)2	206
C-(O)(CB)(C)(H)	207

Functional Group	Group Number
Oxygen-Containing Compounds	
C-(O)(CD)(H)2	208
C-(O)(C)3	209
C-(O)(C)2(H)	210
C-(O)(C)(H)2	211
C-(O)(H)3	212
C-(O)(CT)(H)2	403
C-(O)(C)2(CT)	404
Strain and Ring Corrections for Oxygen-Containing Compounds	
Ether Oxygen, Gauche	213
Ditertiary Ethers	214
Ethylene Oxide	215
Trimethylene Oxide	216
Tetrahydrofuran	217
Tetrahydropyran	218
1,3-Dioxane	219
1,4-Dioxane	220
1,3,5-Trioxane	221
Furan	222
Dihydropyran	223
Cyclopentanone	224
Cyclohexanone	225
Succinic Anhydride	226
Glutaric Anhydride	227
Maleic Anhydride	228
Nitrogen-Containing Compounds	
C-(N)(H)3	229
C-(N)(C)(H)2	230
C-(N)(C)2(H)	231
C-(N)(C)3	232
N-(C)(H)2	233
N-(C)2(H)	234
N-(C)3	235
N-(N)(H)2	236
N-(N)(C)(H)	237
N-(N)(C)2	238
N-(N)(CB)(H)	239
NI-(H) [9]	240

Functional Group	Group Number
Nitrogen-Containing Compounds	
NI-(C)	241
NI-(CB)	242
NA-(H) [10]	243
NA-(C)	244
N-CB)(H)2	245
N-(CB)(C)(H)	246
N-(CB)(C)2	247
N-(CB)2(H)	248
CB-(N)	249
NA-(N)	250
CO-(N)(H)	251
CO-(N)(C)	252
N-(CO)(H)2	253
N-(CO)(C)(H)	254
N-(CO)(C)2	255
N-(CO)(CB)(H)	256
N-(CO)2(H)	257
N-(CO)2(C)	258
N-(CO)2(CB)	259
C-(CN)(C)(H)2	260
C-(CN)(C)2(H)	261
C-(CN)(C)3	262
C-(CN)2(C)2	263
CD-(CN)(H)	264
CD-(CN)(C)	265
CD-(CN)2	266
CD-(NO2)(H)	267
CB-(CN)	268
CT-(CN)	269
C-(NO2)(C)(H)2	270
C-(NO2)(C)2(H)	271
C-(NO2)(C)3	272
C-(NO2)2(C)(H)	273
O-(NO)(C)	274
O-(NO2)(C)	275

Functional Group	Group Number
Ring Corrections for Nitrogen-Containing Compounds	
Ethyleneimine	276
Azetidine	277
Pyrrolidine	278
Piperidine	279
Succinimide	280
Halogen Groups	
C-(F)3(C)	281
C-(F)2(H)(C)	282
C-(F)(H)2(C)	283
C-(F)2(C)2	284
C-(F)(H)(C)2	285
C-(F)(C)3	286
C-(F)2(CL)(C)	287
C-(CL(3(C)	288
C-(CL)2(H)(C)	289
C-(CL)(H)2(C)	290
C-(CL)2(C)2	291
C-(CL)(H)(C)2	292
C-(CL)(C)3	293
C-(BR)3(C)	294
C-(BR)(H)2(C)	295
C-(BR)(H)(C)2	296
C-(BR)(C)3	297
C-(I)(H)2(C)	298
C-(I)(H)(C)2	299
C-(I)(C)(CD)(H)	300
C-(I)(CD)(H)2	301
C-(I)(C)3	302
C-(CL)(BR)(H)(C)	303
N-(F)2(C)	304
C-(CL)(C)(O)(H)	305
C-(I)2(C)(H)	306
C-(I)(O)(H)2	307
CD-(F)2	308
CD-(CL)2	309
CD-(BR)2	310
CD-(F)(CL)	311

Functional Group	Group Number
Halogen Groups	
CD-(F)(BR)	312
CD-(CL)(BR)	313
CD-(F)(H)	314
CD-(CL)(H)	315
CD-(BR)(H)	316
CD-(I)(H)	317
CD-(C)(CL)	318
CD-(C)(I)	319
CD-(CD)(CL)	320
CD-(CD)(I)	321
CT-(CL)	322
CT-(BR)	323
CT-(I)	324
CB-(F)	325
CB-(CL)	326
CB-(BR)	327
CB-(I)	328
C-(CB)(F)3	329
C-(CB)(BR)(H)2	330
C-(CB)(I)(H)2	331
C-(CL)2(CO)(H)	332
C-(CL)3(CO)	333
CO-(CL)(C)	334
Corrections for Next-Nearest-Neighbor Halogen Compounds	
Ortho (F)(F)	335
Ortho (CL)(CL)	336
Ortho (alkane)(halogen) [11]	337
Cis (halogen)(halogen) [11]	338
Cis (alkane)(halogen) [11]	339
Organosulfur Groups	
C-(H)3(S)	340
C-(C)(H)2(S)	341
C-(C)2(H)(S)	342
C-(C)3(S)	343
C-(CB)(H)2(S)	344
C-(CD)(H)2(S)	345
CB-(S)	346

Functional Group	Group Number
Organosulfur Groups	
CD-(H)(S)	347
CD-(C)(S)	348
S-(C)(H)	349
S-(CB)(H)	350
S-(C)2	351
S-(C)(CD)	352
S-(CD)2	353
S-(CB)(C)	354
S-(CB)2	355
S-(S)(C)	356
S-(S)(CB)	357
S-(S)2	358
C-(SO)(H)3	359
C-(C)(SO)(H)2	360
C-(C)3(SO)	361
C-(CD)(SO)(H)2	362
CB-(SO)	363
SO-(C)2	364
SO-(CB)2	365
C-(SO2)(H)3	366
C-(C)(SO2)(H)2	367
C-(C)2(SO2)(H)	368
C-(C)3(SO2)	369
C-(CD)(SO2)(H)2	370
C-(CB)(SO2)(H)2	371
CB-(SO2)	372
CD-(H)(SO2)	373
CD-(C)(SO2)	374
SO2-(CD)(CB)	375
SO2-(CD)2	376
SO2-(C)2	377
SO2-(C)(CB)	378
SO2-(CB)2	379
SO2-(SO2)(CB)	380
CO-(S)(C)	381
S-(H)(CO)	382
C-(S)(F)3	383
CS-(N)2	384

Functional Group	Group Number
Organosulfur Groups	
N-(CS)(H)2	385
S-(S)(N)	386
N-(S)(C)2	387
SO-(N)2	388
N-(SO)(C)2	389
SO2-(N)2	390
N-(SO2)(C)2	391
Ring Corrections for Sulfur-Containing Compounds	
Thiirane	392
Trimethylene Sulfide	393
Tetrahydrothiophene	394
Thiacyclohexane	395
Thiacycloheptane	396
3-Thiocyclopentene	397
2-Thiocyclopentene	398
Thiophene	399
Symmetry and Optical Isomers Corrections [12]	
Symmetry	405
Optical Isomers	406
Other	
Ortho or Para Substitution on Pyridine	400
O-(CD)(H)	401
C-(CT)(C)3	402
C-(O)(CT)(H)2	403
C-(O)(C)2(CT)	404
Silicon Groups	
SI-(C)(H)3	407
SI-(C)2(H)2	408
SI-(C)3(H)	409
SI-(C)4	410
SI-(SI)(H)3	411
SI-(SI)2(H)2	412
SI-(SI)2(C)2	413
SI-(SI)(C)3	414
SI-(SI)4	415
C-(SI)(C)(H)2	416

Functional Group	Group Number
Silicon Groups	
C-(SI)(C)2(H)	417
C-(SI)(H)3	418
SI-(C)(CL)3	419
SI-(C)2(CL)2	420
SI-(C)3(CL)	421
SI-(C)(F)3	422
SI-(C)3(BR)	423
SI-(C)3(I)	424
SI-(C)(H)(CL)2	425
SI-(C)2(H)(CL)	426
SI-(O)(F)3	427
SI-(O)3(CL)	428
SI-(SI)(F)3	429
SI-(SI)2(F)2	430
SI-(SI)(CL)3	431
SI-(SI)(O)3	432
SI-(O)3(H)	433
SI-(C)(O)3	434
SI-(C)2(O)2	435
SI-(C)3(O)	436
SI-(O)4	437
O-(SI)(O)	438
O-(SI)2	439
O-(SI)(C)	440
O-(SI)(H)	441
SI-(SI)(C)(O)2	442
C-(SI)(O)(H)2	443
SI-(CB)4	444
SI-(CB)2(CL)2	445
SI-(CB)(O)3	446
SI-(CB)2(C)(H)	447
CB-(SI)	448
O-(SI)(CB)	449
Boron Groups	
B-(C)3	450
C-(B)(C)(H)2	451
C-(B)(C)2(H)	452
C-(B)(H)3	453

Functional Group	Group Number
Boron Groups	
B-(CB)3	454
CB-(B)	455
B-(O)3	456
B-(O)2(H)	457
B-(O)(H)2	458
B-(B)(O)2	459
O-(B)(C)	460
O-(B)(H)	461
O-(B)(CB)	462
O-(B)(O)	463
B-(C)2(O)	464
B-(CB)(O)2	465
B-(S)3	466
S-(B)(C)	467
S-(B)(CB)	468
B-(N)3	469
B-(C)2(N)	470
B-(C)(N)(O)	471
N-(B)(C)2	472
N-(B)(C)(H)	473
B-(O)(F)2	474
B-(O)2(F)	475
B-(B)(F)2	476
B-(C)(F)2	477
B-(N)2(CL)	478
B-(N)(CL)2	479
B-(B)(CL)2	480
B-(O)2(CL)	481
B-(O)(CL)2	482
B-(C)2(CL)	483
B-(CB)2(CL)	484
B-(CB)(CL)2	485
B-(C)2(BR)	486
B-(CB)2(BR)	487
B-(CB)(BR)2	488
B-(C)2(I)	489

Functional Group	Group Number
Aluminum Groups	
AL-(C)3	490
C-(AL)(C)(H)2	491
AL-(C)2(H)	492
C-(AL)(H)3	494
AL-(AL)(CL)2	495
Silicon in Ring Correction	
SI (ring-4)	496
SI (ring-5)	497

Table 3.2A BensonR8 Method Functional Groups

Functional Group	Group Number
Hydrocarbon Groups	
C-(C)(H)3	100
C-(C)2(H)2	101
C-(C)3(H)	102
C-(C)4	103
CD-(H)2 [4]	104
CD-(C)(H)	105
CD-(C)2	106
CD-(CD)(H)	107
CD-(CD)(C)	108
CD-(CD)2	109
CD-(CB)(H)	110
CD-(CB)(C)	111
CD-(CB)2	112
CD-(CT)(H)	113
CD-(CT)(C)	114
C-(CD)(H)3	115
C-(CD)2(H)2	116
C-(CD)(C)(H)2	117
C-(CD)(C)3	118
C-(CD)(C)(H)2	119
C-(CD)(C)2(H)	120
C-(CD)2(C)(H)	121
C-(CT)(H)3	122
C-(CT)(C)(H)2	123
C-(CT)(C)2(H)	124
C-(CT)(C)3	402

Functional Group	Group Number
Hydrocarbon Groups	
C-(CB)(H)3	125
C-(CB)(C)(H)2	126
C-(CB)(C)2(H)	127
C-(CB)(C)3	128
C-(CB)2(C)(H)	129
C-(CB)2(C)2	130
C-(CB)(CD)(H)2	131
CT-(H) [5]	132
CT-(C)	133
CT-(CD)	134
CT-(CB)	135
CB-(H) [6]	136
CB-(C)	137
CB-(CD)	138
CB-(CT)	139
CB-(CB)	140
CA [7]	141
CBF-(CB)2(CBF) [8]	142
CBF-(CB)(CBF)2	143
CBF-(CBF)3	144
Next-Nearest-Neighbor Correction	
Alkane Gauche	145
Alkene Gauche	146
Cis	147
Ortho	148
Corrections for Ring Compounds	
Cyclopropane	149
Cyclopropene	150
Cyclobutane	151
Cyclobutene	152
Cyclopentane	153
Cyclopentene	154
Cyclopentadiene	155
Cyclohexane	156
Cyclohexene	157
Cycloheptane	158
Cyclooctane	159
Naphthalene	160

Functional Group	Group Number
Oxygen-Containing Compounds	
CO-(CO)(H)	161
CO-(CO)(C)	162
CO-(O)(CD)	163
CO-(O)(CB)	164
CO-(O)(C)	165
CO-(O)(H)	166
CO-(CD)(H)	167
CO-(CB)2	168
CO-(CB)(C)	169
CO-(CB)(H)	170
CO-(C)2	171
CO-(C)(H)	172
CO-(H)2	173
O-(CB)(CO)	174
O-(CO)2	175
O-(CO)(O)	176
O-(CO)(CD)	177
O-(CO)(C)	178
O-(CO)(H)	179
O-(O)(C)	180
O-(O)2	181
O-(O)(H)	182
O-(CD)2	183
O-(CD)(C)	184
O-(CD)(H)	401
O-(CB)2	185
O-(CB)(C)	186
O-(CB)(H)	187
O-(C)2	188
O-(C)(H)	189
CD-(CO)(O)	190
CD-(CO)(C)	191
CD-(CO)(H)	192
CD-(O)(CD)	193
CD-(O)(C)	194
CD-(O)(H)	195
CB-(CO)	196
CB-(O)	197

Functional Group	Group Number
Oxygen-Containing Compounds	
C-(CO)2(H)2	198
C-(CO)(C)2(H)	199
C-(CO)(C)(H)2	200
C-(CO)(C)3	201
C-(CO)(H)3	202
C-(O)2(C)2	203
C-(O)2(C)(H)	204
C-(O)2(H)2	205
C-(O)(CB)(H)2	206
C-(O)(CB)(C)(H)	207
C-(O)(CD)(H)2	208
C-(O)(C)3	209
C-(O)(C)2(H)	210
C-(O)(C)(H)2	211
C-(O)(H)3	212
C-(O)(CT)(H)2	403
C-(O)(C)2(CT)	404
Strain and Ring Corrections for Oxygen-Containing Compounds	
Ether Oxygen, Gauche	213
Ditertiary Ethers	214
Ethylene Oxide	215
Trimethylene Oxide	216
Tetrahydrofuran	217
Tetrahydropyran	218
1,3-Dioxane	219
1,4-Dioxane	220
1,3,5-Trioxane	221
Furan	222
Dihydropyran	223
Cyclopentanone	224
Cyclohexanone	225
Succinic Anhydride	226
Glutaric Anhydride	227
Maleic Anhydride	228

Functional Group	Group Number
Nitrogen-Containing Compounds	
C-(N)(H)3	229
C-(N)(C)(H)2	230
C-(N)(C)2(H)	231
C-(N)(C)3	232
N-(C)(H)2	233
N-(C)2(H)	234
N-(C)3	235
N-(N)(H)2	236
N-(N)(C)(H)	237
N-(N)(C)2	238
N-(N)(CB)(H)	239
NI-(H) [9]	240
NI-(C)	241
NI-(CB)	242
NA-(H) [10]	243
NA-(C)	244
N-CB)(H)2	245
N-(CB)(C)(H)	246
N-(CB)(C)2	247
N-(CB)2(H)	248
CB-(N)	249
NA-(N)	250
CO-(N)(H)	251
CO-(N)(C)	252
N-(CO)(H)2	253
N-(CO)(C)(H)	254
N-(CO)(C)2	255
N-(CO)(CB)(H)	256
N-(CO)2(H)	257
N-(CO)2(C)	258
N-(CO)2(CB)	259
C-(CN)(C)(H)2	260
C-(CN)(C)2(H)	261
C-(CN)(C)3	262
C-(CN)2(C)2	263
CD-(CN)(H)	264
CD-(CN)(C)	265
CD-(CN)2	266

Functional Group	Group Number
Nitrogen-Containing Compounds	
CD-(NO2)(H)	267
CB-(CN)	268
CT-(CN)	269
C-(NO2)(C)(H)2	270
C-(NO2)(C)2(H)	271
C-(NO2)(C)3	272
C-(NO2)2(C)(H)	273
O-(NO)(C)	274
O-(NO2)(C)	275
Ring Corrections for Nitrogen-Containing Compounds	
Ethyleneimine	276
Azetidine	277
Pyrrolidine	278
Piperidine	279
Succinimide	280
Halogen Groups	
C-(F)3(C)	281
C-(F)2(H)(C)	282
C-(F)(H)2(C)	283
C-(F)2(C)2	284
C-(F)(H)(C)2	285
C-(F)(C)3	286
C-(F)2(CL)(C)	287
C-(CL(3(C)	288
C-(CL)2(H)(C)	289
C-(CL)(H)2(C)	290
C-(CL)2(C)2	291
C-(CL)(H)(C)2	292
C-(CL)(C)3	293
C-(BR)3(C)	294
C-(BR)(H)2(C)	295
C-(BR)(H)(C)2	296
C-(BR)(C)3	297
C-(I)(H)2(C)	298
C-(I)(H)(C)2	299
C-(I)(C)(CD)(H)	300
C-(I)(CD)(H)2	301

Functional Group	Group Number
Halogen Groups	
C-(I)(C)3	302
C-(CL)(BR)(H)(C)	303
N-(F)2(C)	304
C-(CL)(C)(O)(H)	305
C-(I)2(C)(H)	306
C-(I)(O)(H)2	307
CD-(F)2	308
CD-(CL)2	309
CD-(BR)2	310
CD-(F)(CL)	311
CD-(F)(BR)	312
CD-(CL)(BR)	313
CD-(F)(H)	314
CD-(CL)(H)	315
CD-(BR)(H)	316
CD-(I)(H)	317
CD-(C)(CL)	318
CD-(C)(I)	319
CD-(CD)(CL)	320
CD-(CD)(I)	321
CT-(CL)	322
CT-(BR)	323
CT-(I)	324
CB-(F)	325
CB-(CL)	326
CB-(BR)	327
CB-(I)	328
C-(CB)(F)3	329
C-(CB)(BR)(H)2	330
C-(CB)(I)(H)2	331
C-(CL)2(CO)(H)	332
C-(CL)3(CO)	333
CO-(CL)(C)	334

Functional Group	Group Number
Corrections for Next-Nearest-Neighbor Halogen Compounds	
Ortho (F)(F)	335
Ortho (CL)(CL)	336
Ortho (alkane)(halogen) [11]	337
Cis (halogen)(halogen) [11]	338
Cis (alkane)(halogen) [11]	339
Organosulfur Groups	
C-(H)3(S)	340
C-(C)(H)2(S)	341
C-(C)2(H)(S)	342
C-(C)3(S)	343
C-(CB)(H)2(S)	344
C-(CD)(H)2(S)	345
CB-(S)	346
CD-(H)(S)	347
CD-(C)(S)	348
S-(C)(H)	349
S-(CB)(H)	350
S-(C)2	351
S-(C)(CD)	352
S-(CD)2	353
S-(CB)(C)	354
S-(CB)2	355
S-(S)(C)	356
S-(S)(CB)	357
S-(S)2	358
C-(SO)(H)3	359
C-(C)(SO)(H)2	360
C-(C)3(SO)	361
C-(CD)(SO)(H)2	362
CB-(SO)	363
SO-(C)2	364
SO-(CB)2	365
C-(SO2)(H)3	366
C-(C)(SO2)(H)2	367
C-(C)2(SO2)(H)	368
C-(C)3(SO2)	369
C-(CD)(SO2)(H)2	370

Functional Group	Group Number
Organosulfur Groups	
C-(CB)(SO2)(H)2	371
CB-(SO2)	372
CD-(H)(SO2)	373
CD-(C)(SO2)	374
SO2-(CD)(CB)	375
SO2-(CD)2	376
SO2-(C)2	377
SO2-(C)(CB)	378
SO2-(CB)2	379
SO2-(SO2)(CB)	380
CO-(S)(C)	381
S-(H)(CO)	382
C-(S)(F)3	383
CS-(N)2	384
N-(CS)(H)2	385
S-(S)(N)	386
N-(S)(C)2	387
SO-(N)2	388
N-(SO)(C)2	389
SO2-(N)2	390
N-(SO2)(C)2	391
Ring Corrections for Sulfur-Containing Compounds	
Thiirane	392
Trimethylene Sulfide	393
Tetrahydrothiophene	394
Thiacyclohexane	395
Thiacycloheptane	396
3-Thiocyclopentene	397
2-Thiocyclopentene	398
Thiophene	399
Symmetry and Optical Isomers Corrections [12]	
Symmetry	405
Optical Isomers	406

Functional Group	Group Number
Other	
Ortho or Para Substitution on Pyridine	400
O-(CD)(H)	401
C-(CT)(C)3	402
C-(O)(CT)(H)2	403
C-(O)(C)2(CT)	404
SYMMETRY	405
OPTICAL-ISOMER	406

Table 3.3 Bondi Method Functional Groups

Functional Group	Group Number
Carbon Increments	
-CH3	100
>CH2	101
>CH-	102
>C<	103
=CH2	104
=CH-	105
=C<	106
=C= (allene)	107
≡CH	108
≡C-	109
-C≡ (diacetylene)	110
=CH- (aromatic)	111
=C<(aromatic, aliphatic)	112
=C<(aromatic)	113
Naphthyl	114
Nitrogen Increments	
-NH2	115
>NH	116
>N-	117
=N-	118
-CN	119
-NO2	120
Oxygen Increments	
-O- (aliphatic)	121
-O- (aromatic)	122
-OH	123
>C=O	124

Functional Group	Group Number
Oxygen Increments	
O=CH- (aldehyde)	125
-COO- (ester)	126
Sulfur Increments	
-S- (aliphatic)	127
-S- (hetero, aromatic)	128
2-Thiophenyl	129
3-Thiophenyl	130
-S-S- (aliphatic)	131
-SH	132
>S=O (aliphatic)	133
>SO2 (aliphatic)	134
-O-SO2-O- (aliphatic)	135
Halogen Increments	
-F (aliphatic) [13]	136
-F (aromatic)	137
-F (other)	138
-CL (aliphatic) [13]	139
-CL (aromatic, per)	140
-CL (aromatic, mono, di, tri)	141
-CL (other)	142
-BR (aliphatic) [13]	143
-BR (aromatic)	144
-BR (other)	145
-I (aliphatic) [13]	146
-I (aromatic)	147
-I (other)	148
Corrections for Intramolecular Effects	
Single bond between conjugated double bonds	149
Single bond adjacent to carboxyl group (>C=O)	150
Single bond adjacent to amide group (=NH)	151
Cyclopropyl ring in single bond attachment	152
Cyclopentyl or cyclohexyl ring in single bond attachment	153
Methylene ring condensed to aromatic ring system as in tetralin	154
Dioxane ring	155

Table 3.3A Ducros Method Functional Groups

Functional Group	Group Number
Hydrocarbon Groups	
C-(C)(H)3	100
C-(C)2(H)2	101
C-(C)3(H)	102
C-(C)4	103
CD-(H)2	104
CD-(C)(H)	105
CD-(C)2	106
CD-(CD)(H)	107
CD-(CD)(C)	108
CD-(CD)2	109
C-(CD)(H)3	115
C-(CD)2(H)2	116
C-(CD)(C)3	118
C-(CD)(C)(H)2	119
C-(CD)(C)2(H)	120
C-(CT)(H)3	122
C-(CT)(C)(H)2	123
C-(CT)(C)2(H)	124
C-(CB)(H)3	125
C-(CB)(C)(H)2	126
C-(CB)(C)2(H)	127
C-(CB)(C)3	128
C-(CB)(CH3)(H)2	129
C-(CB)(CH2CH3)(H	130
C-(CB)(CH3)2(H)	131
C-(CB)(CH3)(CH2C	132
CT-(H)	133
CT-(C)	134
CB-(H)	135
CB-(C)	136
Benzene Substitution	
ORTHO	145
META	146
Corrections for Ring Compounds	
Cyclopentane	147
Cyclopentene	148
Cyclopentadiene	149
Cyclohexane	150

Functional Group	Group Number
Corrections for Ring Compounds	
Cyclohexene	151
Cyclohexadiene	152
Oxygen-Containing Compounds	
CO-(O)(C)	165
CO-(C)(H)	172
O-(CO)(C)	178
O-(CO)(H)	179
C-(CO)(C)2(H)	199
C-(CO)(C)(H)2	200
C-(CO)(C)3	01
C-(CO)(H)3	202
C-(O)2(C)2	203
C-(O)2(C)(H)	204
C-(O)2(H)2	205
C-(O)(C)3	209
C-(O)(C)2(H)	210
C-(O)(C)(H)2	211
C-(O)(H)3	212
O-(C)(H)	400
O-(CO)(C)	402
O-(C)2 (nonring)	403
CO-(C)2	421
O-(C)2 (ring)	445
Corrections for Next-Nearest-Neighbor of Oxygen-Containing Groups Containing Groups	
O-(C)(H) (primary)	401
O-(C)2 (2-alkoxyethanol)	404
O-(C)2 (2-alkoxyethyl acetate)	405
NC1 (number of primary carbons of alpha carbons for group 403)	406
NC2 (number of secondary carbons of alpha carbons for group 403)	407
NC3 (number of third carbons of alpha carbons for group 403)	408
NCALPHA(>CH-) (number of alpha carbons with three-way branch for groups 403)	409
NCALPHA(>C<) (number of alpha carbons with four-way branch for groups 403)	410

Functional Group	Group Number
Corrections for Next-Nearest-Neighbor of Oxygen-Containing Groups Containing Groups	
O-(C)2 (noring structure -C-O-C-O-C-)	417
O-(C)2 (nonring structure -C-O-C-C-O-C-)	418
1,3-DIOXANE (6-member ring)	419
1,4-DIOXANE (6-member ring)	420
NC1 (number of primary carbons of alpha carbons for group 421)	422
NC2 (number of secondary carbons of alpha carbons for group 421)	423
NC3 (number of third carbons of alpha carbons for group 431)	424
NC4 (number of fourth carbons of alpha carbons for group 421)	425
NCALPHA(>CH-) (number of alpha carbons with three-way branch for groups 421)	426
NCALPHA(>C<) (number of alpha carbons with three-way branch for groups 421)	427
O-(C)2 (ring structure -C-O-C-O-C-)	446
O-(C)2 (ring structure -C-O-C-C-O-C-)	447
NCT (total number of carbons in compound for groups 404,417,418)	448
NCT (total number of carbons in compound for group 405)	449
O-(C)(H) (secondary)	450
Nitrogen-Containing Compounds	
C-(N)(H)3	229
C-(N)(C)(H)2	230
C-(N)(C)2(H)	231
C-(N)(C)3	232
C-(CN)(C)(H)2	506
C-(CN)(C)2(H)	507
C-(CN)(C)3	508
N-(C)3	428
N-(C)2(H)	429
N-(C)(H)2	432

Functional Group	Group Number
Corrections for Next-Nearest-Neighbor of Nitrogen-Containing Groups	
NCALPHA(>CH-) (number of alpha carbons with three-way branch for groups 428, 429)	430
NCALPHA(>C<) (number of alpha carbons with four-way branch for groups 428, 429)	431
NC1 (number of primary carbons of alpha carbons for group 429)	434
NC2 (number of seconadry carbons of alpha carbons for group 429)	435
NC1 (number of primary carbons of alpha carbons for group 428)	437
NC2 (number of primary carbons of alpha carbons for group 428)	438
N-(C)(H)2 (primary)	433
N-(C)(H)2 (secondary)	436
Organosulfur Groups	
C-(H)3(S)	340
C-(C)(H)2(S)	341
C-(C)2(H)(S)	342
C-(C)3(S)	343
C-(C)2(H)(S)	342
C-(C)3(S)	343
S-(C)(H)	349
S-(C)2	411
S-(S)(C)	439
Corrections for Next-Nearest-Neighbor of Organosulfur Groups	
NC1 (number of primary carbons of alpha carbons for group 411)	412
NC2 (number of secondary carbons of alpha carbons for group 411)	413
NC3 (number of third carbons of alpha carbons for group 411)	414
NCALPHA(>CH-) (number of alpha carbons with three-way branch for group 411)	415
NCALPHA(>C<) (number of alpha carbons with four-way branch for group 411)	416
NC1 (number of primary carbons of alpha carbon for group 439)	440
NC2 (number of secondary carbons of alpha carbon for group 439)	441

Functional Group	Group Number
Corrections for Next-Nearest-Neighbor of Organosulfur Groups	
NC3 (number of primary carbons of alpha carbon for group 439)	442
NCALPHA(>CH-) (number of alpha carbons with three-way branch for group 439)	451
NCALPHA(>C<) (number of alpha carbons with four-way branch for group 439)	452
Halogen Compounds	
C-(C)(BR)(H)2	500
C-(C)2(BR)(H)	501
C-(C)3(BR)	502
C-(C)(CL)(H)2	503
C-(C)2(CL)(H)	504
C-(C)3(CL)	505
Silicon Groups	
SI-(C)(H)3	601
SI-(C)2(H)2	602
SI-(C)3(H)	603
SI-(C)4	604
SI-(SI)(H)3	605
SI-(SI)2(H)2	606
SI-(SI)2(C)2	607
SI-(SI)(C)3	608
SI-(SI)4	609
C-(SI)(C)(H)2	610
C-(SI)(C)2(H)	611
C-(SI)(H)3	612
SI-(C)(CL)3	613
SI-(C)2(CL)2	614
SI-(C)3(CL)	615
SI-(C)(F)3	616
SI-(C)3(BR)	617
SI-(C)(H)(CL)2	618
SI-(C)2(H)(CL)	619
SI-(O)3(CL)	620
SI-(SI)(F)3	621
SI-(SI)2(F)2	622
SI-(SI)(CL)3	623
SI-(C)(O)3	624

Functional Group	Group Number
Silicon Groups	
SI-(C)2(O)2	625
SI-(C)3(O)	626
SI-(O)4	627
O-(SI)2	628
O-(SI)(C)	629
O-(SI)(H)	630
CB-(SI)	631
C-(SI)2(H)2	632
SI-(CB)2(CL)2	633
Corrections for Silicon Ring	
SI (4-member)	443
SI (5-member)	444
Boron Groups	
B-(B)(N)2	650
B-(B)(O)2	651
B-(B)(CL)2	652
B-(B)(C)2	653
B-(N)3	654
B-(N)2(F)	655
B-(N)2(CL)	656
B-(N)2(H)	657
B-(N)(CL)2	658
B-(N)(C)2	659
B-(O)3	660
B-(O)2(CL)	661
B-(O)2(C)	662
B-(O)(CL)2	663
B-(O)(N)(C)	664
B-(O)(C)2	665
B-(S)3	666
B-(CB)(CL)2	667
B-(CB)(BR)2	668
B-(CB)2(CL)	669
B-(C)(CL)2	671
B-(C)2(CL)	672
B-(C)(BR)2	673
B-(C)2(BR)	674
B-(C)2(I)	675

Functional Group	Group Number
Boron Groups	
B-(C)3	676
N-(B)(C)(H)	677
N-(B)(C)2	678
O-(B)(H)	679
O-(B)(C)	680
S-(B)(C)	681
CB-(B)	682
CD-(B)(H)	683
C-(B)(H)3	684
C-(B)(C)(H)2	685
C-(B)(C)2(H)	686
Aluminum Groups	
AL-(C)2(O)	687
AL-(C)2(CL)	688
AL-(C)2H	689
AL-(C)3	690
O-(AL)(C)	691
C-(AL)(H)3	692
C-(AL)(C)(H)2	693
Gallium Groups	
GA-(C)3	694
C-(H)3(GA)	695
C-(C)(H)2(GA)	696
Cadmium Groups	
Cd-(C)2	697
C-(H)3(Cd)	698
C-(C)(H)2(Cd)	699
Zinc Groups	
ZN-(C)2	700
C-(H)3(ZN)	701
C-(C)(H)2(ZN)	702
Mercury Groups	
HG-(C)2	703
C-(H)3(HG)	704
C-(C)(H)2(HG)	705
C-(C)2(H)(HG)	706

Functional Group	Group Number
Germanium Groups	
GE-(C)3(GE)	707
GE-(N)(C)3	708
GE-(O)(C)3	709
GE-(C)4	710
O-(GE)2	711
N-(C)2(GE)	712
C-(H)3(GE)	713
C-(C)(H)2(GE)	714
Tin Groups	
SN-(C)3(SN)	715
SN-(C)3(N)	716
SN-(C)3(O)	717
SN-(C)(CL)3	718
SN-(C)2(CL)2	719
SN-(C)3(CL)	720
SN-(C)3(BR)	721
SN-(C)3(I)	722
SN-(C)3(CB)	723
SN-(C)3(CD)	724
SN-(CD)4	725
SN-(C)4	726
N-(SN)(C)2	727
O-(SN)2	728
CB-(SN)	729
CD-(H)(SN)	730
C-(CB)(H)2(SN)	731
C-(H)3(SN)	732
C-(C)(H)2(SN)	733
C-(C)2(H)(SN)	734
C-(C)3(SN)	735
Lead Groups	
PB-(C)4	736
C-(H)3(PB)	737
C-(C)(H)2(PB)	738

Functional Group	Group Number
Phosphorus Groups	
P-(C)3	739
C-(H)3(P)	740
C-(C)(H)2(P)	741
Arsenic Groups	
AS-(C)3	742
C-(H)3(AS)	743
C-(C)(H)2(AS)	744
Antimony Groups	
SB-(C)3	745
C-(H)3(SB)	746
C-(C)(H)2(SB)	747
Bismuth Groups	
BI-(C)3	748
C-(H)3(BI)	749
C-(C)(H)2(BI)	750

Table 3.4 Fedors Method Functional Groups

Functional Group	Group Number
Carbon Increments	
-CH3	100
>CH2	101
>CH [14]	102
>C<	103
=CH2	104
=CH-	105
=C<	106
=C=	107
≡CH	108
≡C-	109
Oxygen Increments	
-COOH (acid)	110
-CO-O-CO- (anhydride)	111
-COO- (ester)	112
-O-OC-CO-O- (oxalate)	113
>C=O	114
-O-	115
-O- (aromatic)	116

Functional Group	Group Number
Oxygen Increments	
-OH (alcohols)	117
-OH (aromatic)	118
O=CH- (aldehyde)	119
Nitrogen Increments	
-NH2	120
-NH2 (aromatic)	121
>NH	122
>NH (aromatic)	123
>N-	124
>N- (aromatic)	125
-N=	126
-CN	127
-CN (aromatic)	128
Sulfur Increments	
-SH	129
-S-	130
-S-S-	131
Halogen Increments	
-F [15]	132
-F (disubstituted)	133
-F (trisubstituted)	134
-F (aromatic)	135
-F (perfluoro)	136
-CL	137
-CL (disubstituted)	138
-CL (trisubstituted)	139
-BR	140
-I	141
-I (aromatic)	142
Corrections for Ring Compounds	
3-Member	143
4-Member	144
5-Member	145
6-Member	146
Heteroatom in the ring	147
Substitution on carbon in a double bond (nonaromatic)	148

Functional Group	Group Number
Corrections for Ring Compounds	
Orthosubstitution in a benzene ring	149
Ring-Ring attached	150
Other corrections	
Conjugation, per double bond	151
Other Increments	
Adjacent pairs of >CH-	152
-F (C=C)	153
Silicon	
>SI<	154
>SI< (Siloxane)	155
>SI< (Siloxane, ring)	156

Table 3.4A Gani Method Functional Groups

The First-Order Groups

Functional Group	Group Number
Nonring Increments	
-CH3	1015
>CH2	1010
>CH-	1005
>C<	1000
-CH=CH2	1070
-CH=CH-	1065
>C=CH2	1060
-CH=C<	1055
>C=C<	1050
CH2=C=CH	4995
-C#CH (alkine)	2655
-C#C (alkine)	2650
Benzene Ring Increments	
-ACH=	1105
>AC=	1100
CH3-AC	1160
-CH2-AC	1155
>CH-AC	1150

Functional Group	Group Number
Oxygen Increments	
-OH (alcohol)	1200
HO-AC (phenol)	1350
CH3-CO-(C)	1405
-CH2-CO-(C)	1400
O=CH- (aldehyde)	1450
CH3-COO-(C) (ester)	1505
-CH2-COO-(C) (ester)	1500
HCOO-(C) (formate)	1550
CH3-O-(C) (nonring)	1615
-CH2-O-(C) (nonring)	1610
>CH-O-(C) (nonring)	1605
-CH2-O-(C) (ring)	1600
-COOH (acid)	1955
-COO- (ester)	3300
-OC2H3OH-	3605
-O(CH2)2OH	3600
Nitrogen Increments	
-CH2-NH2	1655
>CH-NH2	1650
CH3-NH-	1710
-CH2-NH-	1705
>CH-NH-	1700
CH3-N<	1755
-CH2-N<	1750
NH2-AC (benzene ring)	1800
C5H4N- (pyridine ring)	1855
C5H3N< (pyridine ring)	1850
-CH2-C#N (nitrile)	1900
-CH2-NO2	2255
>CH-NO2	2250
NO2-AC (benzene ring)	2300
-CONH2	3550
-CONHCH3	3555
-CONHCH2-	3560
-CON(CH3)2	3565
-CONCH3CH2-	3570
-CON(CH2)2<	3575
HCON(CH2)2	4996

Functional Group	Group Number
Halogen Increments	
-CH2-CL	2010
>CH-CL	2005
->C-CL	2000
-CH<CL2	2055
>C-CL2	2050
-CCL3	2100
CL-AC (benzene ring)	2200
-I	2550
-BR	2600
CL-(C=C)	2800
F-AC (benzene ring)	2850
-CF3	2960
>CF2	2955
>C<F	2950
-CCL2F	3505
-HCCLF	3515
-CCLF2	3520
-F (except as above)	3535
Sulfur Increments	
-CH2-SH	2400
CH3S-	3650
-CH2S-	3655
>CHS-	3660
-C4H3S	3755
>C4H2S	3760

Second-Order Groups Corrections

Functional Group	Group Number
Nonring Corrections	
(CH3)2CH-	5000
(CH3)3C-	5005
-CH(CH3)CH(CH3)-	5010
-CH(CH3)C(CH3)<	5015
-C(CH3)2C(CH3)2-	5020
CH3CH3	5050
>C=C-C=C<	5090
-CH=C-C=C<	5095
CH2=C-C=C	5100

Functional Group	Group Number
Nonring Corrections	
C=CH-C=C	5105
CH=CH-C=C	5110
CH2=CH-C=C	5115
CH=C-C=CH	5120
CH=C-C=CH2	5125
CH2=C-C=CH2	5130
CH2=CH-C=CH2	5135
CH2=CH-C=CH	5140
CH2=CH-CH=CH2	5145
CH3-C=C	5150
CH3-CH=C	5155
CH3-CH=CH	5160
CH3-CH=CH2	5165
CH3-C=CH	5170
CH3-C=CH2	5175
CH2-C=C	5180
CH2-CH=C	5185
CH2-CH=CH	5190
CH2-CH=CH2	5195
CH2-C=CH	5200
CH2-C=CH2	5205
CH-C=C	5210
CH-CH=C	5215
CH-CH=CH	5220
CH-CH=CH2	5225
CH-C=CH	5230
CH-C=CH2	5235
C-C=C	5240
C-CH=C	5245
C-C=CH	5250
C-C=CH2	5255
C-CH=CH	5260
C-CH=CH2	5265
c-C-CMH2:(M>1)	5310

Functional Group	Group Number
Ring Corrections	
3-Member	5025
4-Member	5030
5-Member	5035
6-Member	5040
7-Member	5045
Oxygen Corrections	
CHCHO	5055
CCHO	5060
CH3COCH2	5065
CH3COCH	5070
CH3COC	5075
c-C=O	5080
ACCHO (benzene ring)	5085
CHCOOH	5270
CCOOH	5275
ACCOOH (benzene ring)	5280
CH3COOCH	5285
CH3COOC<-	5290
COCH2COO-	5295
COCHCOO	5300
COCCOO	5305
CO-O-CO	5315
ACCOO (benzene ring)	5320
CHOH	5325
COH	5330
C(OH)C(OH)	5335
CH(OH)C(OH)	5340
CH2(OH)C(OH)	5345
CH(OH)CH(OH)	5350
CH2(OH)CH(OH)	5355
CH2(OH)CH2(OH)	5360
c-COH	5365
c-CHOH	5370
C-O-C=C	5490
CH-O-C=C	5495
CH2-O-C=C	5500
C-O-CH=C	5505
C-O-C=CH	5510

Functional Group	Group Number
Oxygen Corrections	
C-O-C=CH2	5515
CH-O-CH=CH	5520
CH-O-CH=CH2	5525
CH-O-C=CH	5530
CH-O-C=CH2	5535
CH2-O-C=C	5440
CH2-O-CH=C	5545
CH2-O-CH=CH	5550
CH2-O-CH=CH2	5555
AC-O-C (benzene ring)	5560
AC-O-CH (benzene ring)	5565
AC-O-CH2 (benzene ring)	5570
AC-O-CH3 (benzene ring)	5575
Nitrogen Corrections	
C(OH)CN	5375
CH(OH)-CN	5380
CH(OH)-CNH	5385
CH2(OH)-CN	5390
CH(OH)-CNH	5395
CH(OH)-CNH2	5400
CH2(OH)-CNH	5405
CH2(OH)-CHNH2	5410
CH(OH)-CHNH	5415
CH(OH)-CH2NH2	5420
CH2(OH)-CHNH	5425
CH2(OH)-CH2NH2	5430
C(NH2)-C(NH2)	5435
CH(NH2)-C(NH2)	5440
CH2(NH2)-C(NH2)	5445
CH(NH2)-CH(NH2)	5450
CH(NH2)-CH2(NH2)	5455
CH2(NH2)-CH2(NH2	5460
c-C-N-c-C	5465
c-CH-N-c-C	5470
c-CH-N-c-CH	5475
c-CH-NH-c-C	5480
c-CH-NH-c-CH	5485
C(NH2)-COOH	5705

Functional Group	Group Number
Nitrogen Corrections	
CH(NH2)-COOH	5710
CH2(NH2)-COOH	5715
Sulfur Corrections	
c-C-S-c-C	5580
c-CH-S-c-C	5585
c-CH2-S-c-C	5590
c-CH2-S-c-CH	5595
c-CH2-S-c-CH2	5600
Halogen Corrections	
C=CF	5605
CH=CF	5610
CH2=CF	5615
C=CHF	5620
CH=CHF	5625
CH2=CHF	5630
C=CBr	5635
CH=CBr	5640
CH2=CBr	5645
C=CHBr	5650
CH=CHBr	5655
CH2=CHBr	5660
C=CI	5665
CH=CI	5670
CH2=CI	5675
C=CHI	5680
CH=CHI	5685
CH2=CHI	5690
ACBr (benzene ring)	5695
ACI (benzene ring)	5700

Table 3.5 Joback Method Functional Groups

Functional Group	Group Number
Nonring Increments	
-CH3	100
>CH2	101
>CH-	102
>C<	103
=CH2	104

Functional Group	Group Number
Nonring Increments	
=CH-	105
=C<	106
=C=	107
≡CH	108
≡C-	109
Ring Increments	
>CH2	110
>CH-	111
>C<	112
=CH-	113
=C<	114
Halogen Increments	
-F-	115
-CL	116
-BR	117
-I	118
Oxygen Increments	
-OH (alcohols)	119
-OH (phenols)	120
-O- (nonring)	121
-O- (ring)	122
>C=O (nonring)	123
>C=O (ring)	124
O=CH- (aldehyde)	125
-COOH (acid)	126
-COO- (ester)	127
=O (except as above)	128
Nitrogen Increments	
-NH2	129
>NH (nonring	130
>NH (ring)	131
>N- (nonring)	132
-CN	133
-NO2	134
-N= (nonring) [16]	135
-N= (ring)	136
=NH	137

Functional Group	Group Number
Sulfur Increments	
-SH	138
-S- (nonring)	139
-S- (ring)	140

Table 3.6 Le Bas Method Functional Groups

Functional Group	Group Number
Carbon	100
Hydrogen	101
Oxygen (except as follows)	102
In methyl esters and ethers	103
In ethyl esters and ethers	104
In higher esters and ethers	105
In acids	106
Joined to S, or N	107
=NH, =N-	108
-NH2	109
>NH	110
-F	111
-CL	112
-BR	113
-I	114
S	115
Corrections for Ring Compounds	
3-Member	116
4-Member	117
5-Member	118
6-Member	119
Naphthalene	120
Anthracene	121

Table 3.6A Li-Ma Method Functional Groups

Functional Group	Group Number
Sulfur Increments	
>SO4	100
>SO3	101
-SO2CL	102
-CSO-	103
>S=O	104
-N=C=S	105

Functional Group	Group Number
Sulfur Increments	
-S-S-	106
-S- (ring)	107
-S- (connect benzene ring)	108
-S- (connect ring)	109
-S- (nonring)	110
-SH (connect benzene ring)	111
-SH (connect ring)	112
-SH	113
Nitrogen Increments	
-NO2 (connect benzene ring)	114
-N=C=O (connect benzene ring)	115
-NO3	116
-NO2	117
=N-OH	118
>N-N=O	119
-HN-CHO	120
>N-CHO	121
-CO-NH2	122
-CO-N<	123
>N-OH	124
-O-NH-	125
-NH-NH2	126
>N-NH2	127
-NH-NH-	128
>N-NH-	129
-C#N (connect ring)	130
-C#N	131
=N- (naphthalene ring)	132
=N- (benzene ring)	133
-NH- (ring)	134
>N- (ring)	135
-NH2 (connect benzene ring)	136
-NH- (connect benzene ring)	137
>N- (connect benzene ring)	138
-NH2 (connect ring)	139
-NH- (connect ring)	140
-NH2	141
-NH-	142

Functional Group	Group Number
Nitrogen Increments	
>N-	143
Oxygen Increments	
-COOH (acid)	144
-COO- (carbon atom connects benzene ring)	145
-COO- (oxygen atom connects benzene ring)	146
-COO- (carbon atom connects ring)	147
-COO- (carbon atom connects ring)	148
-COO- (ester)	149
HCOO- (formate)	150
>C=O (connect benzene ring)	151
>C=O (ring)	152
>C=O (nonring)	153
-CHO (connect benzene ring)	154
-CHO	155
-O- (ring)	156
-O- (connect benzene ring)	157
-O- (nonring)	158
-OH (connect naphthalene ring)	159
-OH (connect benzene ring)	160
-OH (connect ring)	161
-OH	162
Halogen Increments	
=CF- (benzene ring)	165
=CCL- (benzene ring)	166
=CBR- (benzene ring)	167
=CI- (benzene ring)	168
=CFCL	175
=CF2	176
=CF-	177
=CCL2	178
=CCL-	179
=CHCL	180
=CHBR	181
-CF2- (ring)	188
>CF- (ring)	189
-CFH- (ring)	190
-CHCL- (ring)	191
-CHBR- (ring)	192

Functional Group	Group Number
Halogen Increments	
-CHI- (ring)	193
-BR (connect naphthalene ring)	197
-CF3 (connect benzene ring)	198
-CF3 (connect ring)	199
-CF2- (connect ring)	200
-CF2CL	211
-CFCL2	212
-CHFCL	213
-CFCL-	214
-CF2BR	215
-CHCLBR	216
-CF3	217
-CF2-	218
>CF-	219
-CHF2	220
-CH2F	221
-CCL3	222
>CCL-	223
-CHCL2	224
-CH2CL	225
-CHCL-	226
>CBR-	227
-CHBR2	228
-CH2BR	229
-CHBR-	230
>CI-	231
-CH2I	232
-CHI-	233
Nonring Increments	
#CH	163
#C-	164
=CH- (connect benzene ring)	182
=CH- (connect ring)	183
=C=	184
=CH2	185
=CH-	186
=C<	187
-CH3 (connect naphthalene ring)	201

Functional Group	Group Number
Nonring Increments	
-CH2- (connect naphthalene ring)	202
-CH3 (connect benzene ring)	203
-CH2- (connect benzene ring)	204
>CH- (connect benzene ring)	205
>C< (connect benzene ring)	206
-CH3 (connect ring)	207
-CH2- (connect ring)	208
>CH- (connect ring)	209
>C< (connect ring)	210
-CH3	234
-CH2-	235
>CH-	236
>C<	237
Ring Increments	
=CH- (naphthalene ring)	169
=C< (naphthalene ring)	170
=CH- (benzene ring)	171
=C< (benzene ring)	172
=CH- (ring)	173
=C< (ring)	174
-CH2- (ring)	194
>CH- (ring)	195
>C< (ring)	196

Table 3.7 Lydersen Method Functional Groups

Functional Group	Group Number
Nonring Increments	
-CH3	100
>CH2	101
>CH-	102
>C<	103
=CH2	104
=CH-	105
=C<	106
=C=	107
≡CH	108
≡C-	109

Functional Group	Group Number
Ring Increments	
>CH2	110
>CH-	111
>CH [17]	112
>C<	113
=CH-	114
=C<	115
=C=	116
Halogen Increments	
-F-	117
-CL	118
-BR	119
-I	120
Oxygen Increments	
-OH (alcohols)	121
-OH (phenols)	122
-O- (nonring)	123
-O- (ring)	124
>C=O (nonring)	125
>C=O (ring)	126
O=CH- (aldehyde)	127
-COOH (acid)	128
-COO- (ester)	129
=O (except as above)	130
Nitrogen Increments	
-NH2	131
>NH (nonring)	132
>NH (ring)	133
>N- (nonring)	134
>N- (ring)	135
-CN	136
-NO2	137
Sulfur Increments	
-SH	138
-S- (nonring)	139
-S- (ring)	140
=S	141

Functional Group	Group Number
Other Increments	
>SI< [18]	142
>B- [19]	143
>SIH-	144
>SIH3	145
-SI-O-	146
-SI-O- (ring)	147

Table 3.7A Mostafa Method Functional Groups

Cations	Group Number
Ac+3	1001
Ag+1	1002
Ag+2	1003
Al+3	1005
Am+3	1007
Am+4	1008
As+3	1011
As+5	1012
Au+1	1017
Au+3	1018
B+3	1019
Ba+2	1020
Be+2	1022
Bi+3	1023
Bi+5	1024
C+4	1030
Ca+2	1031
Cd+2	1033
Ce+3	1034
Ce+4	1035
Cl+1	1039
Cm+3	1043
Cm+4	1044
Co+2	1046
Co+3	1047
Co+4	1048
Cr+2	1050
Cr+3	1051
Cr+4	1052
Cr+6	1054

Cations	Group Number
Cs+1	1055
Cu+1	1056
Cu+2	1057
Dy+2	1059
Dy+3	1060
Er+3	1061
Eu+2	1064
Eu+3	1065
Fe+1	1066
Fe+2	1067
Fe+3	1068
Fe+4	1069
Fe+5	1070
Fe+6	1071
Ga+3	1076
Gd+3	1077
Ge+2	1078
Ge+4	1079
H+1	1080
Hf+2	1082
Hf+4	1084
Hg+1	1085
Hg+2	1086
Ho+3	1087
I+1	1088
I+5	1089
In+1	1091
In+2	1092
In+3	1093
Ir+3	1095
Ir+4	1096
K+1	1098
La+3	1101
Li+1	1102
Lu+3	1104
Mg+2	1108
Mn+2	1110
Mn+3	1111
Mn+4	1112
Mn+5	1113

Cations	Group Number
Mn+6	1114
Mn+7	1115
Mo+2	1117
Mo+3	1118
Mo+4	1119
Mo+5	1120
Mo+6	1121
N+3	1124
N+4	1125
Na+1	1127
Nb+3	1130
Nb+4	1131
Nb+5	1132
Nd+2	1133
Nd+3	1134
NH4+1	1136
Ni+2	1138
Ni+3	1139
Ni+4	1140
Np+3	1143
Np+4	1144
Np+6	1146
Os+3	1149
Os+4	1150
P+3	1154
P+4	1155
P+5	1156
Pa+4	1158
Pa+5	1159
Pb+2	1160
Pb+4	1161
Pd+2	1162
Pd+3	1163
Pd+4	1164
Po+2	1166
Po+4	1168
Pr+3	1170
Pr+4	1171
Pt+2	1172
Pt+3	1173

Cations	Group Number
Pt+4	1174
Pu+3	1177
Pu+4	1178
Pu+6	1180
Ra+2	1182
Rb+1	1183
Re+2	1185
Re+4	1187
Re+5	1188
Re+6	1189
Re+7	1190
Rh+3	1194
Ru+3	1199
Ru+4	1200
Ru+6	1202
S+4	1205
S+6	1206
Sb+3	1207
Sc+2	1209
Sc+3	1210
Se+4	1211
Se+5	1212
Se+6	1213
Si+4	1215
Sm+2	1216
Sm+3	1217
Sn+2	1218
Sn+4	1219
Sr+2	1220
Sr+4	1221
Ta+3	1223
Ta+4	1224
Ta+5	1225
Tb+3	1226
Tb+4	1227
Tc+4	1231
Tc+6	1233
Tc+7	1234
Te+4	1235
Te+6	1236

Cations	Group Number
Th+4	1238
Ti+2	1239
Ti+3	1240
Ti+4	1241
Tl+1	1242
Tl+3	1243
Tm+2	1244
Tm+3	1245
U+3	1246
U+4	1247
U+5	1248
U+6	1249
V+2	1251
V+3	1252
V+4	1253
V+5	1254
W+2	1256
W+4	1258
W+5	1259
W+6	1260
Y+3	1264
Yb+2	1265
Yb+3	1266
Zn+2	1267
Zr+2	1268
Zr+3	1269
Zr+4	1270
Br+1	1271
Co+6	1272
Ho+2	1274
Pd+1	1275
Pt+1	1276
Y+2	1277
B+5	1278
Gd+2	1279
F+1	1280
Ce+2	1281
La+2	1282
Pr+2	1283
Pu+2	1284

Cations	Group Number
Th+2	1286
Er+2	1287
CH2+2	1727

Anions	Group Number
As-3	1301
Br-1	1303
C-4	1304
Cl-1	1305
F-1	1309
I-1	1311
N-3	1315
O-1	1317
O-2	1318
P-3	1319
Re-1	1321
S-2	1323
Sb-3	1324
Se-2	1325
Te-2	1327
H-1	1330
Si-4	1334
BrO3-1	1601
BrO4-1	1602
CO3-2	1603
HCO3-1	1604
ClO2-1	1605
ClO3-1	1606
ClO4-1	1607
IO3-1	1608
IO4-1	1609
IO6-5	1610
NO2-1	1611
NO3-1	1612
OH-1	1613
PO2-1	1614
PO3-1	1615
PO4-3	1617
PO3-3	1616
P2O7-4	1618

Anions	Group Number
H2PO2-1	1619
SO3-2	1627
SO4-2	1628
S2O3-2	1629
S2O8-2	1633
S2O7-2	1634
S2O6-2	1635
S2O5-2	1636
S2O4-2	1637
S3O6-2	1638
S4O6-2	1639
N2O2-2	1641
S5O6-2	1640
N2O3-2	1642
HOCHOHCOO-1	1701
NH2CH2COO-1	1702
CONH2COO-1	1703
C2H3O2N2-1	1704
ClCHCHCl-2	1705
CH2OHCOO-1	1706
CCl3COO-1	1707
OCH2COO-2	1708
OCH2CH2-2	1709

Table 3.8 Ogata-Tsuchida Method Functional Groups

Functional Group	Group Number	Radical, R, showing deviations > 5K
RH [20]	100	Me, t-Bu
RCL	101	
RBR	102	
RI	103	
ROH	104	Me, t-Bu
MeOR	105	Me
EtOR	106	
ROR	107	Me, Hep
PhOR	108	
RONO2	109	
RSH	110	
RSMe	111	Me

Functional Group	Group Number	Radical, R, showing deviations > 5K
RSET	112	
RSR	113	Me, Hep
RNH2	114	
RNHMe	115	
RNHEt	116	
RNHPr	117	
RNMe2	118	Me
RNO2	119	Me, Et
HCOR	120	
MeCOR	121	
EtCOR	122	
RCN	123	
RCOCL	124	
HCOOR	125	
MeCOOR	126	
EtCOOR	127	
PhCOOR	128	
RCOOH	129	
RCOOMe	130	
RCOOEt	131	
RCOOPr	132	
RCOOPh	133	
(RCO)20	134	Hep
CLCH2COOR [20]	135	
CL2CHCOOR	136	
BRCH2COOR	137	
NCCH2COOR	138	
CH2=CHCOOR	139	

Radical Type	Group Number	Radical, R, showing deviations > 5K
METHYL	140	
ETHYL	141	
N-PROPYL	142	
ISOPROPYL	143	
N-BUTYL	144	
SEC-BUTYL	145	

Radical Type	Group Number	Radical, R, showing deviations > 5K
ISOBUTYL	146	
T-BUTYL	147	
N-AMYL	148	
ISOAMYL	149	
T-AMYL	150	
NEOPENTYL	151	
N-HEXYL	152	
ISOHEXYL	153	
N-HEPTYL	154	
N-OCTYL	155	
VINYL	156	
ALLYL	157	
2-BUTENYL	158	
PHENYL	159	

Table 3.9 Orrick-Erbar Method Functional Groups

Functional Group	Group Number
C	100
Special Corrections	
-C(R)3	101
C(R)4	102
Double bond (nonaromatic)	103
5-Member ring	104
6-Member ring	105
Aromatic ring	106
Ortho substitution	107
Meta substitution	108
Para substitution	109
-CL	110
-BR	111
-I	112
-OH	113
-COO- (ester)	114
-O-	115
>C=O	116
-COOH (acid)	117

Table 3.10 Parachor Method Functional Groups

Functional Group	Group Number
Carbon Increments	
-CH3	100
>CH2	101
>CH-	102
>C<	103
=CH2	104
=CH-	105
=C<	106
=C=	107
≡CH	108
≡C-	109
Halogen Increments	
F	110
-CL	111
-BR	112
-I	113
Oxygen Increments	
-OH (alcohol)	114
-O-	115
O=CH- (aldehyde)	116
-COOH (acid)	117
-COO- (ester)	118
=O (except as above)	119
Nitrogen and Sulfur Increments	
-NH2	120
>NH	121
>N-	122
-CN	123
-NO2 (nitrite)	124
S	125
Alkyl Groups	
CH3-CH(CH3)-	126
CH3-CH2-CH(CH3)-	127
CH3-CH2CH2-CH(CH3)-	128
CH3-CH(CH3)-CH2-	129
CH3-CH2-CH(C2H5)-	130
CH3-C(CH3)2-	131
CH3-CH2-C(CH3)2-	132

Functional Group	Group Number
Alkyl Groups	
CH3CH(CH3)-CH(CH3)-	133
CH3CH(CH3)-C(CH3)2-	134
C6H5-	135
Ketone Groups	
R1-(C=O)-R2 for R1+R2=2	136
R1-(C=O)-R2 for R1+R2=3	137
R1-(C=O)-R2 for R1+R2=4	138
R1-(C=O)-R2 for R1+R2=5	139
R1-(C=O)-R2 for R1+R2=6	140
R1-(C=O)-R2 for R1+R2=7	141
-NO3 (nitrate)	142
-CO(NH2)	143
N (except as above)	144
Corrections for Ring Compounds	
3-Member	145
4-Member	146
5-Member	147
6-Member	148

Table 3.11
Reichenberg Method Functional Groups

Functional Group	Group Number
Nonring Increments	
-CH3	100
>CH2	101
>CH-	102
>C<	103
=CH2	104
=CH-	105
=C<	106
ºCH	107
ºC-	108
Ring Increments	
>CH2	109
>CH-	110
>C<	111
=CH-	112
=C<	113

Functional Group	Group Number
Halogen Increments	
-F	114
-CL	115
-BR	116
Oxygen Increments	
-OH (alcohols)	117
-O- (nonring)	118
>C=O (nonring)	119
O=CH- (aldehyde)	120
-COOH (acid)	121
-COO- (ester)	122
Nitrogen Increments	
-NH2	123
>NH (nonring)	124
-N= (ring)	125
-CN	126
Other Increments	
-S- (ring)	127
HCOO- (formates)	128

Table 3.11A Ruzicka Method Functional Groups

Functional Group	Group Number
Hydrocarbon Groups	
C-(C)(H)3	100
C-(C)2(H)2	101
C-(C)3(H)	102
C-(C)4	103
CD-(H)2	104
CD-(C)(H)	105
CD-(C)2	106
CD-(CD)(H)	107
CD-(CD)(C)	108
CD-(CB)(H)	110
CD-(CB)(C)	111
C-(CD)(H)3	115
C-(CD)2(H)2	116
C-(CD)(C)3	118
C-(CD)(C)(H)2	119

Functional Group	Group Number
Hydrocarbon Groups	
C-(CD)(C)2(H)	120
C-(CT)(H)3	122
C-(CT)(C)(H)2	123
C-(CB)(CD)(H)2	124
C-(CB)(H)3	125
C-(CB)(C)(H)2	126
C-(CB)(C)2(H)	127
C-(CB)(C)3	128
C-(CB)2(H)2	129
C-(CB)3(H)	130
C-(CB)(N)(H)2	131
CT-(H)	132
CT-(C)	133
CT-(CB)	135
CB-(H)	136
CB-(C)	137
CB-(CD)	138
CB-(CT)	139
CB-(CB)	140
CA	141
CBF-(CB)2(CBF)	142
CBF-(CB)(CBF)2	143
CBF-(CBF)3	144
Corrections for Ring Compounds	
Cyclopropane	149
Cyclobutane	151
Cyclopentane	153
Cyclopentene	154
Cyclohexane	156
Cyclohexene	157
Cycloheptane	158
Cyclooctane	159
Cylcopentane with subtituting groups	500
Spiropentane	501
Indene	502
Cyclooctatetraene	503
Cyclooctadiene	504
Cyclooctene	505

Functional Group	Group Number
Corrections for Ring Compounds	
Cycloheptatriene	506
Cycloheptene	507
Cyclohexadiene	508
Indan	509
Tetralin	510
Hexadecahydropyrene	511
Tetradecahydrophonanthrene	512
Dodecahydrofluorene	513
Decahydronaphthalene	514
Hexahydroindan	515
Oxygen-Containing Compounds	
CO-(CO)(O)	162
CO-(O)(CD)	163
CO-(O)(CB)	164
CO-(O)(C)	165
CO-(O)(H)	166
CO-(CD)(H)	167
CO-(CD)(C)	168
CO-(CB)(C)	169
CO-(CB)(H)	170
CO-(C)2	171
CO-(C)(H)	172
O-(CO)(C)	178
O-(CO)(H)	179
O-(CB)2	185
O-(CB)(C)	186
O-(CB)(H)	187
O-(C)2	188
O-(C)(H)	189
CD-(CO)(C)	191
CD-(CO)(H)	192
CB-(CO)	196
CB-(O)	197
C-(CO)(C)2(H)	199
C-(CO)(C)(H)2	200
C-(CO)(C)3	201
C-(CO)(H)3	202
C-(O)2(C)2	203

Functional Group	Group Number
Oxygen-Containing Compounds	
C-(C)2(O)(H) (ester)	204
C-(O)2(H)2	205
C-(O)(CB)(H)2	206
C-(O)(C)3 (ester,ether)	207
C-(O)(CD)(H)2	208
C-(O)(C)3 (alcohol)	209
C-(O)(C)2(H) (alcohol)	210
C-(O)(C)(H)2	211
C-(O)(H)3	212
Strain and Ring Corrections for Oxygen-Containing Compounds	
Ethylene Oxide	215
Trimethylene Oxide	216
Tetrahydrofuran	217
Tetrahydropyran	218
1,3-Dioxane	219
Furan	222
Glycols	516
Diphenol	517
Nitrogen-Containing Compounds	
C-(N)(H)3	229
C-(N)(C)(H)2	230
C-(N)(C)2(H)	231
C-(N)(C)3	232
N-(C)(H)2	233
N-(C)2(H)	234
N-(C)3	235
N-(N)(H)2	236
N-(N)(C)(H)	237
N-(N)(C)2	238
N-(N)(CB)(H)	239
N-(CD)2(H) (ring)	241
NI-(CB)	242
N-(CB)(H)2	245
N-(CB)(C)(H)	246
N-(CB)(C)2	247
N-(CB)2(C)	248
CB-(N)	249

Functional Group	Group Number
Nitrogen-Containing Compounds	
C-(CN)(C)(H)2	260
C-(CN)(C)3	262
CD-(CN)(H)	264
CB-(CN)	268
C-(NO2)(C)(H)2	270
O-(NO2)(C)	275
CD-(H)(N)	348
CB-(NO2)	372
Ring Corrections for Nitrogen-Containing Compounds	
Pyrrole	109
Ethyleneimine	276
Pyrrolidine	278
Piperdine	279
Halogen Groups	
C-(F)3(C)	281
C-(F)2(BR)(C)	282
C-(F)(CL)2(C)	283
C-(F)2(C)2	284
C-(F)2(CL)(C)	287
C-(CL)3(C)	288
C-(CL)2(H)(C)	289
C-(CL)(H)2(C)	290
C-(CL)(H)(C)2	292
C-(BR)(H)2(C)	295
C-(BR)(H)(C)2	296
C-(I)(H)2(C)	298
CD-(F)2	308
CD-(CL)2	309
CD-(F)(CL)	311
CD-(H)(CL)	318
CB-(F)	325
CB-(CL)	326
CB-(BR)	327
CB-(I)	328
C-(CB)(F)3	329
C-(CB)(CL)(H)2	330
C-(CD)(CL)(H)2	331

Functional Group	Group Number
Organosulfur Groups	
C-(H)3(S)	340
C-(C)(H)2(S)	341
C-(C)2(H)(S)	342
C-(C)3(S)	343
CB-(S)	346
CD-(H)(S)	347
S-(C)(H)	349
S-(CB)(H)	350
S-(C)2	351
S-(CB)2	355
S-(S)(C)	356
S-(S)(CB)	357
S-(CD)2 (ring)	358
Ring Corrections for Sulfur-Containing Compounds	
Trimethylene Sulfide	393
Tetrahydrothiophene	394
Thiacyclohexane	395
Thiophene	399

UNIFAC Functional Groups

Tables 3.12 and 3.13 list the UNIFAC groups built into the Aspen Physical Property System. The group number and an example of group usage is provided for each group listed. Values of the van der Waals area and volume parameters (GMUFQ and GMUFR) are built in for all groups. The AC symbol in Table 3.12 denotes a carbon atom in an aromatic ring. The symbol FCH_2O denotes the $CH_2\text{-}O$ group in a furan ring.

An X in the L-L column of Table 3.12 indicates liquid-liquid group interaction parameters are available. A dash (–) indicates parameters are not available.

An X in the LBY column of Table 3.12 indicates that the functional group has been defined for the Lyngby modified UNIFAC model. A dash (–) indicates that the group cannot be used for this model. The DMD column is for the Dortmund modified UNIFAC model.

Table 3.13 lists six groups with liquid-liquid parameters, but no vapor-liquid parameters. The propanols are a special case. For the vapor-liquid option sets such as UNIFAC and UNIF-HOC, propanol is described by three CH_n groups and one *OH* group. For UNIF-LL, 1-propanol is described by the independent propanol group P1, and 2-propanol is described by the independent propanol group P2.

Table 3.12 UNIFAC Method Functional Groups

Main Group	Group	V-L	L-L	LBY [21]	DMD [22]	Group Number	Example Component	Example Component Constituent Groups
CHn	C	X	X	X	X	1000	2,2-Dimethylpropane	4 CH3, 1 C
	CH	X	X	X	X	1005	2-Methylpropane	3 CH3, 1 CH
	CH2	X	X	X	X	1010	Hexane	2 CH3, 4 CH2
	CH3	X	X	X	X	1015	Hexane	2 CH3, 4 CH2
	CH4	X	—	X	X	1020	Methane	1 CH4
c-CHn	c-C [23]	—	—	—	X	1025	1,1 - dimethyl cyclohexane	2 CH3, 5 c-CH2; 1 c-C
	c-CH	—	—	—	X	1030	methylcyclohexane	1 CH3, 5 c-CH2, 1 c-CH
	c-CH2	—	—	—	X	1035	cyclohexane	6 c-CH2
CHm=CHn	C=C	X	—	X	X	1050	2,3 - Dimethylbutene-2	4 CH3, 1 C=C
	CH=C	X	X	X	X	1055	2-Methyl-2-butene	3 CH3, 1 CH=C
	CH2=C	X	X	X	X	1060	2-Methyl-1-butene	2 CH3, 1 CH2, 1 CH2=C
	CH=CH	X	X	X	X	1065	2-Hexene	2 CH3, 2 CH2, 1 CH=CH
	CH2=CH	X	X	X	X	1070	1-Hexene	1 CH3, 3 CH2, 1 CH2=CH
	CH2=CH2	X	—	—	—	1075	Ethylene	1 CH2=CH2
ACHn	AC [24]	X	X	X	X	1100	Styrene	1 CH2=CH, 5 ACH, 1 AC
	ACH	X	X	X	X	1105	Benzene	6 ACH
ACCHn	ACCH	X	X	—	X	1150	Cumene	2 CH3, 5 ACH, 1 ACCH
	ACCH2	X	X	—	X	1155	Ethylbenzene	1 CH3, 5 ACH, 1 ACCH2
	ACCH3	X	X	—	X	1160	Toluene	5 ACH, 1 ACCH3
OH	OH (P) [25]	X	X	X	X	1200	1-Propanol	2 CH3, 1 CH2, 1 OH (P)
	OH (S)	—	—	—	X	1210	2-Propanol	2 CH3, 1 CH, 1 OH (S)
	OH (T)	—	—	—	X	1220	tert-Butanol	3 CH3, 1C, 1 OH (T)
CH3OH	—	X	—	X	X	1250	Methanol	1 CH3OH
H2O	—	X	X	X	X	1300	Water	1 H2O
ACOH	—	X	X	—	X	1350	Phenol	5 ACH, 1 ACOH
CHnCO	CH2CO	X	X	X	X	1400	3-Pentanone	2 CH3, 1 CH2, 1 CH2CO

Main Group	Group	V-L	L-L	LBY[21]	DMD[22]	Group Number	Example Component	Example Component Constituent Groups
	CH3CO	X	X	X	X	1405	2-Butanone	1 CH3, 1 CH2, 1 CH3CO
CHO	CHO	X	X	X	X	1450	Acetaldelhyde	1 CH3, 1 CHO
CHnCOO	CH2COO	X	X	X	X	1500	Butyl propanoate	2 CH3, 3 CH2, 1 CH2COO
	CH3COO	X	X	X	X	1505	Butyl acetate	1 CH3, 3CH2, 1 CH3COO
HCOO	—	X	—	—	X	1550	Ethyl formate	1 CH3, 1 CH2, 1 HCOO
CHnO	FCH2O [26]	X	X	X	—	1600	Tetrahydrofuran	3 CH2, 1 FCH2O
	CHO	X	X	X	X	1605	Diisopropyl ether	4 CH3, 1 CH, 1 CHO
	CH2O	X	X	X	X	1610	Diethyl ether	2 CH3, 1 CH2, 1 CH2O
	CH3O	X	X	X	X	1615	Dimethyl ether	1 CH3, 1 CH3O
c-CHnO	c-CH2O CH2 [23]	—	—	—	X	1620	Tetrahydrofuran	2 c-CH2, 1 c-CH2OCH2
	c-CH2O (CH2)[1]/2	—	—	—	X	1625	1,3 - dioxane	1 c-CH2, 2 c-CH2O(CH2)[1]/2
	c-(CH2)[1]/2 O(CH2)[1]/2	—	—	—	X	1630	1,3,5 - trioxane	3 c-(CH2)[1]/2O(CH2)[1]/2
CHnNH2	CHNH2	X	—	—	X	1650	Isopropylamine	2 CH3, 1 CHNH
	CH2NH2	X	—	—	X	1655	Propylamine	1 CH3, 1 CH2, 1 CH2NH2
	CH3NH2	X	—	—	X	1660	Methylamine	1 CH3NH2
	CNH2	X	—	—	X	1670	tert-butylamine	3 CH3, 1 CNH2
NH2	NH2	—	—	X	—	1680	Isopropylamine	2 CH3, 1 CH, 1 NH2
CHnNH	CHNH	X	—	X	X	1700	Diisopropylamine	4 CH3, 1 CH, 1 CHNH
	CH2NH	X	—	X	X	1705	Diethylamine	2 CH3, 1 CH2, 1 CH2NH
	CH3NH	X	—	X	X	1710	Dimethylamine	1 CH3, 1 CH3NH
ChnN	CH2N	X	—	X	X	1750	Triethylamine	3 CH3, 2 CH2, 1 CH2N
	CH3N	X	—	X	X	1755	Trimethylamine	2 CH3, 1 CH3N
ACNH2	—	X	X	X	X	1800	Aniline	5 ACH, 1 ACNH2
C5HnN	C5H3N	X	X	X	X	1850	2,3-Dimethylpyridine	2 CH3, 1 C5H3N
	C5H4N	X	X	X	X	1855	3-Methylpyridine	1 CH3, 1 C5H4N
	C5H5N	X	X	X	X	1860	Pyridine	1 C5H5N
CHnCN	CH2CN	X	X	X	X	1900	Propionitrile	1 CH3, 1 CH2CN
	CH3CN	X	X	X	X	1905	Acetonitrile	1 CH3CN
CHnOOH	HCOOH	X	X	—	X	1950	Formic acid	1 HCOOH
	COOH	X	X	X	X	1955	Acetic acid	1 CH3, 1 COOH

Main Group	Group	V-L	L-L	LBY[21]	DMD[22]	Group Number	Example Component	Example Component Constituent Groups
CHnCl	CCl	X	X	X	X	2000	2-Chloro-2-methylpropane	3 CH3, 1 CCl
	CHCl	X	X	X	X	2005	2-Chloropropane	2 CH3, 1 CHCl
	CH2Cl	X	X	X	X	2010	1-Chlorobutane	1 CH3, 2 CH2, 1 CH2Cl
CHnCl2	CCl2	X	X	X	X	2050	2,2-Dichloropropane	2 CH3, 1 Ccl2
	CHCl2	X	X	X	X	2055	1,1-Dichloroethane	1 CH3, 1 CHCl2
	CH2Cl2	X	X	X	X	2060	Dichloromethane	1 CH2Cl2
CHnCl3	CCl3	X	X	X	X	2100	1,1,1-Trichloroethane	1 CH3, 1 CCl3
	CHCl3	X	X	X	X	2105	Chloroform	1 CHCl3
CCl4	—	X	X	X	X	2150	Tetrachloromethane	1 CCl4
ACCl	—	X	X	—	X	2200	Chlorobenzene	5 ACH, 1 ACCl
CHnNO2	CHNO2	X	X	—	X	2250	2-Nitropropane	2 CH3, 1 CHNO2
	CH2NO2	X	X	—	X	2255	1-Nitropropane	1 CH3, 1 CH2, 1 CH2NO2
	CH3NO2	X	X	—	X	2260	Nitromethane	1 CH3NO2
ACNO2	—	X	X	—	X	2300	Nitrobenzene	5 ACH, 1 ACNO2
CS2	—	X	—	—	X	2350	Carbon-disulfide	1 CS2
CHnSH	CH2SH	X	—	—	X	2400	Ethanethiol	1 CH3, 1 CH2SH
	CH3SH	X	—	—	X	2405	Methanethiol	1 CH3SH
Furfural	—	X	X	—	X	2450	Furfural	1 Furfural
(CH2OH)2	(CH2OH)2	X	X	—	X	2500	1,2-Ethanediol	1 (CH2OH)2
I	—	X	—	—	X	2550	1-Iodoethane	1 CH3, 1 CH2, 1 I
Br	—	X	—	—	X	2600	1-Bromoethane	1 CH3, 1 CH2, 1 Br
CHn≡C	C≡C	X	—	—	X	2650	2-Hexyne	2 CH3, 2 CH2, 1 C≡C
	CH≡C	X	—	—	X	2655	1-Hexyne	1 CH3, 3 CH2, 1 CH≡C
	CH≡CH	X	—	—	—	2660	Acetylene	1 CH≡CH
DMSO	(CH3)2SO	X	X	—	X	2700	Dimethyl-Sulfoxide	1 DMSO
Acrylonitrile	—	X	—	—	X	2750	Acrylonitrile	1 Acrylonitrile
Cl(C=C)	—	X	—	—	X	2800	Trichloroethylene	1 CH=C, 3 Cl(C=C)
ACF	—	X	—	—	X	2850	Hexafluorobenzene	6 ACF
Dimethyl-formamide (DMF)	DMF-1	X	—	—	X	2900	Dimethylformamide	1 DMF-12 CH3, 1 DMF-2
	DMF-2	X	—	—	X	2905	Diethylformamide	
CFn	CF	X	—	—	X	2950	Perfluormethyl-cyclohexane	1 CH3, 5 CH2, 1 CF
	CF2	X	—	—	X	2955	Perfluorohexane	2 CF3, 4 CF2
	CF3	X	—	—	X	2960	Perfluorohexane	2 CF3, 4 CF2

Main Group	Group	V-L	L-L	LBY[21]	DMD[22]	Group Number	Example Component	Example Component Constituent Groups
COO	COO	X	—	—	X	3300	Dimethyl oxalate	2 CH3, 2 COO
SiH2	Si	X	—	—	—	3350	Hexamethyl disiloxane	6 CH3, 1 SiO, 1 Si
	SiH	X	—	—	—	3355	Heptamethyl trisiloxane	7 CH3, 2 SiO, 1 SiH
	SiH2	X	—	—	—	3360	Diethylsilane	2 CH3, 2 CH2, 1 SiH2
	SiH3	X	—	—	—	3365	Methylsilane	1 CH3, 1 SiH3
SiO	SiO	X	—	—	—	3400	Octamethyl cyclotetrasiloxane	8 CH3, 4 SiO
	SiHO	X	—	—	—	3405	1,1,3,3-Tetramethyl disiloxane	4 CH3, 1 SiHO, 1 SiH
	SiH2O	X	—	—	—	3410	1,3-Dimethyldisiloxane	2 CH3, 1 SiH2O, 1 SiH2
NMP	NMP	X	—	—	—	3450	N-methylpyrrolidone	1 NMP
CClF	CCl3F	X	—	—	—	3500	Trichloro fluoromethane	1 CCl3F
	CCl2F	X	—	—	—	3505	Tetrachloro-1,2-difluoroethane	2 CCl2F
	HCCl2F	X	—	—	—	3510	Dichloro fluoromethane	1 HCCl2F
	HCClF	X	—	—	—	3515	1-Chloro-1,2,2,2,-tetrafluoroethane	1 CF3, 1HCClF
	CClF2	X	—	—	—	3520	1,2 Dichloro tetrafluoroethane	2 HCClF2
	HCClF2	X	—	—	—	3525	Chloro difluoromethane	1 HCCl2F
	CClF3	X	—	—	—	3530	Chloro trifluoromethane	1 CClF3
	CCl2F2	X	—	—	—	3535	Dichloro difluoromethane	1 CCl2F2
CON	CONH2	X	—	—	—	3550	Acetamid	1 CH3, 1 CONH2
	CONHCH3	X	—	—	—	3555	N-Methylacetamid	1 CH3, 1 CONHCH3
	CONHCH2	X	—	—	—	3560	N-Ethylacetamid	2 CH3, 1 CONHCH2
	CON(CH3)2	X	—	—	—	3565	N,N-Dimethylacetamid	1 CH3, 1 CON(CH3)2
	CONCH3CH2	X	—	—	—	3570	N,N-Methylethyl acetamid	2 CH3, 1 CONCH3CH2
	CON(CH2)2	X	—	—	—	3575	N,N-Diethylacetamid	3 CH3, 1 CON(CH2)2
OCCOH	C2H5O2	X	—	—	—	3600	2-Ethoxyethanol	1 CH3, 1 CH2, 1 C2H5O2

Main Group	Group	V-L	L-L	LBY[21]	DMD[22]	Group Number	Example Component	Example Component Constituent Groups
	C2H4O2	X	—	—	—	3605	2-Ethoxy-1-propanol	2 CH3, 1 CH2, 1 C2H4O2
CH2S	CH3S	X	—	—	—	3650	Dimethylsulfide	1 CH3, 1 CH3S
	CH2S	X	—	—	—	3655	Diethylsulfide	2 CH3, 1 CH2, 1 CH2S
	CHS	X	—	—	—	3660	Diisopropylsulfide	4 CH3, 1 CH, 1 CHS
Morpholine	MORPH	X	—	—	—	3700	Morpholine	1 MORPH
Thiophene	C4H4S	X	—	—	—	3750	Thiophene	1 C4H4S
	C4H3S	X	—	—	—	3755	2 - Methylthiophene	1 CH3, 1 C4H3S
	C4H2S	X	—	—	—	3760	2,3 - Dimethylthiophene	2 CH3, 1 C4H2S
NH3 [27]	NH3	—	—	X	X	3800	Ammonia	1 NH3
H2 [27]	H2	—	—	X	X	3810	Hydrogen	1 H2
N2 [27]	N2	—	—	X	X	3820	Nitrogen	1 N2
O2 [27]	O2	—	—	X	X	3830	Oxygen	1 O2
CO [27]	CO	—	—	X	X	3840	Carbon monoxide	1 CO
CO2 [27]	CO2	—	—	X	X	3850	Carbon dioxide	1 CO2
H2S [27]	H2S	—	—	X	X	3860	Hydrogen sulfide	1 H2S
AR [27]	AR	—	—	X	X	3870	Argon	1 AR
C2H6 [28]	C2H6	—	—	X	—	3880	Ethane	1 C2H6
C3H6 [28]	C3H6	—	—	X	—	3890	Propylene	1 C3H6
C3H8 [28]	C3H8	—	—	X	—	3900	Propane	1 C3H8
C4H10 [28]	C4H10	—	—	X	—	3910	n-Butane	1 C4H10

Table 3.13 Special UNIFAC Liquid-Liquid Functional Groups

Main Group	Group	Group Number	Example Components	Example Component Constituent Groups
P1	P1	3000	1-Propanol	1 P1
P2	P2	3050	2-Propanol	1 P2
DEOH	(HOCH2CH2)2O	3100	Diethylene glycol	1 HOCH2CH2)2O
TCE	CCL2=CHCL	3150	Trichlorethylene	1 CCL2=CHCL
MFA	HCONHCH3	3200	Methylformamide	1 HCONHCH3
TMS	(CH2)4SO2	3250	Tetramethylene Sulfone (Sulfolane)	1 (CH2)4SO2

Table 3.14 Vapor-Liquid Systems UNIFAC Group Interaction Parameters

From H. K. Hansen, P. Rasmussen, Aa. Fredenslund, M. Schiller, and J. Gmehling, Ind. Eng. Chem. Res.30 (10), (1991), p. 2352.

MAIN GROUP	CCH=2	ACH2O	CH3OH	H2O	ACOH	CH2CO	CHO	CH2COO	HCOO	CH2O	CH2NH2	CH2NH	CH2N	ACNH2	C5H4N	CH2CN	COOH	CCL	CCL2	CCL3	CCL4	ACCL	CH2NO2	ACNO2	CS2	CH2SH	FURFURAL	(CH2OH)2	I	BR	CH#C	DMSO	ACRYLONI	CL(C=C)	ACF	DMF	CF2	COO	SIH2	SIO	NMP	CCLF	CON	OCCOH	CH4S	MORPHOLI	THIOPHEN
CH2																																															
C=C	X																																													
ACH	X	X																																												
ACCH2	X	X	X																																											
OH	X	X	X	X																																										
CH3OH	X	X	X	X	X																																									
H2O	X	X	X	X	X	X																																								
ACOH	X	X	X	X	X	X	X																																							
CH2CO	X	X	X	X	X	X	X																																							
CHO	X	X	X	X	X	X	X																																							
CH2COO	X	X	X	X	X	X	X	X																																						
HCOO	X	X	X	X	X	X	-	-	X	X																																				
CH2O	X	X	X	X	X	X	X	X	X	X	X																																			
CH2NH2	X	X	X	X	X	X	X	-	-	-	-	X																																		
CH2NH	X	X	X	X	X	X	X	-	X	-	X	-	X	X																																	
CH2N	X	X	X	X	X	X	X	-	X	-	X	-	X	X	X																																
ACNH2	X	X	X	X	X	X	X	-	X	X	X	-	X	-	-	X																															
C5H4N	X	X	X	X	X	X	X	-	-	X	X	-	-	X	-	X	X																														
CH2CN	X	X	X	X	X	X	X	-	X	-	X	-	X	X	X	X	X	X																													
COOH	X	X	X	X	X	X	X	X	X	X	X	-	-	X	X	-																															
CCL	X	X	X	X	X	X	X	-	X	-	X	X	-	X	X	-	X	-	X	X																											
CCL2	X	X	X	X	X	X	X	-	X	-	X	X	-	X	-	-	X	X	X	X	X	X																								
CCL3	X	X	X	X	X	X	X	-	X	-	X	X	X	X	-	-	X	-	X	X	X	X	X																							
CCL4	X	X	X	X	X	X	X	-	X	X	X	X	X	X	-	X	X	X	X	X	X	X	X	X																						
ACCL	X	X	X	X	X	X	X	-	X	X	X	X	X	X	-	X	X	X	X	X	X	X	X	X	X																					
CH2NO2	X	X	X	X	X	X	X	-	X	-	X	-	-	-	-	X	-	X	-	X	X																								
ACNO2	X	-	X	X	X	-	X	-	X	-	-	-	-	-	-	-	X	X	-	-	X	X	X																						
CS2	X	X	X	X	X	X	X	X	X	-	X	-	X	-	-	-	X	-	X	-	X	X	-	X	-																				
CH2SH	X	-	X	X	X	X	-	-	X	-	-	X	X	X	-	-	-	X	-	-	-	-	-	-	-																				
FURFURAL	X	X	X	X	X	-	X	-	X	-	X	-	-	-	-	-	X	-	-	X	X	-	-	-	-																				
(CH2OH)2	X	-	X	X	X	X	X	X	X	-	X	-	X	-	-	X	-	-	-	-	-	-	X	-	-	-																			
I	X	-	X	X	X	X	-	-	X	X	X	-	X	-	-	-	X	-	X	X	X	-	X	X	X	-	-																		
BR	X	X	X	X	X	X	-	-	X	-	X	-	-	-	X	X	X	X	-	X	X	-	X	X	-	-	-																		
CH#C	X	X	-	-	X	-	-	-	X	-	-	-	-	-	X	-	-	-	-	-	-	-	X	-	-	-	-	-																
DMSO	X	X	X	X	X	X	X	X	-	X	-	X	-	-	-	X	-	X	-	X	X	-	-	-	X	-	X	-	X															
ACRYLONI	X	X	X	X	X	X	X	-	-	X	X	-	-	-	-	X	-	-	-	X	-	-	-	X	-	-	-	-	-	-														
CL(C=C)	X	X	X	X	X	X	-	-	X	X	X	X	-	-	-	X	X	X	X	-	-	-	X	-	X	-	-	-	X	-	X													
ACF	X	X	X	X	X	X	-	-	-	-	X	-	X	X	-	X	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-													
DMF	X	X	X	X	X	X	X	-	X	X	X	X	X	-	X	-	X	-	X	X	-	-	-	X	-	-	X	-	X	-	X	X											
CF2	X	X	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	X									
COO	X	X	X	X	X	X	X	X	X	X	X	X	-	X	-	X	-	X	-	X	X	X	X	X	-	X	-	X	-	X	-	X	-	-									
SIH2	X	-	X	-	X	-	X	-	X	-	-	X	X	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-								
SIO	X	-	X	-	-	-	-	-	-	-	-	X	X	-	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X							
NMP	X	X	X	X	X	X	-	X	X	-	-	-	-	-	-	-	-	-	X	-	X	-	-	X	-	X	-	-	-	X	-	-	-	-	-	-	-						
CCLF	X	-	X	-	X	X	-	-	-	-	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	X	-	-	-	-					
CON	X	X	-	-	X	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-				
OCCOH	X	X	X	X	X	X	-	X	-	X	-	-	X	-	-	X	-	-	X	-	X	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
CH4S	X	X	-	-	-	X	-	-	-	-	-	-	-	X	-	-	X	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-		
MORPHOLI	X	X	X	X	X	X	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
THIOPHEN	X	-	X	X	X	-	X	X	-	-	-	-	-	-	-	-	-	-	-	X	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Table 3.15 Liquid-Liquid Systems UNIFAC Group Interaction Parameters

From T. Magnussen, P. Rasmussen, and Aa. Fredenslund, Ind. Eng. Chem.Process Des. Dev. 20, (1980), pp. 331–339.

MAIN GROUP	CH*	CH*=CH*	ACH*	ACCH*	H	H2O	ACOH	CH*CO	CHO	CH*COO	CH*O	ACNH2	C5H*N	CH*CN	CH*OOH	CH*CL	CH*CL2	CH*CL3	CCL4	ACCL	CH*NO2	ACNO2	FURFURAL	(CH2OH)2	DMSO	DMF	P1	P2	DEOH	TCE	MFA	TMS
CH*																																
CH*=CH*	X																															
ACH*	X	X																														
ACCH*	X	X	X																													
H	X	X	X	X																												
H2O	X	X	X	X	X																											
ACOH	X	-	X	X	X	X																										
CH*CO	X	X	X	X	X	X	X																									
CHO	X	X	X	X	X	X	-	X																								
CH*COO	X	X	X	X	X	X	X	X	X																							
CH*O	X	X	X	X	X	X	-	X	-	X																						
ACNH2	X	-	X	X	X	X	X	X	-	-	-																					
C5H*N	X	-	X	X	X	X	X	-	-	-	-	X																				
CH*CN	X	X	X	X	X	X	X	-	X	-	-	-	X																			
CH*OOH	X	X	X	X	X	X	X	-	X	X	X	X	-	-																		
CH*CL	X	X	X	X	X	X	X	-	X	X	-	X	-	-	-	X																
CH*CL2	X	X	-	-	X	X	X	-	X	-	X	X	-	-	-	X	X															
CH*CL3	X	X	X	X	X	X	X	-	X	-	X	X	X	X	X	X	-															
CCL4	X	X	X	X	X	X	X	X	X	-	X	X	-	X	X	X	X	X														
ACCL	X	-	X	X	X	X	X	-	X	-	X	-	-	X	X	X	-	-	X													
CH*NO2	X	X	X	X	X	X	X	-	X	-	-	X	-	-	-	X	-	-	-	X	X											
ACNO2	X	-	X	X	X	X	X	X	-	-	-	-	X	-	-	-	-	-	-	X	-	-										
FURFURAL	X	-	X	X	X	X	X	-	X	X	X	-	-	X	-	X	-	X	X	X	-	-	-									
(CH2OH)2	X	-	X	X	X	X	X	X	-	X	-	X	-	-	X	-	-	-	-	-	X	X	X	X								
DMSO	X	X	X	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-							
DMF	X	X	X	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	-	-							
P1	X	X	X	X	X	X	X	X	X	X	X	X	-	-	-	X	X	X	X	X	-	X	-	X	-	-	-					
P2	X	X	X	X	X	X	X	X	X	X	X	X	-	-	-	X	X	X	X	X	-	X	-	X	-	-	-	X				
DEOH	X	-	X	X	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
TCE	X	-	-	-	X	X	-	X	-	-	-	-	-	-	-	X	-	-	-	-	-	-	X	-	-	-	-	-	-	-		
MFA	X	X	X	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
TMS	X	X	X	X	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Table 3.16 Group Interaction Parameters for Lyngby Modified UNIFAC

From B. L. Larsen, P. Rasmussen, and Aa. Fredenslund, Ind. Eng. Chem. Res. 26, (1987), p. 2274.

MAIN GROUP	CH2 2	C=C 3	ACH 4	ACCH2 5	OH 6	CH3OH 7	H2O 8	ACOH 9	CH2CO 10	CHO 11	CH2COO 12	HCOO 13	CH2O 14	CH2NH2 15	NH2 16	CH2NH 17	CH2N 18	ACNH2 19	C5H4N 20	CH2CN 21	COOH 22	CCL 23	CCL2 24	CCL3 25	CCL4 26
CH2 2																									
C=C 3	X																								
ACH 4	X	X																							
ACCH2 5	X	X	X																						
OH 6	X	X	X	X																					
CH3OH 7	X	X	X	X	X																				
H2O 8	X	X	X	X	X	X																			
ACOH 9	X	X	X	X	X	X	X																		
CH2CO 10	X	X	X	X	X	X	X	X																	
CHO 11	X	X	X	X	X	X	-	X	X																
CH2COO 12	X	X	X	X	X	X	X	X	X	X															
HCOO 13	X	X	X	X	X	X	X	X	X	X	X														
CH2O 14	X	X	X	X	X	X	X	X	X	X	X	X													
CH2NH2 15	X	X	X	X	X	X	X	X	X	X	X	X	X												
NH2 16	X	X	X	X	X	X	X	X	-	-	-	X	-	X											
CH2NH 17	X	X	X	X	X	X	X	X	-	-	X	X	X	X	X										
CH2N 18	X	X	X	X	X	X	X	X	-	-	-	X	-	X	X	X									
ACNH2 19	X	-	X	X	X	X	X	X	X	-	-	X	-	X	-	-	-								
C5H4N 20	X	-	X	X	X	X	X	X	X	-	-	X	-	X	-	X	-	-							
CH2CN 21	X	X	X	X	X	X	X	X	X	-	X	X	-	X	-	-	-	X	X						
COOH 22	X	X	X	X	X	X	X	X	X	-	X	X	X	X	-	-	-	-	-	-					
CCL 23	X	X	X	X	X	X	X	X	X	X	-	X	X	X	X	-	-	-	-	-	-				
CCL2 24	X	X	X	X	X	X	X	X	X	-	X	X	X	X	-	-	X	-	X	-	-	X			
CCL3 25	X	X	X	X	X	X	X	X	X	-	X	X	X	X	-	-	X	-	X	X	-	X	X		
CCL4 26	X	X	X	X	X	X	X	X	X	-	X	X	X	X	X	X	X	X	X	X	-	X	X	X	

Table 3.17 Group Interaction Parameters for Dortmund Modified UNIFAC Model

From J. Gmehling, J. Li, and M. Schiller, Ind. Eng. Chem. Res. 32, (1993), pp. 178-193.

MAIN GROUP	CH2	C=C	ACH	ACCH2	OH	CH3OH	H2O	ACOH	CH2CO	CHO	CH2COO	HCOO	CH2O	CH2NH2	CH2NH	CH2N	ACNH2	C5H4N	CH2CN	COOH	CCL	CCL2	CCL3	CCL4	ACCL	CH2NO2	ACNO2	CS2	CH3SH	FURFURAL	(CH2OH)2	I	BR	CH#C	DMSO	ACRY	CL(C=C)	ACF	DMF	CF2	COO	CY-CH2	CY-CH2O	HCOOH	CHCL3
CH2																																													
C=C	X																																												
ACH	X	X																																											
ACCH2	X	X	X																																										
OH	X	X	X	X																																									
CH3OH	X	X	X	X	X																																								
H2O	X	X	X	X	X	X																																							
ACOH	X	X	X	X	X	X	X																																						
CH2CO	X	X	X	X	X	X	X	X																																					
CHO	X	X	X	X	X	X	X	-	X																																				
CH2COO	X	X	X	X	X	X	X	X	X	X																																			
HCOO	X	X	X	X	X	X	-	-	X	X	X																																		
CH2O	X	X	X	X	X	X	X	X	X	X	X	X																																	
CH2NH2	X	X	X	X	X	X	X	-	-	-	-	-	-																																
CH2NH	X	X	X	X	X	X	X	-	X	-	X	-	-	X																															
CH2N	X	X	X	X	X	X	X	-	X	-	X	-	-	X	X																														
ACNH2	X	X	X	X	X	X	X	-	X	X	X	-	-	-	-	-																													
C5H4N	X	X	X	X	X	X	X	-	-	X	X	-	-	-	X																														
CH2CN	X	X	X	X	X	X	X	-	X	-	X	X	X	X	X	X	-	X	X																										
COOH	X	X	X	X	X	X	X	X	X	X	X	-	X	-	-	X	-																												
CCL	X	X	X	X	X	X	X	-	X	X	X	-	X	-	-	X	-	X	X																										
CCL2	X	X	X	X	X	X	X	-	X	X	X	-	X	-	-	X	-	X	X	X																									
CCL3	X	X	X	X	X	X	-	-	X	-	X	-	-	X	-	-	-	-	-	X	X																							
CCL4	X	X	X	X	X	X	X	X	X	-	X	X	X	X	X	X	-	X	X	X	X	X																						
ACCL	X	X	X	X	X	X	X	X	X	-	X	X	X	X	X	X	-	X	X	X	X	X	-	X																				
CH2NO2	X	X	X	X	X	X	X	-	X	-	X	-	-	-	X	-	-	X	X	-	X	X	-	X	X																		
ACNO2	X	-	X	X	X	-	-	-	X	-	-	-	-	-	-	-	-	X	-	-	-	X	-	-	X	X																	
CS2	X	X	X	X	-	X	-	-	X	-	X	-	-	-	X	-	-	X	-	-	-	X	-	-	X	-	X																
CH3SH	X	-	X	-	-	X	-	-	X	X	-	X	X	X	-	-	-	X	-	-	-	-	-	-	-	-	-	-															
FURFURAL	X	X	X	X	X	X	X	-	X	X	X	-	X	-	-	-	-	-	-	-	-	X	X	-	X	-	-	-	-														
(CH2OH)2	X	-	X	X	X	X	X	X	-	X	-	-	-	-	X	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-													
I	X	-	X	X	X	X	-	-	X	X	X	-	-	-	-	-	-	X	-	X	-	X	-	X	-	X	-	-														
BR	X	X	X	X	X	X	X	-	X	-	X	-	-	-	X	X	-	X	X	X	X	X	X	-	-	-	-																
CH#C	X	X	-	-	X	-	-	-	X	-	-	-	-	-	X	-	-	-	-	-	-	X	-	-	-	-																	
DMSO	X	X	X	X	X	X	X	X	-	X	-	-	-	-	-	-	-	X	-	X	-	-	-	X	-	X	-																
ACRY	X	X	-	-	X	X	X	-	-	-	X	-	-	-	X	-	-	-	X	-	-	-	-	-	-	-	-	-															
CL(C=C)	X	X	X	X	X	X	-	-	X	X	X	-	-	-	X	X	X	X	X	-	X	-	X	-	X	-	-	-	-														
ACF	X	X	X	X	X	X	-	-	-	-	X	-	X	-	X	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-													
DMF	X	X	X	X	X	X	X	-	X	X	-	X	-	X	-	X	-	X	-	X	-	-	-	X	-	-	X	-	X	-	-												
CF2	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-												
COO	X	X	X	X	X	X	X	-	X	-	X	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	X	-	-	X	-	-										
CY-CH2	X	X	X	X	X	X	X	X	X	X	X	-	X	X	X	X	-	X	X	-	X	X	X	X	X	-	-	X	-	-	X	X	X	X								
CY-CH2O	X	X	X	X	X	X	X	-	X	-	X	X	-	-	X	X	-	X	X	-	X	X	-	X	-	-	-	X	-	-	X	X	X	-	-							
HCOOH	X	-	X	X	-	-	X	-	-	-	X	X	X	-	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-							
CHCL3	X	X	X	X	X	X	X	-	X	-	X	X	-	-	X	-	-	X	-	X	X	X	-	X	-	-	X	-	-	-	X	-	-	-	-	-						

Table 3.18 Group Interaction Parameters for UNIFAC Model Revision 3

From E. A. Macedo, U. Weidlich, J. Gmehling, and P. Rasmussen, Ind. Eng. Chem. Process Des. Dev., 22, (1983), p. 676.

MAIN GROUP	CH2	C=C	ACH	ACCH2	OH	CH3OH	H2O	ACOH	CH2CO	CHO	CH2COO	HCOO	CH2O	CH2NH2	CH2NH	CH2N	ACNH2	C5H4N	CH2CN	COOH	CCL	CCL2	CCL3	CCL4	ACCL	CH2NO2	ACNO2	CS2	CH2SH	FURFURAL	(CH2OH)2	I	BR	CH#C	DMSO	ACRYLONI	CL(C=C)	ACF	DMF	CF2	COO
CH2																																										
C=C	X																																									
ACH	X	X																																								
ACCH2	X	X	X																																							
OH	X	X	X	X																																						
CH3OH	X	X	X	X	X																																				
H2O	X	X	X	X	X	X																																			
ACOH	X	X	X	X	X	X	X																																		
CH2CO	X	X	X	X	X	X	X	X																																	
CHO	X	-	-	-	X	X	X	-	X																																
CH2COO	X	X	X	X	X	X	X	X	X	-																															
HCOO	X	X	-	-	X	X	-	-	-	-	X																														
CH2O	X	X	X	X	X	X	X	-	X	X	X	-																													
CH2NH2	X	X	X	-	X	X	X	-	-	-	-	-	-																												
CH2NH	X	X	X	X	X	X	X	-	-	-	X	-	X	X																												
CH2N	X	X	X	X	X	X	X	-	-	-	-	-	-	X	X																											
ACNH2	X	-	X	X	X	X	X	-	X	-	-	-	-	-	-	-																										
C5H4N	X	-	X	X	X	X	X	X	X	-	-	-	-	-	-	-	-																									
CH2CN	X	X	X	X	X	X	X	-	X	-	X	-	-	-	-	-	X	X																								
COOH	X	X	X	X	X	X	X	-	X	-	X	X	X	-	-	-	X	-																								
CCL	X	X	X	X	X	X	X	-	X	X	-	-	X	-	-	-	-	-	-	X																						
CCL2	X	X	X	-	X	X	X	-	X	-	X	-	X	-	-	X	-	X	-	X	X																					
CCL3	X	X	X	X	X	X	X	-	X	-	X	X	X	-	-	X	-	X	X	X	X	X																				
CCL4	X	X	X	X	X	X	X	X	X	-	X	-	X	X	X	X	X	X	X	X	X	X	X																			
ACCL	X	X	X	X	X	X	X	-	X	-	X	-	-	X	X	X	X	-	X	-	-	X																				
CH2NO2	X	X	X	X	X	X	X	-	X	-	-	-	X	-	-	-	-	-	-	-	-	X	X																			
ACNO2	X	-	X	X	X	-	X	-	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-	X	-	X															
CS2	X	X	X	X	X	X	X	-	X	-	X	-	X	-	-	-	-	-	X	-	X	-	X	X	-	-	-														
CH2SH	X	-	X	-	X	X	-	-	X	-	-	X	X	X	-	-	-	-	X	-	X	-	-	-	-	-	-	-													
FURFURAL	X	-	X	X	X	-	X	-	X	-	X	-	-	-	-	-	-	-	-	-	-	X	X	-	-	-	-	-	-												
(CH2OH)2	X	-	X	X	X	-	X	X	-	-	X	-	X	-	-	-	X	-	-	-	-	-	-	X	-	-	-	-													
I	X	-	X	-	X	-	-	-	X	-	X	-	X	-	-	-	-	-	-	-	X	X	X	-	X	-	-	-	-	-											
BR	X	-	X	X	X	-	-	-	X	-	-	X	-	-	-	-	-	-	-	X	-	-	X	X	X	-	-	-	-	-	-										
CH#C	X	X	-	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-	-	X	-	-	-	-	-	-									
DMSO	X	X	X	X	X	X	X	-	X	-	X	-	X	-	-	-	-	-	-	-	X	X	X	-	-	-	X	-	X	-	-	X									
ACRYLONI	X	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-								
CL(C=C)	X	X	X	-	X	X	-	-	X	-	X	-	X	-	-	-	X	X	X	-	X	X	-	X	-	X	-	-	-	-	-	-	-	-							
ACF	X	-	X	X	X	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-						
DMF	X	X	X	X	X	X	X	-	X	-	-	X	-	-	X	-	-	-	-	-	X	-	-	-	X	-	X	-	-	X	X	-	-	-	-	-					
CF2	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-				
COO	X	X	X	X	X	X	X	X	X	-	X	X	X	-	X	-	X	X	X	X	X	-	-	X	-	-	-	X	-	-	X	X	X	-	-	-	-				

Table 3.19 Group Interaction Parameter for UNIFAC Model Revision 4

From D. Tiegs, P. Rasmussen, J. Gmehling, and Aa. Fredenslund, Ind. Eng. Chem. Res. 26, (1987), p. 159.

MAIN GROUP	CH2	C=C	ACH	ACCH2	OH	CH3OH	H2O	ACOH	CH2CO	CHO	CH2COO	HCOO	CH2O	CH2NH2	CH2NH	CH2N	ACNH2	C5H4N	CH2CN	COOH	CCL	CCL2	CCL3	CCL4	ACCL	CH2NO2	ACNO2	CS2	CH2SH	FURFURAL	(CH2OH)2	I	BR	CH#C	DMSO	ACRYLONI	CL(C=C)	ACF	DMF	CF2	COO	SIH2	SIO	NMP
CH2																																													
C=C	X																																												
ACH	X	X																																											
ACCH2	X	X	X																																										
OH	X	X	X	X																																									
CH3OH	X	X	X	X	X																																								
H2O	X	X	X	X	X	X																																							
ACOH	X	X	X	X	X	X	X																																						
CH2CO	X	X	X	X	X	X	X	X																																					
CHO	X	X	X	X	X	X	X	-	X																																				
CH2COO	X	X	X	X	X	X	X	X	X	X																																			
HCOO	X	X	X	X	X	X	-	-	X	X	X																																		
CH2O	X	X	X	X	X	X	X	-	X	X	X	-																																	
CH2NH2	X	X	X	-	X	X	X	-	-	-	-	-	-																																
CH2NH	X	X	X	X	X	X	X	-	-	-	X	-	X	X																															
CH2N	X	X	X	X	X	X	X	-	X	-	-	-	-	X	X																														
ACNH2	X	X	X	X	X	X	X	X	X	-	X	-	-	X	-	-																													
C5H4N	X	-	X	X	X	X	X	X	X	-	-	-	-	-	-	-	-																												
CH2CN	X	X	X	X	X	X	X	-	X	-	X	-	X	-	-	-	X	X																											
COOH	X	X	X	X	X	X	X	-	X	-	X	X	X	-	-	-	-	X	-																										
CCL	X	X	X	X	X	X	X	-	X	X	X	-	X	-	-	-	X	-	X	X																									
CCL2	X	X	X	X	X	X	X	-	X	-	X	-	X	-	-	X	-	X	X	X	X																							
CCL3	X	X	X	X	X	X	X	-	X	X	X	X	X	-	-	X	-	X	X	X	X	X																						
CCL4	X	X	X	X	X	X	X	X	X	-	X	X	X	X	X	X	X	X	X	X	X	X	X																					
ACCL	X	X	X	X	X	X	X	-	X	-	X	-	X	X	X	X	X	-	X	-	-	X																						
CH2NO2	X	X	X	X	X	X	X	-	X	-	X	-	X	-	-	-	-	X	-	X	-	X	X																					
ACNO2	X	-	X	X	X	-	X	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-	X	-	X																		
CS2	X	X	X	X	X	X	X	-	X	-	X	-	X	-	-	-	-	X	-	X	-	X	X	-	-	-																	
CH2SH	X	-	X	-	X	X	-	-	X	-	-	X	X	X	-	-	-	-	X	-	X	-	-	-	-	-	-																
FURFURAL	X	-	X	X	X	-	X	-	X	-	X	-	-	-	-	-	-	-	-	-	-	X	X	-	-	-	-	-															
(CH2OH)2	X	-	X	X	X	-	X	X	-	-	X	-	X	-	-	-	X	-	-	-	-	-	-	-	X	-	-	-	-														
I	X	-	X	-	X	-	-	-	X	-	X	-	X	-	-	-	-	-	-	-	X	X	X	-	X	-	-	-	-	-												
BR	X	-	X	X	X	X	-	-	X	-	X	-	X	-	-	-	-	-	X	X	-	-	X	X	X	-	-	-	-	-	-											
CH#C	X	X	-	-	-	-	-	-	X	-	-	-	-	-	-	-	X	-	-	-	-	-	-	-	X	-	-	-	-	-	-	-										
DMSO	X	X	X	X	X	X	X	-	X	-	X	-	X	-	-	-	X	-	-	-	X	-	X	X	X	-	-	-	X	-	X	-	-	-								
ACRYLONI	X	-	-	-	-	-	X	-	-	-	X	-	-	-	-	-	-	X	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-							
CL(C=C)	X	X	X	-	X	X	-	-	X	-	X	-	X	-	-	-	X	X	X	-	X	X	-	X	-	X	-	-	-	-	-	-	-	-	-	-						
ACF	X	-	X	X	X	X	-	-	-	-	-	-	X	-	-	X	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-					
DMF	X	X	X	X	X	X	X	-	X	-	-	-	X	-	-	-	X	-	-	X	-	-	-	X	-	-	-	X	-	X	-	-	X	X	-	-	-					
CF2	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	-			
COO	X	X	X	X	X	X	X	X	X	-	X	X	X	-	X	-	X	-	X	X	X	X	X	X	-	X	-	-	-	X	-	-	X	X	X	-	-	-				
SIH2	X	-	X	-	X	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
SIO	X	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	
NMP	X	-	X	X	X	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	

Notes

1 The contributions for PC are missing for the following groups: 120, 124, 148, and 151. The contributions for VC are missing for the following groups: 120, 146, 147, 148, 149, 150, and 151.

2 Used only for branched alkanes. The delta Platt number is defined as the Platt number of the isomer, minus the Platt number of the corresponding alkane. The Platt number is the total number of groups with four carbon atoms, three bonds apart. For n-alkanes, the Platt number is n-3.

3 Includes naphthenic alcohols and glycols, but not aromatic alcohols, such as xylenol.

4 CD represents a carbon atom joined to another carbon atom by a double bond.

5 CT represents a carbon atom joined to another carbon atom by a triple bond.

6 CB represents a carbon atom in an aromatic ring.

7 CA represents the central carbon atom of an allene group, >C=C=C<. The end carbons are treated as normal CD atoms.

8 CBF represents a carbon atom at the border of two or three fused aromatic rings.

9 NI represents a double-bonded nitrogen in imines; NI-(CB) represents a pyridine nitrogen.

10 NA represents a double-bonded nitrogen in azo compounds.

11 Halogen refers to CL, BR, and I.

12 Required to estimate absolute entropy, which is used to estimate standard Gibbs free energy of formation.

13 Substitution on 1, normal-aliphatic.

14 For adjacent pairs of >CH-, use group 152.

15 For -F substitution on nonaromatic C=C, use group 153.

16 The contributions for VC, DGFORM, and CPIG are missing.

17 This >CH- group represents a carbon atom common to two condensed saturated rings.

18 The contribution for VC is missing for groups 142, >Si< and 143, >B-.

19 The contribution for VC is missing for groups 142, >Si< and 143, >B-.
The contribution for PC is missing for group 143, >B-.

20 R represents radicals, such as Methyl. Groups 140 through 159 are valid radical types.

21 Lyngby modified UNIFAC model.

22 Dortmund modified UNIFAC model.

23 c denotes cyclic functional group.

24 AC denotes a carbon atom in an aromatic ring.

25 P denotes primary alcohol, S for secondary, and T for tertiary.

26 FCH2O denotes CH2-O group in a furan ring.

27 Functional groups used in Henry's Law application and in PSRK and MHV2 equations of state.

28 Functional groups used in MHV2 equation of state.

CHAPTER 4

Property Sets

Overview

A property set is a list of properties that you can use for:

- Heating and cooling curve reports
- Distillation column stage property reports and performance specifications
- Reactor profile reports
- Design specifications and constraints
- FORTRAN blocks
- Sensitivity blocks
- Optimization
- Stream reports and report scaling
- Physical property tables

The properties for these applications are defined indirectly. Define a property set listing the properties. Each property set is assigned an ID. Use the Prop-Set ID on other forms, such as heating and cooling curve forms.

Use the Prop-Sets form to list the properties for a property set. You can specify the phase as follows:

Phase	Description
V	Vapor
L1	First liquid phase
L2	Second liquid phase
L	Total liquid phase
S	Solid phase
T	Total mixture for mixed substream

For the property set you can also define:

- Temperature at which to calculate the property
- Pressure at which to calculate the property
- Whether to include or exclude water from the calculation
- Units for the property
- Components for which the properties are to be calculated (for pure component properties and properties of components in a mixture)

When you use multiple qualifiers, the property is computed for each valid combination of qualifiers.

The tables in this chapter describe the properties available in the Aspen Physical Property System. These tables show the phase qualifiers and indicate if the temperature, pressure, and basis qualifiers are applicable. A point (•) in the tables indicates that you can use the qualifier for that property.

The properties listed in a property set are calculated only for the substream specified. Table 4.9 lists properties that can be calculated for all substreams.

Table 4.1 Mixture Thermodynamic Properties

Volume

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
RHOLSTD	Standard liquid density	V L L1 L2 T			•	MOLE-DENSITY or MASS-DENSITY
RHOMX	Density	V L L1 L2 S T	•	•	•	MOLE-DENSITY or MASS-DENSITY
VLSTDMX	Standard liquid volume	V L L1 L2 T		•		MOLE-VOLUME or VOLUME-FLOW
VMX	Volume	V L L1 L2 S T	•	•	•	MOLE-VOLUME or VOLUME-FLOW
VVSTDMX	Standard vapor volume	V L L1 L2 T	•	•	•	MOLE-VOLUME or VOLUME-FLOW

Flow Rates, Fractions

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
BETA	Molar fraction of liquid that is L1					—
LFRAC	Liquid fraction					—
MASSFLMX	Mass flow rate	V L L1 L2 S T			•	MASS-FLOW
MASSVFRAC	Mass vapor fraction					—
MASSSFRAC	Mass solid fraction					
MOLEFLMX	Mole flow rate	V L L1 L2 S T			•	MOLE-FLOW
SFRAC	Solid fraction					—
VFRAC	Mole vapor fraction					—
VOLFLMX	Volume flow rate	V L L1 L2 S T			•	VOLUME-FLOW

Enthalpy, Entropy, Gibbs Energy, Heat Capacity

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
AVAILMX	Availability, H-ToS To=298.15 K	V L L1 L2 S T	•	•	•	MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
CPCVMX	Heat capacity ratio (CPMX/CVMX)	V L L1 L2 S T	•	•	•	—
CPIGMX [1]	Ideal gas heat capacity	V	•		•	MOLE-HEAT-CAPACITY or MASS-HEAT-CAPACITY
CPMX	Constant pressure heat capacity	V L L1 L2 S T	•	•	•	MOLE-HEAT-CAPACITY or MASS-HEAT-CAPACITY
CSATMX	Specific heat at saturation	V L L1 L2	•	•	•	MOLE-HEAT-CAPACITY or MASS-HEAT-CAPACITY
CVMX	Constant volume heat capacity	V L L1 L2 S T	•	•	•	MOLE-HEAT-CAPACITY or MASS-HEAT-CAPACITY
DGMIX	Gibbs free energy of mixing	L L1 L2 T	•	•	•	MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
DGMX	Free energy departure	V L L1 L2 S T	•	•	•	MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
DHMX	Enthalpy departure	V L L1 L2 S T	•	•	•	MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
DSMX	Entropy departure	V L L1 L2 S T	•	•	•	MOLE-ENTROPY or MASS-ENTROPY
GIGMX [1]	Ideal gas free energy	V	•		•	MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
GMX	Free energy	V L L1 L2 S T	•	•	•	MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
GXS [2]	Excess free energy	L L1 L2 S	•	•	•	MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
HIGMX [1]	Ideal gas enthalpy	V	•		•	MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
HMX	Enthalpy	V L L1 L2 S T	•	•	•	MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
HXS [2]	Excess enthalpy	L L1 L2 S	•	•	•	MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
SIGMX [1]	Ideal gas entropy	V	•		•	MOLE-ENTROPY or MASS-ENTROPY
SMX	Entropy	V L L1 L2 S T	•	•	•	MOLE-ENTROPY or MASS-ENTROPY

Other Properties

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
ABSHUMID	Absolute humidity	V				—
COMB-O2	Amount of O2 needed to completely combust a given material	V L L1 L2 S				MOLES or MASS
MWMX	Molecular weight	V L L1 L2 S T			•	—
PBUB	Bubble point pressure	V L L1 L2 T	•		•	PRESSURE
PCMX [3]	Pseudo-critical pressure	V L L1 L2 S T			•	PRESSURE
PDEW	Dew point pressure	V L L1 L2 T	•		•	PRESSURE
PH2OTDEW	Dew point temperature for water at the partial pressure of water	V			•	TEMPERATURE
PRES	Pressure					PRESSURE
PRMX [4]	Reduced pressure (based on PCMX)	V L L1 L2 S T			•	—
RAT-MLFR [5]	Ratio of mole fractions	V L L1 L2 T			•	—
RAT-MSFR [5]	Ratio of mass fractions	V L L1 L2 T			•	—

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
RAT-VLFR [5]	Ratio of liquid volume fractions	L L1 L2 T			•	—
RELHUMID	Percent relative humidity	V				—
SONVELMX	Sonic velocity	V L L1 L2 T	•	•	•	
SUM-MLFR [6]	Sum of mole fractions	V L L1 L2 T			•	—
SUM-MSFR [6]	Sum of mass fractions	V L L1 L2 T			•	—
SUM-VLFR [6]	Sum of liquid volume fractions	L L1 L2 T			•	—
TBUB	Bubble point temperature	V L L1 L2 T		•	•	TEMPERATURE
TCMX [3]	Pseudo-critical temperature	V L L1 L2 S T			•	TEMPERATURE
TDEW	Dew point temperature	V L L1 L2 T		•	•	TEMPERATURE
TEMP	Temperature					TEMPERATURE
TRMX [4]	Reduced temperature (based on TCMX)	V L L1 L2 S T			•	—
VCMX [3]	Pseudo-critical volume	V L L1 L2 S T			•	MOLE-VOLUME
ZCMX [3]	Pseudo-critical compressibility factor	V L L1 L2 S T			•	—
ZMX	Compressibility factor	V L L1 L2 S	•	•	•	—

Table 4.2 Thermodynamic Properties of Components in Mixtures

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
GAMMA [2]	Activity coefficient	L L1 L2 S	•	•	•	—
GAMPC [2]	Activity coefficient pressure correction	L L1 L2 S	•	•	•	—
GAMUS [2]	Unsymmetrically normalized activity coefficient	L L1 L2	•	•	•	—
KLL2	Liquid-liquid K-value		•	•	•	—
KVL [7]	Vapor-liquid K-value		•	•	•	—
KVL2	Vapor-liquid2 K-value		•	•	•	—
MASSCONC	Mass concentration	V L L1 L2 S T			•	MASS-CONC
MASSFLOW	Mass flow rate	V L L1 L2 S T			•	MASS-FLOW

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
MASSFRAC	Mass fraction	V L L1 L2 S T			•	—
MOLECONC	Molar concentration	V L L1 L2 S T			•	MOLE-CONC
MOLEFLOW	Mole flow rate	V L L1 L2 S T			•	MOLE-FLOW
MOLEFRAC	Mole fraction	V L L1 L2 S T			•	—
PHIMX [2]	Fugacity coefficient	V L L1 L2 S	•	•	•	—
PPMX	Partial pressure	V			•	PRESSURE
SSOLFACT	Solubility safety factor [8]	V L L1 L2	•	•	•	—
SSOLUB	Equilibrium solubility of a freeze-out component	V L L1 L2	•	•	•	—
TFREEZ	Freeze-out temperature of a component [9]	V L L1 L2	•	•	•	TEMPERATURE
TFRZMARG	Temperature safety margin [10]	V L L1 L2	•	•	•	—
VLSTD	Standard liquid volume	V L L1 L2 T			•	MOLE-VOLUME or VOLUME-FLOW
VLSTDFR	Standard liquid volume fraction	V L L1 L2 T			•	—
VVSTD	Standard vapor volume	V	•	•	•	MOLE-VOLUME or VOLUME-FLOW
VVSTDFR	Standard vapor volume fraction	V			•	—

Table 4.3 Pure Component Thermodynamic Properties

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
AVAIL	Availability, H-ToS To=298.15 K	V L L1 L2 S T	•	•		MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
CP	Constant pressure heat capacity	V L L1 L2 S T	•	•		MOLE-HEAT-CAPACITY or MASS-HEAT-CAPACITY
CPCV	Heat capacity ratio (CP/CV)	V L L1 L2 S T	•	•		—
CPIG [1]	Ideal gas heat capacity	V	•			MOLE-HEAT-CAPACITY or MASS-HEAT-CAPACITY
CV	Constant volume heat capacity	V L L1 L2 S T	•	•		MOLE-HEAT-CAPACITY or MASS-HEAT-CAPACITY
DG	Free energy departure	V L L1 L2 S	•	•		MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
DGPC	Free energy departure pressure correction	L L1 L2 S	•	•		—

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
DH	Enthalpy departure	V L L1 L2 S	•	•		MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
DHVL [11]	Enthalpy of vaporization	L	•	•		MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
DHPC	Enthalpy departure pressure correction	L L1 L2 S	•	•		—
DS	Entropy departure	V L L1 L2 S	•	•		MOLE-ENTROPY or MASS-ENTROPY
G	Free energy	V L L1 L2 S T	•	•		MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
GIG [1]	Ideal gas free energy	V	•			MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
H	Enthalpy	V L L1 L2 S T	•	•		MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
HIG [1]	Ideal gas enthalpy	V	•			MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
PHI	Fugacity coefficient	V L L1 L2 S	•	•		—
PHIPC	Fugacity coefficient pressure correction	L L1 L2 S	•	•		—
PL [12]	Vapor pressure	L	•			PRESSURE
RHO	Density	V L L1 L2 S T	•	•		MOLE-DENSITY or MASS-DENSITY
S	Entropy	V L L1 L2 S T	•	•		MOLE-ENTROPY or MASS-ENTROPY
SIG [1]	Ideal gas entropy	V	•			MOLE-ENTROPY or MASS-ENTROPY
SONVEL	Sonic velocity	V L L1 L2 T	•	•	•	—
V	Volume	V L L1 L2 S T	•	•		MOLE-VOLUME or VOLUME-FLOW

Table 4.4 Electrolyte Properties

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
FAPP	Apparent component molar flow rate	L L1 L2 S	•	•		MOLE-FLOW
FTRUE	True species molar flow rates	L L1 L2 S	•	•		MOLE-FLOW
GXTRUE	Activity coefficient of a true species (mole fraction scale)	L L1 L2	•	•	•	—
GMTRUE	Activity coefficient of a true species (molality scale)	L L1 L2	•	•	•	—
IONSM	Ionic strength (molality scale)	L L1 L2	•	•		—

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
IONSX	Ionic strength (mole fraction scale)		•	•		—
MAPP	Apparent component molality	L L1 L2	•	•		—
MTRUE	True species molality	L L1 L2	•	•		—
OSMOT	Osmotic coefficient	L L1 L2	•	•		—
PH25	pH at 25°C	L L1 L2		•		—
PH	pH	L L1 L2	•	•		—
POH25	pOH at 25°C	L L1 L2			•	—
POH	pOH	L L1 L2	•	•		—
SOLINDEX	Solubility index (ratio of activity in mixture to activity at saturation)	L L1 L2	•	•		—
WAPP	Apparent component mass flow rate	L L1 L2 S	•	•		MASS-FLOW
WTRUE	True species mass flow rate	L L1 L2 S	•	•		MASS-FLOW
WXAPP	Apparent component mass fraction	L L1 L2 S	•	•		—
WXTRUE	True species mass fraction	L L1 L2 S	•	•		—
XAPP	Apparent component mole fraction	L L1 L2 S	•	•		—
XTRUE	True species mole fraction	L L1 L2 S	•	•		—

Table 4.5 Transport Properties

Mixture [2]

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
KINVISC	Kinematic viscosity	V L L1 L2	•	•	•	DIFFUSIVITY
KMX	Thermal conductivity	V L L1 L2 S	•	•	•	THERMAL-CONDUCTIVITY
MUMX	Viscosity	V L L1 L2	•	•	•	VISCOSITY
PR	Prandtl Number	V L L1 L2	•	•	•	—
RE [13]	Dimensional Reynolds Number	V L L1 L2	•	•	•	LENGTH
SIGMAMX	Surface tension	L L1 L2	•	•	•	SURFACE-TENSION
THRMDIFF	Thermal diffusivity	V L L1 L2 S	•	•	•	DIFFUSIVITY

Component in a Mixture [2]

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
DMX	Diffusion coefficient	V L L1 L2	•	•	•	DIFFUSIVITY

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
K	Thermal conductivity	V L L1 L2	•	•		THERMAL-CONDUCTIVITY
MU	Viscosity	V L L1 L2	•	•		VISCOSITY
SIGMA	Surface tension	L L1 L2	•	•		SURFACE-TENSION

Table 4.6 Petroleum-Related Properties for Mixtures

PROPNAME	Description	PHASE [14]	TEMP	PRES	BASIS	Units
ANILPT	Aniline point	V L L1 L2 T			•	TEMPERATURE
API	API gravity	V L L1 L2 T	•	•	•	—
CHRATIO	Carbon to hydrogen ratio	V L L1 L2 T			•	—
FLPT-API	Flash point, API method	V L L1 L2 T			•	TEMPERATURE
FLPT-PM	Flash point, Pennsky-Martens method	V L L1 L2 T			•	TEMPERATURE
FLPT-TAG	Flash point, Tag method	V L L1 L2 T			•	TEMPERATURE
MABP	Mean average boiling point	V L L1 L2 T			•	TEMPERATURE
PHYDRATE [15]	Hydrate formation pressure	V			•	PRESSURE
PRPT-API	Pour point, API method	V L L1 L2 T			•	TEMPERATURE
QVALGRS	Gross heating value	V L L1 L2 T			•	MASS-ENTHALPY
QVALNET	Net heating value	V L L1 L2 T			•	MASS-ENTHALPY
REFINDEX	Refractive index	V L L1 L2 T	•		•	—
REIDVP	Reid vapor pressure	L L1 L2			•	PRESSURE
RVP-API	Reid vapor pressure, API method	V L L1 L2 T	•			PRESSURE
RVP-P2	Reid vapor pressure, ASTM method, PML implementation	V L L1 L2 T			•	PRESSURE
SG	Specific gravity	V L L1 L2 T			•	—
SGAIR	Specific gravity (ref. AIR at 60°F)	V	•	•	•	—
THYDRATE [15]	Hydrate formation temperature	V			•	TEMPERATURE

PROPNAME	Description	PHASE [14]	TEMP	PRES	BASIS	Units
VABP	Volume average boiling point	V L L1 L2 T			•	TEMPERATURE
VISINDEX	Liquid viscosity index	L L1 L2			•	—
WAT	Watson UOP K-factor	V L L1 L2 T			•	—

Distillation Curves

PROPNAME	Description	PHASE [14]	TEMP	PRES	BASIS	Units
APICRV	API curve	V L L1 L2 T			•	—
APICRVWT	API curve as a function of weight percent	V L L1 L2 T			•	—
D2887CRV	ASTM D2887 curve as a function weight percent	V L L1 L2 T			•	TEMPERATURE
D86CRK	ASTM D86 curve with cracking correction	V L L1 L2 T			•	TEMPERATURE
D86CRV [16]	ASTM D86 curve	V L L1 L2 T			•	TEMPERATURE
D86CRVWT	ASTM D86 curve as a function of weight percent	V L L1 L2 T			•	TEMPERATURE
D86WTCRK	ASTM D86 weight curve with cracking correction	VLL1 L2T			•	TEMPERATURE
D1160CRV	ASTM D1160 curve	V L L1 L2 T		•	•	TEMPERATURE
D1160CVW	ASTM D1160 curve as a function of weight percent	V L L1 L2 T		•	•	TEMPERATURE
GRVCRV	Gravity curve	V L L1 L2 T			•	—
GRVCRVWT	Gravity curve as a function of weight percent	V L L1 L2 T			•	—
MWCRV	Molecular weight curve	V L L1 L2 T			•	—
MWCRVWT	Molecular weight curve as a function of weight percent	V L L1 L2 T			•	—
TBPCRV [16]	True boiling point curve	V L L1 L2 T			•	TEMPERATURE
TBPCRVWT	True boiling point curve as a function of weight percent	V L L1 L2 T			•	TEMPERATURE
VACCRV [16]	Vacuum curve	V L L1 L2 T			•	TEMPERATURE
VACCRVWT	Vacuum curve as a function of weight percent	V L L1 L2 T			•	TEMPERATURE

Distillation Temperature

PROPNAME	Description	PHASE [14]	TEMP	PRES	BASIS	Units
D2887T	ASTM D2887 temperature	V L L1 L2 T			•	TEMPERATURE
D86T [17]	ASTM D86 temperature	V L L1 L2 T			•	TEMPERATURE
D86TCK	ASTM D86 temperature with cracking correction	V L L1 L2 T			•	TEMPERATURE
D86TWT	ASTM D86 temperature at a given weight percent	V L L1 L2 T			•	TEMPERATURE
D86TWTCK	ASTM D86 temperature with cracking correction at a given weight percent	V L L1 L2 T				TEMPERATURE
D1160T [17]	ASTM D1160 temperature	V L L1 L2 T		•	•	TEMPERATURE
D1160TWT	ASTM D1160 temperature at a given weight percent	V L L1 L2 T		•	•	TEMPERATURE
TBPT [17]	True boiling point temperature	V L L1 L2 T			•	TEMPERATURE
TBPTWT	True boiling point temperature at a given weight percent	V L L1 L2 T			•	TEMPERATURE
VACT [17]	Vacuum temperature	V L L1 L2 T			•	TEMPERATURE
VACTWT	Vacuum Temperature at a given weight percent	V L L1 L2 T			•	TEMPERATURE

Distillation Volume and Weight Percent

PROPNAME	Description	PHASE [14]	TEMP	PRES	BASIS	Units
D2887WT	ASTM D2887 weight percent	V L L1 L2 T	•		•	—
D86LV [18]	ASTM D86 liquid volume percent	V L L1 L2 T	•		•	—
D86LVCK	ASTM D86 liquid volume percent with cracking correction	V L L1 L2 T	•		•	—
D86WT	ASTM D86 weight percent	V L L1 L2 T	•		•	—
D86WTCK	ASTM D86 weight percent with cracking correction	V L L1 L2 T	•		•	—
D1160LV [18]	ASTM D1160 liquid volume percent	V L L1 L2 T	•	•	•	—
D1160WT	ASTM D1160 weight percent	V L L1 L2 T	•	•	•	—
TBPLV [18]	True boiling point liquid volume percent	V L L1 L2 T	•		•	—
TBPWT	True boiling point weight percent	V L L1 L2 T	•		•	—

PROPNAME	Description	PHASE [14]	TEMP	PRES	BASIS	Units
VACLV [18]	Vacuum liquid volume percent	V L L1 L2 T	•		•	—
VACWT	Vacuum weight percent	V L L1 L2 T		•	•	—

Flow Rates for Petroleum Cuts

PROPNAME	Description	PHASE [14]	TEMP	PRES	BASIS	Units
CUTS-E [19]	Flow rates for petroleum cuts and light ends in Deg. F	V L L1 L2 T	•		•	MOLE-FLOW, MASS-FLOW, or VOLUME-FLOW
CUTS-M [19]	Flow rates for petroleum cuts and light ends in Deg. C	V L L1 L2 T	•		•	MOLE-FLOW, MASS-FLOW, or VOLUME-FLOW

Petroleum Property from ASSAY Analysis

PROPNAME	Description	PHASE [14]	TEMP	PRES	BASIS	Units
ANILPT	Aniline point	V L L1 L2 T			•	TEMPERATURE
AROMATIC	Aromatic content	V L L1 L2 T			•	—
ASPHALTE	Asphaltene content	V L L1 L2 T			•	—
BASIC-N2	Basic nitrogen	V L L1 L2 T			•	—
BROMINE	Bromine number	V L L1 L2 T			•	—
CARBON	Carbon content	V L L1 L2 T			•	TEMPERATURE
CETANENO	Cetane number	V L L1 L2 T			•	—
CLOUDPT	Cloud point	V L L1 L2 T			•	TEMPERATURE
COCARBON	Conradson carbon content	V L L1 L2 T			•	—
FLASHPT	Flash point	V L L1 L2 T			•	TEMPERATURE
FREEZEPT	Freeze point	V L L1 L2 T			•	TEMPERATURE
HYDROGEN	Hydrogen content	V L L1 L2 T			•	—
IRON	Iron content	V L L1 L2 T			•	—
KNOCKIDX	Antiknock index	V L L1 L2 T			•	—
KVISC	Kinematic viscosity	V L L1 L2 T	•		•	DIFFUSIVITY
LUMI-NO	Luminometer number	V L L1 L2 T			•	—

PROPNAME	Description	PHASE [14]	TEMP	PRES	BASIS	Units
MERCAPTA	Mercaptan content	V L L1 L2 T			•	—
METAL	Metal content	V L L1 L2 T			•	—
MOC-NO	Motor octane number	V L L1 L2 T			•	—
NAPHTHENE	Naphthene content	V L L1 L2 T			•	—
NICKEL	Nickel content	V L L1 L2 T			•	—
OLEFIN	Olefin content	V L L1 L2 T			•	—
OXYGEN	Oxygen content	V L L1 L2 T			•	—
PARAFFIN	Paraffin content	V L L1 L2 T			•	—
POURPT	Pour point	V L L1 L2 T			•	TEMPERATURE
REFINDEX	Refractive index	V L L1 L2 T			•	—
ROC-NO	Research octane number	V L L1 L2 T			•	—
RVP	Reid vapor press.	V L L1 L2 T			•	PRESSURE
SMOKEPT	Smoke point	V L L1 L2 T			•	LENGTH
SULFUR	Sulfur content	V L L1 L2 T			•	—
TOTAL-N2	Total nitrogen	V L L1 L2 T			•	—
VANADIUM	Vanadium content	V L L1 L2 T			•	—
VISC	Viscosity	V L L1 L2 T	•		•	VISCOSITY
VLOCKIDX	Vapor knock index	V L L1 L2 T			•	—
WARMIDX	Warm-up index	V L L1 L2 T			•	—

Petroleum Property Curves

PROPNAME	Description	PHASE [14]	TEMP	PRES	BASIS	Units
ANILCRV	Aniline point curve	V L L1 L2 T			•	TEMPERATURE
AROMCRV	Aromatic content curve	V L L1 L2 T			•	—
ASPHACRV	Asphaltene content curve	V L L1 L2 T			•	—
BAS-NCRV	Basic Nitrogen content	V L L1 L2			•	—

PROPNAME	Description	PHASE [14]	TEMP	PRES	BASIS	Units
	curve	T				
BROMICRV	Bromine number curve	V L L1 L2 T			•	—
CARBCRV	Carbon content curve	V L L1 L2 T			•	—
CETANCRV	Cetane number curve	V L L1 L2 T			•	—
CLOUDCRV	Cloud point curve	V L L1 L2 T			•	TEMPERATURE
COCARCRV	Conradson carbon content curve	V L L1 L2 T			•	—
FLASHCRV	Flash point curve	V L L1 L2 T			•	TEMPERATURE
FREEZCRV	Freeze point curve	L L1 L2 T			•	TEMPERATURE
HYDROCRV	Hydrogen content curve	V L L1 L2 T			•	—
IRONCRV	Iron content curve	V L L1 L2 T			•	—
KNOCKCRV	Antiknock index curve	V L L1 L2 T			•	—
KVISCCRV	Kinematic viscosity curve	V L L1 L2 T			•	DIFFUSIVITY
LUM-NCRV	Luminometer number curve	V L L1 L2 T			•	—
MERCCRV	Mercaptan content curve	V L L1 L2 T			•	—
METALCRV	Metal content curve	V L L1 L2 T			•	—
MOCNCRV	Motor octane number curve	V L L1 L2 T			•	—
NAPHCRV	Naphthene content curve	V L L1 L2 T			•	—
NICKCRV	Nickel content curve	V L L1 L2 T			•	—
OLEFCRV	Olefin content curve	V L L1 L2 T			•	—
OXYGEN	Oxygen content curve	V L L1 L2 T			•	—
PARACRV	Paraffin content curve	V L L1 L2 T			•	—
POURCRV	Pour point curve	V L L1 L2 T			•	TEMPERATURE
REFICRV	Refractive index curve	V L L1 L2 T			•	—
ROCNCRV	Research octane number curve	V L L1 L2 T	•		•	—
RVPCRV	Reid vapor pressure curve	V L L1 L2 T			•	PRESSURE

PROPNAME	Description	PHASE [14]	TEMP	PRES	BASIS	Units
SMOKCRV	Smoke point curve	V L L1 L2 T			•	LENGTH
SULFCRV	Sulfur content curve	V L L1 L2 T			•	—
TOT-NCRV	Total nitrogen content curve	V L L1 L2 T			•	—
UOPKCRV	Watson UOP K curve	V L L1 L2 T			•	—
VANACRV	Vanadium content curve	V L L1 L2 T			•	—
VISCCRV	Viscosity curve	V L L1 L2 TV	•		•	DIFFUSIVITY
VLOCKCRV	Vapor knock index curve	V L L1 L2 T			•	—
WARMICRV	Warm-up index curve	V L L1 L2 T			•	—

Table 4.7 Elemental Analysis of Mixtures

PROPNAME	Description	PHASE	Units
MOLEFLC	Mole flow of carbon atoms	V L L1 L2 S T	MOLE-FLOW
MOLEFLH	Mole flow of hydrogen atoms	V L L1 L2 S T	MOLE-FLOW
MOLEFLO	Mole flow of oxygen atoms	V L L1 L2 S T	MOLE-FLOW
MOLEFLN	Mole flow of nitrogen atoms	V L L1 L2 S T	MOLE-FLOW
MOLEFLS	Mole flow of sulfur atoms	V L L1 L2 S T	MOLE-FLOW
MOLEFLF	Mole flow of fluorine atoms	V L L1 L2 S T	MOLE-FLOW
MOLEFLCL	Mole flow of chlorine atoms	V L L1 L2 S T	MOLE-FLOW
MOLEFLBR	Mole flow of bromine atoms	V L L1 L2 S T	MOLE-FLOW
MOLEFLI	Mole flow of iodine atoms	V L L1 L2 S T	MOLE-FLOW
MOLEFLAR	Mole flow of argon atoms	V L L1 L2 S T	MOLE-FLOW
MOLEFLHE	Mole flow of helium atoms	V L L1 L2 S T	MOLE-FLOW
MASSFLC	Mass flow of carbon atoms	V L L1 L2 S T	MASS-FLOW
MASSFLH	Mass flow of hydrogen atoms	V L L1 L2 S T	MASS-FLOW
MASSFLO	Mass flow of oxygen atoms	V L L1 L2 S T	MASS-FLOW
MASSFLN	Mass flow of nitrogen atoms	V L L1 L2 S T	MASS-FLOW
MASSFLS	Mass flow of sulfur atoms	V L L1 L2 S T	MASS-FLOW
MASSFLF	Mass flow of fluorine atoms	V L L1 L2 S T	MASS-FLOW
MASSFLCL	Mass flow of chlorine atoms	V L L1 L2 S T	MASS-FLOW
MASSFLBR	Mass flow of bromine atoms	V L L1 L2 S T	MASS-FLOW
MASSFLI	Mass flow of iodine atoms	V L L1 L2 S T	MASS-FLOW
MASSFLAR	Mass flow of argon atoms	V L L1 L2 S T	MASS-FLOW
MASSFLHE	Mass flow of helium atoms	V L L1 L2 S T	MASS-FLOW
MOLEFRC	Mole fraction of carbon atoms	V L L1 L2 S T	—
MOLEFRH	Mole fraction of hydrogen atoms	V L L1 L2 S T	—
MOLEFRO	Mole fraction of oxygen atoms	V L L1 L2 S T	—
MOLEFRN	Mole fraction of nitrogen atoms	V L L1 L2 S T	—
MOLEFRS	Mole fraction of sulfur atoms	V L L1 L2 S T	—
MOLEFRF	Mole fraction of fluorine atoms	V L L1 L2 S T	—
MOLEFRCL	Mole fraction of chlorine atoms	V L L1 L2 S T	—
MOLEFRBR	Mole fraction of bromine atoms	V L L1 L2 S T	—

PROPNAME	Description	PHASE	Units
MOLEFRI	Mole fraction of iodine atoms	V L L1 L2 S T	—
MOLEFRAR	Mole fraction of argon atoms	V L L1 L2 S T	—
MOLEFRHE	Mole fraction of helium atoms	V L L1 L2 S T	—
MASSFRC	Mass fraction of carbon atoms	V L L1 L2 S T	—
MASSFRH	Mass fraction of hydrogen atoms	V L L1 L2 S T	—
MASSFRO	Mass fraction of oxygen atoms	V L L1 L2 S T	—
MASSFRN	Mass fraction of nitrogen atoms	V L L1 L2 S T	—
MASSFRS	Mass fraction of sulfur atoms	V L L1 L2 S T	—
MASSFRF	Mass fraction of fluorine atoms	V L L1 L2 S T	—
MASSFRCL	Mass fraction of chlorine atoms	V L L1 L2 S T	—
MASSFRBR	Mass fraction of bromine atoms	V L L1 L2 S T	—
MASSFRI	Mass fraction of iodine atoms	V L L1 L2 S T	—
MASSFRAR	Mass fraction of argon atoms	V L L1 L2 S T	—
MASSFRHE	Mass fraction of helium atoms	V L L1 L2 S T	—

Table 4.8 Nonconventional Component Properties

PROPNAME	Description	PHASE	Temperature	Units
DENSITY	Density [20]	S	•	MASS-DENSITY
ENTHALPY	Enthalpy [20]	S	•	MASS-ENTHALPY
HEAT-CAPACITY	Heat capacity [20]	S	•	MASS-HEAT-CAPACITY

Table 4.9 Valid Properties for Substream ALL

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
GMX	Free energy of mixture	V L L1 L2 S T	•	•	•	MOLE-ENTHALPY, MASS-ENTHALPY, or ENTHALPY-FLOW
HMX	Enthalpy of mixture	V L L1 L2 S T	•	•	•	MOLE-ENTHALPY, MASS-ENTHALPY
LFRAC	Liquid fraction					
MASSCONC	Mass concentration	V L L1 L2 S T			•	MASS-CONC
MASSFLMX	Mass flow rate of mixture	V L L1 L2 S T			•	MASS-FLOW
MASSFLOW	Mass flow rate of components in mixture	V L L1 L2 S T			•	MASS-FLOW
MASSFRAC	Mass fraction	V L L1 L2 S T			•	—
MASSSFRAC	Mass solid fraction					
MASSVFRAC	Mass vapor fraction					—
MOLECONC	Molar concentration	V L L1 L2 S T			•	MOLE-CONC

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
MOLEFLMX	Mole flow rate of mixture	V L L1 L2 S T			•	MOLE-FLOW
MOLEFLOW	Mole flow rate of components in mixture	V L L1 L2 S T			•	MOLE-FLOW
MOLEFRAC	Mole fraction	V L L1 L2 S T			•	—
MWMX	Molecular weight of mixture	V L L1 L2 S T			•	—
RHOMX	Density of mixture	V L L1 L2 S T	•	•	•	MOLE-DENSITY or MASS-DENSITY
SFRAC	Solid fraction					—
SMX	Entropy of mixture	V L L1 L2 S T	•	•	•	MOLE-ENTROPY or MASS-ENTROPY
VFRAC	Mole vapor fraction					—
VMX	Volume of mixture	V L L1 L2 S T	•	•	•	MOLE-VOLUME or VOLUME-FLOW
VOLFLMX	Volume flow rate of mixture	V L L1 L2 S T			•	VOLUME-FLOW

Notes

1 Ideal gas properties are computed at the specified temperature and the reference pressure of 1 atm.

2 PHASE = L is not allowed if two liquid phases are present.

3 Pseudocritical property; a mole-fraction average of the pure component critical properties. A PT-Envelope should be used to calculate the true mixture critical properties.

4 Based on pseudocritical property (see note 3).

5 Specify components for numerator and denominator of ratio as single component, component group, or boiling point range.

6 Specify single component, component group, or boiling point range.

7 Vapor-liquid K-value for PHASE=L1 is returned if two liquid phases are present.

8 Ratio of equilibrium solubility of the freeze-out component and its mole-fraction

9 Temperature at which a component at its given concentration just begins to freeze out

10 Temperature safety margin is defined as stream temperature — freeze-out temperature (TFREEZ)

11 Should be obtained using FLASHCURVE with VFRAC=0.

12 PL cannot be calculated by the following property option sets: PENG-ROB, PRWS, PRMHV2, PSRK, RK-SOAVE, RKSWS, RKSMHV2, RK-ASPEN, STEAM-TA, STEAMNBS, LK-PLOCK, and SR-POLAR.

13 $RE = \frac{(mass\ flow)}{\frac{\pi}{4} viscosity}$ Dimensionless Reynolds Number can be computed from RE by dividing by pipe diameter (Reynolds Number $\frac{RE}{D}$).

14 Combined phase properties are calculated using the combined phase composition, not by mixing the properties of the individual phases. (PHASE=T, or PHASE=L when two liquid phases are present.)

15 The effect of inhibitors on hydrate formation temperature and pressure is not observed.

16 Temperature calculated for LVPCT=0, 5, 10, 30, 50, 70, 90, 95, 100

17 LVPCT required

18 TEMP required

19 Reports flow rates in 100 deg F or 50 deg C increments.

20 All properties are component properties. Nonconventional component mixture properties cannot be computed using PROP-SET.

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