Aspen Plus®

STEADY STATE SIMULATION

Version 10

Physical Property Data

AspenTech®

REFERENCE MANUAL

Use of Aspen Plus and This Manual

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Contents

About *Physical Property Data*

This manual includes technical reference information and listings for all Aspen Plus 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 *Aspen Plus Physical Property Methods and Models*.

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

For More Information

Online Help Aspen Plus has a complete system of online help and context-sensitive prompts. The help system contains both context-sensitive help and reference information. For more information about using Aspen Plus help, see the *Aspen Plus User Guide*, Chapter 3.

Aspen Plus Getting Started Building and Running a Process Model This tutorial includes several hands-on sessions to familiarize you with Aspen Plus. The guide takes you step-by-step to learn the full power and scope of Aspen Plus.

Aspen Plus Getting Started Modeling Processes with Electrolytes This tutorial includes several hands-on sessions to familiarize you with simulating electrolyte systems with Aspen Plus.

Aspen Plus Getting Started Modeling Petroleum Processes This tutorial includes several hands-on sessions to familiarize you with simulating petroleum processes with Aspen Plus.

Aspen Plus Getting Started Customizing Unit Operation Models This tutorial includes several hands-on sessions to familiarize you with the customization of unit operation models with Aspen Plus.

Aspen Plus User Guide The three-volume *Aspen Plus User Guide* provides step-by-step procedures for developing and using an Aspen Plus process simulation model. The guide is task-oriented to help you accomplish the engineering work you need to do, using the powerful capabilities of Aspen Plus.

Aspen Plus reference manual series Aspen Plus reference manuals provide detailed technical reference information. These manuals include background information about the unit operation models and the physical properties methods and models available in Aspen Plus, tables of Aspen Plus databank parameters, group contribution method functional groups, and a wide range of other reference information. The set comprises:

- *Unit Operation Models*
- *Physical Property Methods and Models*
- *Physical Property Data*
- *User Models*
- *System Management*
- *System Administration*
- *Summary File Toolkit*

Aspen Plus application examples A suite of sample online Aspen Plus simulations illustrating specific processes is delivered with Aspen Plus.

Aspen Plus Installation Guides These guides provide instructions on platform and network installation of Aspen Plus. The set comprises:

- *Aspen Plus Installation Guide* for Windows
- *Aspen Plus Installation Guide* for OpenVMS
- *Aspen Plus Installation Guide* for UNIX

The Aspen Plus manuals are delivered in Adobe portable document format (PDF) on the Aspen Plus Documentation CD.

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 To obtain in-depth technical support information on the Internet, visit the Technical Support homepage. Register at:

http://www.aspentech.com/ts/

Approximately three days after registering, you will receive a confirmation e-mail and you will then be able to access this information.

The most current Hotline contact information is listed. Other information includes:

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1 Databanks

Physical property models require parameters to calculate properties. After you have selected the option set(s) to be used in a simulation, 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 Aspen Plus using the Property Constant Estimation System (PCES).

This chapter discusses:

- Aspen Plus databanks
- Use of the Data File Management System (DFMS) to manage databanks
- Databanks available in Aspen Plus
- 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.

Aspen Plus Databanks

Aspen Plus 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 Aspen Plus and delivered with Aspen Plus. 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 Plus run. 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 and components available in: AQUEOUS, ASPENPCD, INORGANIC, PURE10, PURE856, PURE93,SOLIDS and COMBUST. See Databanks Available in Aspen Plus, this chapter, 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 Aspen Plus. These databanks are independent of the Aspen Plus system databanks. Your Aspen Plus system administrator must create and activate in-house databanks. (See Using DFMS to Manage Databanks, this chapter, 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 Plus users. This may occur when the accuracy of the data is in question, or when data are of a proprietary nature. Use the Aspen Plus Data File Management System (DFMS) to create user databanks. (See Using DFMS to Manage Databanks, this chapter.) These databanks can be used in any Aspen Plus run.

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 Plus *Physical Property Databanks*

System Databanks

Databank Name	Password	Type†	Maximum Parameters	Maximum Components	Maximum Pairs	Description
PURE10	PURE10	PP1	100	1800	—	Main pure component databank
ASPENPCD	ASPENPCD	PP1	40	1000	—	Aspen Plus pure component databank
SOLIDS	SOLIDS	PP1	40	4000	—	SOLIDS databank
AQUEOUS	AQUEOUS	PP1	40	4000	—	AQUEOUS databank
BINARY	BINARY	PP2	20	100	3000	Binary databank
COMBUST	COMBUST	PP1	40	4000	—	Combustion databank
INORGANI	INORGANI	PP1	25	2500	—	Inorganic databank
PURE856	PURE856	PP1	100	1800	—	Pure component databank from release 8.5 – 6
PURE93	PURE93	PP1	100	1800	—	Pure component databank from release 8.5 – 6
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

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

†† *Assigned by the user.*

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 Aspen Plus. 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.

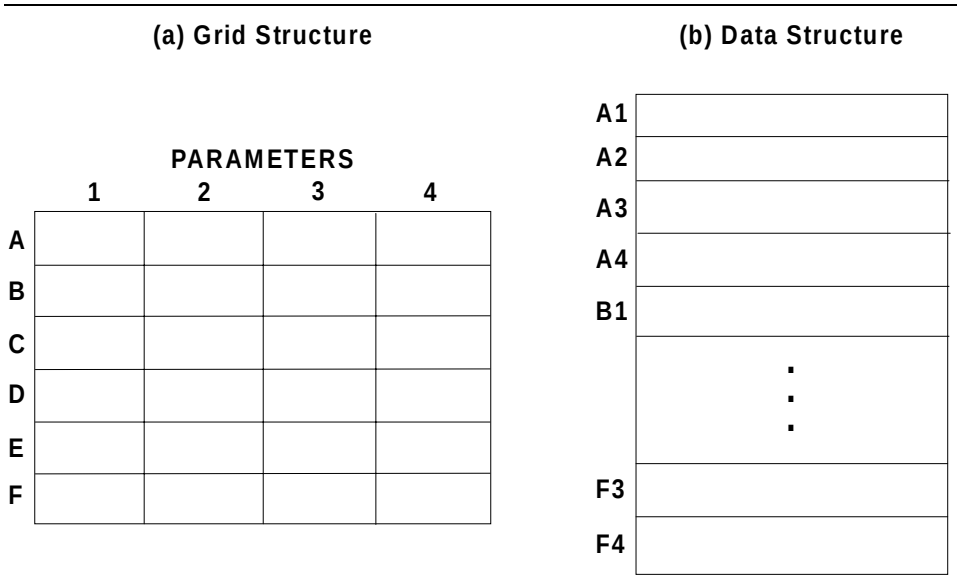

Figure 1.1 Unpacked Structure Databank

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.

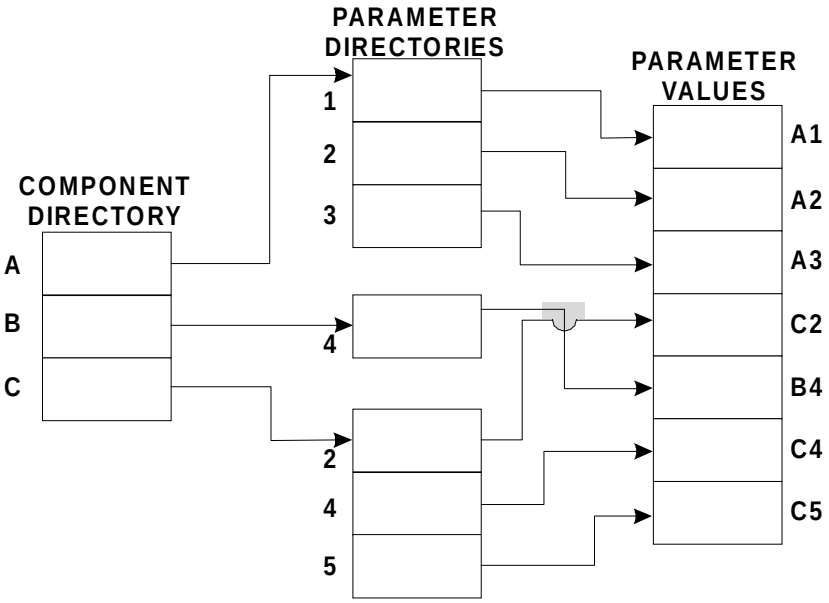

Figure 1.2 Packed Structure Databank

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	DESCRIPTIO	NEW- COMP	PRINT-DIR
CLEAN-	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.

The following section describes the 14 DFMS primary keywords.

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

```
FILE    name    password    [NEW]    /
                            [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 Plus simulation.

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 Aspen Plus system databanks.

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 Plus 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 Plus 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

Input Language Description

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

PRINT-DATA   password   [ cname - list ]
                        [ pair - list  ]
                        [ 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 THE ASPENPCD'

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 Aspen Plus

The following pure component databanks are available in Aspen Plus:

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. Table 1.2 and Table 1.3 list 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. Table 1.3A and Table 1.3B list 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. Table 1.4 and Table 1.5 list the parameters and components available in the 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 Plus 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. Table 1.6 and Table 1.7 list the parameters and components available in the databank.

PURE10 databank Contains parameters for over 1727 (mostly organic) components. This is the main source of pure component parameters for Aspen Plus. 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 simulations, the PURE10 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 and octane numbers
- 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 Aspen Plus to the next, certain parameter values change. This change can cause differences in your simulation results if you use the new, updated databank.

To facilitate upward compatibility (that is, allowing you to obtain the same simulation results as in the previous release), the main pure component databank is named according to the major release of Aspen Plus. For example, the pure component databank from Release 8.5-6 is called PURE856 (see PURE856 databank). The pure component data bank delivered with Release 9.3 is called PURE93 (see PURE93 databank).

Table 1.8 and Table 1.9 list 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 in Aspen Plus for upward compatibility. See PURE10 databank for detailed discussions.

Table 1.10 and Table 1.11 list 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 in Aspen Plus for upward compatibility. See PURE10 databank for detailed discussions.

Table 1.9A and Table 1.9B list 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.

Table 1.12 and Table 1.13 list the parameters and components available in the SOLIDS 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.

Table 1.14 and Table 1.15 list the parameters and components available in the COMBUST data bank.

Table 1.2 Parameters Available in the AQUEOUS Databank

Parameter Name	Description
ATOMNO †	Atomic number of each atom in the compound
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 †	Number of occurences of each atom
PLXANT	Antoine liquid vapor pressure coefficients
PRADII	Pauling ion radius
S025C	Criss-Cobble absolute entropy at 25°C
VLBROC	Partial molal volume at infinite dilution

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

†† *Ideal gas at 25°C*

Table 1.3 Components Available in the AQUEOUS Database

Alias	Component Name	Alias	Component Name
AG+	AG+	AGSCN	SILVER-THIOCYANATE
AG+2	AG++	AG(SCN)2-	AG(CNS)2-
AGOH	SILVER-HYDROXIDE	AG(SCN)3-2	AG(CNS)3--
AG(OH)2-	AG(OH)2-	AG(SCN)4-3	AG(CNS)4---
AGF	SILVER-FLUORIDE	AL+3	AL+++
AGCL	SILVER-CHLORIDE	ALO2-	ALO2-
AGCL2-	AGCL2-	ALOH+2	ALOH++
AGBR	SILVER-BROMIDE	AL(OH)4-	AL(OH)4-
AGBR2-	AGBR2-	ALF+2	ALF++
AGBR3-2	AGBR3--	ALF2+	ALF2+
AGCL3BR-3	AGBRCL3---	ALF3	ALUMINIUM-FLUORIDE
AGCLBR3-3	AGBR3CL---	ALF4-	ALF4-
AGI	SILVER-IODIDE	ALF5-2	ALF5--
AGI2-	AGI2-	ALF6-3	ALF6---
AGI3-2	AGI3--	ALSO4+	ALSO4+
AGI4-3	AGI4---	AL(SO4)2-	AL(SO4)2-
AGSO3-	AGSO3-	AR	ARGON
AGSO4-	AGSO4-	ASO+	ASO+
AG(S2O3)2-3	AG(S2O3)2---	ASO2-	ASO2-
AG2SO3	AG2SO3	ASO4-3	ASO4---
AGNO3	SILVER-NITRATE	HASO2	ARSENOUS-ACID
AG(NO2)2-	AG(NO2)2-	HASO4-2	HASO4--
AG(NH3)+	AG(NH3)+	H2ASO3-	H2ASO3-
AG(NH3)2+	AG(NH3)2+	H2ASO4-	H2ASO4-
AG(NH3)2CL	AG(NH3)2CL	H3ASO3	H3ASO3
AG(NH3)2BR	AG(NH3)2BR	H3ASO4	ARSENIC-ACID
AGC2H4+	AGC2H4+	ASO3F-2	ASO3F--
AGCH3CO2	SILVER-ACETATE	HASO3F-	HASO3F-
AG(CH3CO2)2-	AG(CH3COO)2-	AU+	AU+
AG2(CH3CO2)+	AG2(CH3COO)+	AUO3-3	AUO3---
AG(CN)2-	AG(CN)2-	HAUO3-2	HAUO3--
AG(CN)OH-	AG(CN)OH-	H2AUO3-	H2AUO3-
AG(CH3NH2)2+	AG(CH3NH2)2+	AU(OH)3	GOLD-HYDROXIDE
AG(C2H6NH)2+	AG(C2H6NH)2+	AUCL2-	AUCL2-
AG(C2H4NO2)	AG(NH2CH2COO)	AUCL4-	AUCL4-

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
AUBR2-	AUBR2-	CO	CARBON-MONOXIDE
AUBR4-	AUBR4-	CO2	CARBON-DIOXIDE
AU(CN)2-	AU(CN)2-	CO3-2	CO3--
AU(SCN)2-	AU(CNS)2-	CH4	METHANE
AU(SCN)4-	AU(CNS)4-	CHO2-	HCOO-
AU(SCN)5-2	AU(CNS)5-2	HCO3-	HCO3-
AU(SCN)6-3	AU(CNS)6-3	CH2O2	FORMIC-ACID
BO2-	BO2-	H2CO3	CARBONIC-ACID
B4O7-2	B4O7--	CH4O	METHANOL
BH4-	BH4-	CH3CL	METHYL-CHLORIDE
H3BO3	HYDROGEN-ORTHOBORATE	CN-	CN-
B(OH)4-	B(OH)4-	OCN-	CNO-
H4BO5-	H2BO3.H2O2-	CHN	HYDROGEN-CYANIDE
H9B2O10-	H2BO3.H3BO3.(H2O2)2-	CH3NH3+	CH3NH3+
HB4O7-	HB4O7-	NH4CN	AMMONIUM-CYANIDE
H2B4O7	HYDROGEN-TETRABORATE	HOCN	HYDROGEN-CYANATE
BF4-	BF4-	HCOONH4	AMMONIUM-FORMATE
BF2(OH)2-	BF2(OH)2-	CH3NH3OH	CH3NH3OH
BF3OH-	BF3OH-	NH4CNO	AMMONIUM-CYANATE
BA+2	BA++	CH5N3O	NH2CONHNH2
BAOH+	BA(OH)+	I2CN-	I2CN-
BANO3+	BANO3+	SCN-	CNS-
BE+2	BE++	HSCN	HYDROGEN-THIOCYANATE
BEO2-2	BEO2--	C2O4-2	C2O4--
BR-	BR-	C2H4	ETHYLENE
BR2	BROMINE	C2H6	ETHANE
BR3-	BR3-	HC2O4-	HC2O4-
BR5-	BR5-	C2H2O4	OXALIC-ACID
BRO-	BRO-	CH3COO-	CH3COO-
BRO3-	BRO3-	C2H4O2-1	ACETIC-ACID
BRO4-	BRO4-	C2H5O-	CH3CH2O-
HBR	HYDROGEN-BROMIDE	C2H6O-2	ETHANOL
HBRO	HYDROGEN-HYPOBROMITE	C2H7N-2	DIMETHYLAMINE
HBRO3	HYDROGEN-BROMATE	(CH3)2NH2+	(CH3)2NH2+
BR2CL-	BR2CL-	CH5N	METHYL-AMINE

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
NH2COO-	CARBAMATE	CD(CN)4-2	CD(CN)4--
NH2CH2COO-	NH2CH2COO-	CD(CH5N)2+2	CD(NH2CH3)2++
NH2CH2COOH	NH2CH2COOH	CD(CH5N)4+2	CD(NH2CH3)4++
NH3CH2COOH+	NH3CH2COOH+	CE+3	CE+++
C2H9NO	(CH3)2NH2OH	CE+4	CE++++
I(CN)2-	I(CN)2-	CEOH+3	CEOH+++
C2H6NSO3-	NH2(CH2)2SO3-	CECL+2	CECL++
C2H7NSO3	NH2(CH2)2SO3H	CECLO4+2	CECLO4++
C3H9N-3	TRIMETHYL-AMINE	CESO4+	CESO4+
(CH3)3NH+	(CH3)3NH+	CE(SO4)2-	CE(SO4)2-
C3H11NO	(CH3)3NHOH	CECH3CO2+2	CECH3CO2++
C2H8NO+	MEA+	CE(CH3CO2)2+	CE(CH3CO2)2+
C3H6NO3-	MEACOO-	CE(CH3CO2)3	CERIUM-TRIACETATE
C4H12NO2+	DEA+	CL-	CL-
C5H10NO4-	DEACOO-	CL2	CHLORINE
C4H12NOO+	DGA+	CL3-	CL3-
C5H10NOO3-	DGACOO-	CLO-	CLO-
C5H14NO2+	MDEA+	CLO2	CHLORINE-DIOXIDE
C4H12NO+	AMP+	CLO2-	CLO2-
C4H11NO-1	2-AMINO-2-METHYL-1-PROPANOL	CLO3-	CLO3-
CA+2	CA++	CLO4-	CLO4-
CAOH+	CAOH+	CL2O	DICHLORINE-MONOXIDE
CASO4	CALCIUM-SULFATE	HCL	HYDROGEN-CHLORIDE
CACO3	CALCIUM-CARBONATE	HCLO	HYDROGEN-HYPOCHLORITE
CACH3CO2+	CACH3CO2+	HCLO2	CHLOROUS-ACID
CD+2	CD++	HCLO3	CHLORIC-ACID
CDCL+	CDCL+	HCLO4	PERCHLORIC-ACID
CDCL2	CADMIUM-CHLORIDE	CO+2	CO++
CDCL3-	CDCL3-	CO+3	CO+++
CDBR+	CDBR+	COCL+	COCL+
CDI+	CDI+	CO(NH3)+2	CO(NH3)++
CDI3-	CDI3-	CO(NH3)6+3	CO(NH3)6+3
CDI4-2	CDI4--	CO(NH3)6N3+2	CO(NH3)6N3++
CD(NH3)2+2	CD(NH3)2++	CO(NH3)5NO2	CO(NH3)5NO2++
CD(NH3)4+2	CD(NH3)4++	CO(NH3)5CL+2	CO(NH3)5CL++

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
CO(NH3)6CL+2	CO(NH3)6CL++	CUP2O7-2	CUP2O7--
CO(NH3)6BR+2	CO(NH3)6BR++	CU(P2O7)2-6	CU(P2O7)2-6
CO(NH3)6I+2	CO(NH3)6I++	CUN2H6P2O7-2	CU(NH3)2P2O7-2
CO(NH3)6SO4+	CO(NH3)6SO4+	CUC2O4	COPPER-OXALATE
COC2O4	COBALT-OXALATE	CU(C2O4)2-2	CU(C2O4)2--
CO(C2O4)2-2	CO(C2O4)2--	CUCHO2+	CUHCOO+
COC2H4NO2+	CONH2CH2COO+	CUCH3CO2+	CUCH3COO+
CO(C2H4NO2)2	CO(NH2CH2COO)2	CU(CH3CO2)2	COPPER-DIACETATE
CR+2	CR++	CU(CN)2-	CU(CN)2-
CR+3	CR+++	CU(CN)3-2	CU(CN)3--
CRO4-2	CRO4--	CU(CN)4-3	CU(CN)4---
CR2O7-2	CR2O7--	CU(C2H4NO2)+	CU(NH2CH2COO)+
CROH+2	CROH++	CU(C2H4NO2)2	CU(NH2CH2COO)2
HCRO4-	HCRO4-	CUSCN+	CUCNS+
CRCL2+	CRCL2+	CU(SCN)2	COPPER-THIOCYANATE
CS+	CS+	CU(SCN)4-3	CU(CNS)4-3
CU+	CU+	DY+3	DY+3
CU+2	CU++	DYSO4+	DYSO4+
CUO2-2	CUO2--	DY(SO4)2-	DY(SO4)2-
HCUO2-	HCUO2-	DYCH3CO2+2	DYCH3CO2++
CUF+	CUF+	DY(CH3CO2)2+	DY(CH3CO2)2+
CUCL+	CUCL+	DY(CH3CO2)3	DYSPROSIUM-TRIACETATE
CUCL2	COPPER-DICHLORIDE	ER+3	ER+3
CUCL2-	CUCL2-	ERSO4+	ERSO4+
CUCL3-2	CUCL3--	ER(SO4)2-	ER(SO4)2-
CUBR+	CUBR+	ERCH3CO2+2	ERCH3CO2++
CUSO3-	CUSO3-	ER(CH3CO2)2+	ER(CH3CO2)2+
CUSO4	COPPER-SULFATE	ER(CH3CO2)3	ERBIUM-TRIACETATE
CU(SO3)2-3	CU(SO3)2---	EU+2	EU+2
CU(SO3)3-5	CU(SO3)3-5	EU+3	EU+3
CU(NH3)+2	CU(NH3)++	EUCL+2	EUCL++
CU(NH3)2+2	CU(NH3)2++	EUSO4+	EUSO4+
CU(NH3)3+2	CU(NH3)3++	EU(SO4)2-	EU(SO4)2-
CU(NH3)4+2	CU(NH3)4++	F-	F-
CU(NH3)5+2	CU(NH3)5++	HF	HYDROGEN-FLUORIDE

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
HF2-	HF2-	GABR4-	GABR4-
FE+2	FE++	GE+2	GE++
FE+3	FE+++	GE+4	GE+4
FEO2-2	FEO2--	GEOH+3	GE(OH)+++
FEOH+	FEOH+	GE(OH)2+2	GE(OH)2++
FEOH+2	FEOH++	GE(OH)3+	GE(OH)3+
HFEO2-	HFEO2-	GE(OH)4	GERMANIUM-TETRAHYDROXIDE
FE(OH)2+	FE(OH)2+	GE(OH)5-	GE(OH)5-
FE(OH)3	IRON-TRIHYDROXIDE	GE(OH)6-2	GE(OH)6--
FE(OH)3-	FE(OH)3-	GEF6-2	GEF6--
FE(OH)4-2	FE(OH)4--	GEF5-	GEF5-
FE2(OH)2+4	FE2(OH)2+4	GEF4OH-	GEF4OH-
FEF+2	FEF++	GD+3	GD+3
FEF2+	FEF2+	GDSO4+	GDSO4+
FECL+2	FECL++	GD(SO4)2-	GD(SO4)2-
FECL2	IRON-DICHLORIDE	GDCH3CO2+2	GDCH3CO2++
FECL2+	FECL2+	GD(CH3CO2)2+	GD(CH3CO2)2+
FECL3	IRON-TRICHLORIDE	GD(CH3CO2)3	GADOLINIUM-TRIACETATE
FECLO4+2	FECLO4++	H+	H+
FEBR+2	FEBR++	H2	HYDROGEN
FEI+2	FEI++	OH-	OH-
FESO4+	FESO4+	O2H-	HO2-
FE(SO4)2-	FE(SO4)2-	H2O2	HYDROGEN-PEROXIDE
FEN3+2	FEN3++	H2+	H2+
FENO+2	FENO++	H3O+	H3O+
FENO3+2	FENO3++	HE-4	HELIUM
FEHPO4+	FEHPO4+	HG	MERCURY
FE(CN)6-3	FE(CN)6-3	HG+2	HG++
FE(CN)6-4	FE(CN)6-4	HG2+2	HG2++
HFE(CN)6-3	HFE(CN)6-3	HGOH+	HGOH+
H2FE(CN)6-2	H2FE(CN)6--	HHGO2-	HHGO2-
FESCN+2	FESCN++	HG(OH)2	MERCURY-DIHYDROXIDE
GA+3	GA+3	HGF+	HGF+
GAF+2	GAF++	HGCL+	HGCL+
GAF2+	GAF2+	HGCL2	MERCURY-DICHLORIDE

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
HGCL3-	HGCL3-	HG(CN)2CL-	HG(CN)2CL-
HGCL4-2	HGCL4--	HG(CN)3CL-2	HG(CN)3CL--
HGBR+	HGBR+	HGCLC2H4NO2	HGCL(NH2CH2COO)
HGBR2	MERCURY-DIBROMIDE	HG(CN)3BR-2	HG(CN)3BR--
HGBR3-	HGBR3-	HG(SCN)2	MERCURY-THIOCYANATE
HGBR4-2	HGBR4--	HG(SCN)3-	HG(CNS)3-
HGBRCL	HGCLBR	HGSC4N4-2	HG(CNS)(CN)3--
HGI+	HGI+	HG(SCN)4-2	HG(CNS)4-2
HGI2	MERCURY-DIIODIDE	HG(SCN)CL	HG(CNS)CL
HGI3-	HGI3-	HG(SCN)BR	HG(CNS)BR
HGI4-2	HGI4--	HO+3	HO+3
HGICL	HGCLI	HOSO4+	HOSO4+
HGIBR	HGBRI	HO(SO4)2-	HO(SO4)2-
HGIBR3-2	HGIBR3--	HOCH3CO2+2	HOCH3CO2++
HGI2BR2-2	HGBR2I2--	HO(CH3CO2)2+	HO(CH3CO2)2+
HGI3BR-2	HGBRI3--	HO(CH3CO2)3	HOLMIUM-TRIACETATE
HGS2-2	HGS2--	I-	I-
HGSO4	MERCURY-SULFATE	I2	IODINE
HG(HS)2	HG(HS)2	I3-	I3-
HG(NH3)2+2	HG(NH3)2++	IO-	IO-
HG(NH3)3+2	HG(NH3)3++	IO3-	IO3-
HG(NH3)4+2	HG(NH3)4++	IO4-	IO4-
HG2P2O7-2	HG2P2O7--	I2O-2	I2O--
HG2HP2O8-3	HG2(OH)P2O7---	HI	HYDROGEN-IODIDE
HG(C2O4)2-2	HG(C2O4)2--	HIO	HIO
HGCH3COO+	HGCH3COO+	HIO3	IODIC-ACID
HG2HC2O5-	HG2(OH)C2O4-	H2OI+	H2OI+
HGCN+	HGCN+	I2OH-	I2OH-
HG(CN)2	MERCURY-DICYANIDE	ICL	IODINE-CHLORIDE
HG(CN)3-	HG(CN)3-	ICL2-	ICL2-
HG(CN)4-2	HG(CN)4--	I2CL-	I2CL-
HGCH5N+2	HG(CH3NH2)++	IBR	IODINE-BROMIDE
HG(CH5N)2+2	HG(CH3NH2)2++	IBR2-	IBR2-
HGC2H4NO2+	HG(NH2CH2COO)+	BRI2-	BRI2-
HG(C2H4NO2)2	HG(NH2CH2COO)2	HBRI2	HBRI2

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
IBRCL-	IBRCL-	MGF+	MGF+
IN+	IN+	MGIO3+	MGIO3+
IN+2	IN++	MGSO4	MAGNESIUM-SULFATE
IN+3	IN+++	MGP2O7-2	MGP2O7--
INOH+2	INOH++	MGCO3	MAGNESIUM-CARBONATE
IN(OH)2+	IN(OH)2+	MG(C2O4)2-2	MG(C2O4)2--
INSO4+	INSO4+	MGHCO3+	MGHCO3+
INC2O4+	INC2O4+	MGCH3CO2+	MGCH3CO2+
IN(C2O4)2-	IN(C2O4)2-	MN+2	MN++
INSCN+2	INSCN++	MN+3	MN+++
IN(SCN)2+	IN(CNS)2+	MNO4-	MNO4-
IN(SCN)3	INDIUM-THIOCYANATE	MNO4-2	MNO4--
K+	K+	MNOH+	MNOH+
KSO4-	KSO4-	MN(OH)3-	MN(OH)3-
KS2O8-	KS2O8-	MNCL2	MANGANESE-DICHLORIDE
KP2O7-3	KP2O7-3	MNCL3-	MNCL3-
KR	KRYPTON	MNSO4	MANGANESE-SULFATE
LA+3	LA+3	MNC2O4	MANGANESE-OXALATE
LASO4+	LASO4+	MN(C2O4)2-2	MN(C2O4)2--
LA(SO4)2-	LA(SO4)2-	MNHCO3+	MNHCO3+
LACH3CO2+2	LACH3CO2++	MNCH3CO2+	MNCH3COO+
LA(CH3CO2)2+	LA(CH3CO2)2+	MNSCN+	MNCNS+
LA(CH3CO2)3	LANTHANUM-TRIACETATE	MN(SCN)2	MANGANESE-THIOCYANATE
LI+	LI+	MOO4-2	MOO4--
LIOH	LITHIUM-HYDROXIDE	N2	NITROGEN
LISO4-	LISO4-	N3-	N3-
LINO3	LITHIUM-NITRATE	NO2-	NO2-
LIP2O7-3	LIP2O7---	NO3-	NO3-
LIHPO4-	LIHPO4-	H3N	AMMONIA
LIHP2O7-2	LIHP2O7--	NH4+	NH4+
LU+3	LU+3	H4N2	HYDRAZINE
LUSO4+	LUSO4+	N2H5+	N2H5+
LU(SO4)2-	LU(SO4)2-	HN3	HYDROGEN-AZIDE
MG+2	MG++	NH4N3	AMMONIUM-AZIDE
MGOH+	MGOH+	HNO2	HYDROGEN-NITRITE

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
HNO2-1	NITROUS-ACID(CIS)	ND(CH3CO2)3	NEODYMIUM-TRIACETATE
HNO2-2	NITROUS-ACID(TRANS)	NE	NEON
HNO3	NITRIC-ACID	NI+2	NI++
NH4OH	AMMONIUM-HYDROXIDE	NIOH+	NIOH+
NH4HO2	NH4HO2	NISO4	NICKEL-SULFATE
NH4NO2	AMMONIUM-NITRITE	NI(NH3)2+2	NI(NH3)2++
NH4NO3	AMMONIUM-NITRATE	NI(NH3)4+2	NI(NH3)4++
N2H5OH	N2H5OH	NI(NH3)6+2	NI(NH3)6++
N2H5NO3	N2H5NO3	NIP2O7-2	NIP2O7--
NH4F	AMMONIUM-FLUORIDE	NIC2O4	NICKEL-OXALATE
NH4HF2	NH4HF2	NI(CN)4-2	NI(CN)4--
NOCL	NOCL	NI(CH5N)6+2	NI(CH3NH2)6++
NH4CL	AMMONIUM-CHLORIDE	NISCN+	NICNS+
NH4CL3	AMMONIUM-TRICHLORIDE	O2	OXYGEN
N2H5CL	N2H5CL	O3	OZONE
NH4BR	AMMONIUM-BROMIDE	OSO4	OSMIUM-TETROXIDE
N2H5BR	N2H5BR	PO4-3	PO4---
NH4I	AMMONIUM-IODIDE	P2O7-4	P2O7----
NH4HS	NH4HS	PH3	PHOSPHINE
NA+	NA+	PH4+	PH4+
NASO4-	NASO4-	HPO4-2	HPO4--
NAS2O3-	NAS2O3-	H2PO4-	H2PO4-
NA2P2O7-2	NA2P2O7--	H3PO4	ORTHOPHOSPHORIC-ACID
NAHP2O7-2	NAHP2O7--	PH4OH	PH3.H2O
NACO3-	NACO3-	HP2O7-3	HP2O7---
NAHCO3	SODIUM-HYDROGEN-CARBONATE	H2P2O7-2	H2P2O7--
NACLO	SODIUM-HYPOCHLORITE	H3P2O7-	H3P2O7-
NBO2+	NBO2+	H4P2O7	H4P2O7
NBO3-	NBO3-	PO3F-2	PO3F--
HNBO3	HNBO3	HPO3F-	HPO3F-
ND+3	ND+3	H2PO3F	H2PO3F
NDSO4+	NDSO4+	PB+2	PB++
ND(SO4)2-	ND(SO4)2-	PBOH+	PBOH+
NDCH3CO2+2	NDCH3CO2++	HPBO2-	HPBO2-
ND(CH3CO2)2+	ND(CH3CO2)2+	H2PBO2	H2PBO2

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
PB(OH)3-	PB(OH)3-	PRSO4+	PRSO4+
PB3(OH)4+2	PB3(OH)4++	PR(SO4)2-	PR(SO4)2-
PB4(OH)4+4	PB4(OH)4+4	PRNO3+2	PRNO3+2
PB6(OH)8+4	PB6(OH)8+4	PRCH3CO2+2	PRCH3CO2++
PBF+	PBF+	PR(CH3CO2)2+	PR(CH3CO2)2+
PBF2	LEAD-DIFLUORIDE	PR(CH3CO2)3	PRASEODYMIUM-TRIACETATE
PBCL+	PBCL+	PRMOO4+	PRMOO4+
PBCL2	LEAD-DICHLORIDE	PT+2	PT++
PBCL3-	PBCL3-	PTCL4-2	PTCL4--
PBCLO3+	PBCLO3+	PTCL6-2	PTCL6--
PB(CLO3)2	PB(CLO3)2	PTBR4-2	PTBR4--
PBBR+	PBBR+	PTBR6-2	PTBR6--
PBBR2	LEAD-DIBROMIDE	PTI6-2	PTI6--
PBBR3-	PBBR3-	PT(NH3)4+2	PT(NH3)4++
PBBRO3+	PBBRO3+	PT(NH3)CL3-	PT(NH3)CL3-
PBI+	PBI+	PT(NH3)3CL+	PT(NH3)3CL+
PBI2	LEAD-DIIODIDE	RA+2	RA++
PBI3-	PBI3-	RB+	RB+
PBI4-2	PBI4--	RE-	RE-
PBNO3+	PBNO3+	REO4-	REO4-
PBP2O7-2	PBP2O7--	RECL6-2	RECL6--
PBHCO2+	PBHCO2+	RUO4	RUTHENIUM-TETROXIDE
PB(HCO2)2	PB(HCO2)2	S-2	S--
PB(CH3CO2)+	PB(CH3CO2)+	S2-2	S2--
PB(CH3CO2)2	LEAD-DIACETATE	S3-2	S3--
PBSCN+	PBCNS+	S4-2	S4--
PB(SCN)2	LEAD-THIOCYANATE	S5-2	S5--
PD+2	PD++	O2S	SULFUR-DIOXIDE
PDCL+	PDCL+	SO3-2	SO3--
PDBR4-2	PDBR4--	SO4-2	SO4--
PDCL3(C2H4)-	PDCL3(C2H4)-	S2O3-2	S2O3--
PR+3	PR+3	S2O4-2	S2O4--
PROH+2	PROH+2	S2O8-2	S2O8--
PR(OH)2+	PR(OH)2+	S4O6-2	S4O6--
PRCL+2	PRCL++	HS-	HS-

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
H2S	HYDROGEN-SULFIDE	H7SIO6-	HSI(OH)6-
HSO3-	HSO3-	H8SIO6	H2(SI(OH)6)
HSO4-	HSO4-	SIF6-2	SIF6--
H2SO3	SULFUROUS-ACID	SM+3	SM+3
H2SO4	SULFURIC-ACID	SMSO4+	SMSO4+
HS2O4-	HS2O4-	SM(SO4)2-	SM(SO4)2-
H2S2O4	H2S2O4	SMCH3CO2+2	SMCH3CO2++
H2S2O8	HYDROGEN-PEROXODISULFIDE	SM(CH3CO2)2+	SM(CH3CO2)2+
F6S	SULFUR-HEXAFLUORIDE	SM(CH3CO2)3	SAMARIUM-TRIACETATE
SBO+	SBO+	SN+2	SN++
SBO2-	SBO2-	SNOH+	SNOH+
HSBO2	HSBO2	SNOOH+	SNOOH+
SB(OH)3	ANTIMONY-TRIHYDROXIDE	SNF+	SNF+
SB2S4-2	SB2S4--	SNOOHF	SNO(OH)F
SC+3	SC+3	SNOHCL	SNOHCL
SCOH+2	SCOH++	SNOHBR	SNOHBR
SCCL+2	SCCL++	SNSO4+2	SNSO4++
SCCL2+	SCCL2+	SN(SO4)2	TIN-DISULFATE
SCBR+2	SCBR++	SR+2	SR++
SCBR2+	SCBR2+	SROH+	SR(OH)+
SCSEO4+	SCSEO4+	TAO2+	TAO2+
SC(SEO4)2-	SC(SEO4)2-	TAO3-	TAO3-
SE-2	SE--	HTAO3	HTAO3
SEO3-2	SEO3--	TB+3	TB+3
SEO4-2	SEO4--	TBSO4+	TBSO4+
HSE-	HSE-	TB(SO4)2-	TB(SO4)2-
H2SE	H2SE	H2TEO3	TELLURIC-ACID
HSEO3-	HSEO3-	TE(OH)3+	TE(OH)3+
HSEO4-	HSEO4-	TH+4	TH+4
H2SEO3	SELENIOUS-ACID	THOH+3	THOH+3
SIO4-4	SIO4----	TH(OH)2+2	TH(OH)2++
H2SIO3	H2SIO3	TH2(OH)2+6	TH2(OH)2+6
H2SIO4-2	H2SIO4--	THF+3	THF+3
H3SIO4-	H3SIO4-	THF2+2	THF2++
H4SIO4	H4SIO4	THF3+	THF3+

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
THF4	THORIUM-TETRAFLUORIDE	TLCL4-	TLCL4-
THCL+3	THCL+3	TLCLO3	THALLIUM-CHLORATE
THCL2+2	THCL2++	TLBR+	TLBR+
THCL3+	THCL3+	TLBR+2	TLBR++
THCLO3+	THCLO3+	TLBR2+	TLBR2+
THBRO3+3	THBRO3+3	TLBR2-	TLBR2-
TH(BRO3)2+2	TH(BRO3)2++	TLBR3	THALLIUM-TRIBROMIDE
THIO3+3	THIO3+3	TLBR4-	TLBR4-
TH(IO3)2+2	TH(IO3)2++	TLBRCL-	TLBRCL-
TH(IO3)3+	TH(IO3)3+	TLI	THALLIUM-IODIDE
THSO4+2	THSO4++	TLI2-	TLI2-
TH(SO4)3-2	TH(SO4)3--	TLI4-	TLI4-
TH(SO4)4-4	TH(SO4)4-4	TLIBR-	TLIBR-
THNO3+3	THNO3+3	TLSO4-	TLSO4-
TH(NO3)2+2	TH(NO3)2+2	TLNO3	THALLIUM-NITRATE
THH2PO4+3	THH2PO4+3	TLNO3+2	TLNO3++
TH(H2PO4)2+2	TH(H2PO4)2+2	TLNH3+	TLNH3+
THC2O4+2	THC2O4++	TL(CN)4-	TL(CN)4-
TH(C2O4)3-2	TH(C2O4)3-2	TLCNS	THALLIUM-THIOCYANATE
THCH3COO+3	THCH3COO+3	TM+3	TM+3
THSCN+3	THSCN+3	TMSO4+	TMSO4+
TH(SCN)2+2	TH(SCN)2++	TM(SO4)2-	TM(SO4)2-
TH(SCN)3+	TH(SCN)3+	U+3	U+3
TH(SCN)4	TH(SCN)4	U+4	U+4
TL+	TL+	UO2+	UO2+
TL+3	TL+++	UO2+2	UO2++
TLOH	THALLIUM-HYDROXIDE	UOH+3	UOH+3
TLOH+2	TLOH++	UO2OH+	UO2OH+
TL(OH)2+	TL(OH)2+	UO2(OH)2	UO2(OH)2
TLF	THALLIUM-FLUORIDE	U(OH)4	U(OH)4
TLCL	THALLIUM-CHLORIDE	UO2(OH)3-	UO2(OH)3-
TLCL+2	TLCL++	U(OH)5-	U(OH)5-
TLCL2+	TLCL2+	UO2(OH)4-2	UO2(OH)4--
TLCL2-	TLCL2-	(UO2)2OH+3	(UO2)2OH+3
TLCL3	THALLIUM-TRICHLORIDE	(UO2OH)2+2	(UO2OH)2++

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
U3O10H4+2	U3O10H4++	UO2NO3+	UO2NO3+
U3O11H5+	U3O11H5+	U(NO3)2+2	U(NO3)2++
U3O13H7-	U3O13H7-	UO2PO4-	UO2PO4-
U4O15H7+	U4O15H7+	UO2HPO4	UO2HPO4
UF+3	UF+3	UO2H2PO4+	UO2H2PO4+
UF2+2	UF2++	UO2H3PO4+2	UO2H3PO4++
UF3+	UF3+	UO2(H2PO4)2	UO2(H2PO4)2
UF4	UF4	UO2H5P2O8+	UO2H5P2O8+
UF5-	UF5-	UO2CO3	UO2CO3
UF6-2	UF6--	UO2(CO3)2-2	UO2(CO3)2--
UO2F+	UO2F+	UO2(CO3)3-4	UO2(CO3)3-4
UO2F2	UO2F2	UO2(CO3)3-5	UO2(CO3)3-5
UO2F3-	UO2F3-	U(CO3)4-4	U(CO3)4-4
UO2F4-2	UO2F4--	U(CO3)5-6	U(CO3)5-6
UCL+3	UCL+3	U3O6(CO3)6-6	U3O6(CO3)6-6
UO2CL+	UO2CL+	U2CO7(OH)3-	U2CO7(OH)3-
UO2CL2	UO2CL2	USCN+3	USCN+3
UO2CLO3+	UO2CLO3+	U(SCN)2+2	U(SCN)2++
UBR+3	UBR+3	UO2SCN+	UO2SCN+
UO2BR+	UO2BR+	UO2(SCN)2	UO2(SCN)2
UO2BRO3+	UO2BRO3+	UO2(SCN)3-	UO2(SCN)3-
UI+3	UI+3	V+2	V++
UO2IO3+	UO2IO3+	V+3	V+++
UO2(IO3)2	UO2(IO3)2	VO+2	VO++
USO4+2	USO4++	VO2+	VO2+
UO2SO3	UO2SO3	VO3-	VO3-
UO2S2O3	UO2S2O3	HVO4-2	HVO4--
UO2SO4	UO2SO4	H2VO4-	H2VO4-
U(SO4)2	U(SO4)2	VOSCN+	VOSCN+
UO2(SO4)2-2	UO2(SO4)2--	WO4-2	WO4--
UO2N3+	UO2N3+	HWO4-	HWO4-
UO2(N3)2	UO2(N3)2	H2WO4	H2WO4
UO2(N3)3-	UO2(N3)3-	H7(WO4)6-5	H7(WO4)6-5
UO2(N3)4-2	UO2(N3)4--	XE	XENON
UNO3+3	UNO3+3	Y+3	Y+3

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
YOH+2	YOH++	ZNI2	ZINC-DIIODIDE
Y2(OH)2+4	Y2(OH)2+4	ZNI3-	ZNI3-
YCL+2	YCL++	ZNI4-2	ZNI4--
YBR+2	YBR++	ZNSO4	ZINC-SULFATE
YSO4+	YSO4+	ZNN3+	ZNN3+
Y(SO4)2-	Y(SO4)2-	ZNN6	ZN(N3)2
YNO3+2	YNO3++	ZNNH3+2	ZNNH3++
YC2O4+	YC2O4+	ZNN2H4+2	ZNN2H4++
Y(C2O4)2-	Y(C2O4)2-	ZN(NH3)2+2	ZN(NH3)2++
Y(C2O4)3-3	Y(C2O4)3-3	ZN(NH3)3+2	ZN(NH3)3++
YSCN+2	YCNS++	ZN(N2H4)2+2	ZN(N2H4)2++
YB+3	YB+3	ZN(NH3)4+2	ZN(NH3)4++
YBSO4+	YBSO4+	ZN(N2H4)3+2	ZN(N2H4)3++
YB(SO4)2-	YB(SO4)2-	ZN(N2H4)4+2	ZN(N2H4)4++
YBCH3CO2+2	YBCH3CO2++	ZNC2O4	ZINC-OXALATE
YB(CH3CO2)2+	YB(CH3CO2)2+	ZN(C2O4)2-2	ZN(C2O4)2--
YB(CH3CO2)3	YTTERBIUM-TRIACETATE	ZN(CHO2)2	ZINC-FORMATE
ZN+2	ZN++	ZN(CHO2)3-	ZN(CHO2)3-
ZNO2-2	ZNO2--	ZN(CHO2)4-2	ZN(CHO2)4--
ZNOH+	ZNOH+	ZN(CN)4-2	ZN(CN)4--
HZNO2-	HZNO2-	ZN(SCN)2	ZINC-THIOCYANATE
ZN(OH)2	ZINC-DIHYDROXIDE	ZN(SCN)4-2	ZN(CNS)4--
ZN(OH)3-	ZN(OH)3-	ZR+4	ZR+4
ZN(OH)4-2	ZN(OH)4--	ZROH+3	ZR(OH)+++
ZNF+	ZNF+	ZR(OH)2+2	ZR(OH)2++
ZNCL+	ZNCL+	ZR(OH)3+	ZR(OH)3+
ZNCL2	ZINC-DICHLORIDE	ZR(OH)4	ZIRCONIUM-TETRAHYDROXIDE
ZNCL3-	ZNCL3-	ZRSO4+2	ZRSO4++
ZNCL4-2	ZNCL4--	ZR(SO4)2	ZIRCONIUM-DISULFATE
ZNCLO4+	ZNCLO4+	ZR(SO4)3-2	ZR(SO4)3--
ZN(OH)CL	ZN(OH)CL	C4H11N-1	N-BUTYL-AMINE
ZNBR+	ZNBR+	C4H10O-1	N-BUTANOL
ZNBR2	ZINC-DIBROMIDE	C4H8-1	1-BUTENE
ZNBR3-	ZNBR3-	C4H6-1	1-BUTYNE
ZNI+	ZNI+	C7H17N	1-AMINOHEPTANE

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
C7H16O	1-HEPTANOL	C3H7COO-	BUTANOATE
C7H14-7	1-HEPTENE	C4H8O2-1	N-BUTYRIC-ACID
C7H12-D1	1-HEPTYNE	BACO3	BACO3
C6H15N-D2	N-HEXYLAMINE	BACL+	BACL+
C6H14O-1	1-HEXANOL	BAF+	BAF+
C6H12-3	1-HEXENE	CA(HCO3)+	CA(HCO3)+
C6H10-E2	1-HEXYNE	CACL+	CACL+
C8H19N-D0	N-OCTYLAMINE	CACL2	CACL2
C8H18O-1	1-OCTANOL	CAF+	CAF+
C8H16-16	1-OCTENE	CSBR	CSBR
C8H14-D1	1-OCTYNE	CSCL	CSCL
C5H13N	1-PENTYLAMINE	CSI	CSI
C5H12O-1	1-PENTANOL	C2H7N-1	ETHYL-AMINE
C5H10-2	1-PENTENE	C8H10-4	ETHYLBENZENE
C5H8-5	1-PENTYNE	C2H2	ACETYLENE
C3H9N-1	N-PROPYL-AMINE	FE(CH3COO)+	FE(CH3COO)+
C3H8O-1	1-PROPANOL	FE(CH3COO)2	FE(CH3COO)2
C3H6-2	PROPYLENE	FECL+	FECL+
C3H4-2	METHYL-ACETYLENE	C5H9NO4	L-GLUTAMIC-ACID
C4H8O-2	ISOBUTYRALDEHYDE	C5H10N2O3-G	GLUTAMINE
C7H14O-D2	2-HEPTANONE	C2H5NO2-D1	GLYCINE
C6H12O-D3	2-HEXANONE	C6H13COO-	HEPTANOATE
C8H16O-E2	2-OCTANONE	C7H14O2-D3	N-HEPTANOIC-ACID
C5H10O-2	METHYL-N-PROPYL-KETONE	C5H11COO-	HEXANOATE
C4H9NO2	A-AMINOBUTYRIC	C6H12O2-D5	N-HEXANOIC-ACID
C3H6O-1	ACETONE	HSO5-	HSO5-
C3H7NO2	ALANINE	HSIO3-	HSIO3-
C4H8N2O3-A	ASPARAGINE	C6H13NO2-I	ISOLEUCINE
C4H7NO4	ASPARTIC-ACID	KBR	KBR
AG(CO3)-	AG(CO3)-	KCL	KCL
AG(CO3)2-3	AG(CO3)2---	KHSO4	KHSO4
AGCL3-2	AGCL3--	KI	KI
AGCL4-3	AGCL4---	C6H13NO2	LEUCINE
AU+3	AU+++	LICL	LICL
C6H6	BENZENE	C5H11NO2S	METHIONINE

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
MGCL+	MGCL+	S2O6-2	S2O6--
MNCL+	MNCL+	S3O6-2	S3O6--
C4H10-1	N-BUTANE	S5O6-2	S5O6--
C10H14-1	N-BUTYLBENZENE	C3H7NO3	SERINE
C7H16-1	N-HEPTANE	SIO2	SIO2
C13H20	N-HEPTYLBENZENE	SM+2	SM++
C6H14-1	N-HEXANE	SRCO3	SRCO3
C12H18-D3	N-HEXYLBENZENE	SRCL+	SRCL+
C8H18-1	N-OCTANE	SRF+	SRF+
C14H22	N-OCTYLBENZENE	C4H9NO3	THREONINE
C5H12-1	N-PENTANE	C7H8	TOLUENE
C11H16	N-PENTYLBENZENE	C11H12N2O2	TRYPTOPHAN
C9H12-1	N-PROPYLBENZENE	C9H11NO3	TYROSINE
NABR	NABR	C5H11NO2	VALINE
NACL	NACL	YB+2	YB++
NAF	NAF	ZN(CH3COOH)+	ZN(CH3COO)+
NAHSIO3	NAHSIO3	ZN(CH3COOH)2	ZN(CH3COO)2
NAI	NAI	ZN(CH3COO)3-	ZN(CH3COO)3-
NICL+	NICL+	C4H6N2O2	DIKETOPIPERAZINE
C7H15COO-	OCTANOATE	C4H8N2O3-D	DIGLYCINE
C8H16O2-D3	N-OCTANOIC-ACID	C8H16N2O3	LEUCYLGLYCINE
C4H9COO-	PENTANOATE	C5H10N2O3-A	ALANYLGLYCINE
C5H10O2	NEOPENTANOIC-ACID	C2H4O-1	ACETALDEHYDE
C6H6O	PHENOL	C4H8O-1	N-BUTYRALDEHYDE
C9H11NO2	L-PHENYLALANINE	C10H20O	1-DECANAL
C3H8	PROPANE	CH2O	FORMALDEHYDE
C2H5COO-	PROPANOATE	C7H14O-D1	1-HEPTANAL
C3H6O2-1	PROPIONIC-ACID	C6H12O-D2	1-HEXANAL
PBCL4-2	PBCL4--	C9H18O	1-NONANAL
RBBR	RBBR	C8H16O-E1	1-OCTANAL
RBCL	RBCL	C5H10O-1	VALERALDEHYDE
RBF	RBF	C3H6O-3	N-PROPIONALDEHYDE
RBI	RBI	C2H5NO-D1	ACETAMIDE
RN	RN	C4H8O2-3	ETHYL-ACETATE
S2O5-2	S2O5--	BI(AC)+2	BICH3COO+2

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
BI(AC)2+	BI(CH3COO)2+	NI(AC)+	NICH3COO+
BI(AC)3	BI(CH3COO)3	NI(AC)2	NI(CH3COO)2
TM(AC)+2	TMCH3COO+2	NI(AC)3-	NI(CH3COO)3-
TM(AC)2+	TM(CH3COO)2+	CU(AC)3-	CU(CH3COO)3-
TM(AC)3	TM(CH3COO)3	NH4(AC)	NH4CH3COO
BE(AC)+	BECH3COO+	NH4(AC)2-	NH4(CH3COO)2-
BE(AC)2	BE(CH3COO)2	UO2(AC)+	UO2CH3COO+
RA(AC)+	RACH3COO+	UO2(AC)2	UO2(CH3COO)2
RA(AC)2	RA(CH3COO)2	UO2(AC)3-	UO2(CH3COO)3-
AU(AC)	AUCH3COO	CD(AC)+	CDCH3COO+
AU(AC)2-	AU(CH3COO)2-	CD(AC)2	CD(CH3COO)2
LI(AC)	LICH3COO	CD(AC)3-	CD(CH3COO)3-
LI(AC)2-	LI(CH3COO)2-	HG(AC)2	HG(CH3COO)2
NA(AC)	NACH3COO	HG(AC)3-	HG(CH3COO)3-
NA(AC)2-	NA(CH3COO)2-	SC(AC)+2	SCCH3COO+2
K(AC)	KCH3COO	SC(AC)2+	SC(CH3COO)2+
K(AC)2-	K(CH3COO)2-	SC(AC)3	SC(CH3COO)3
MG(AC)2	MG(CH3COO)2	U(AC)+2	UCH3COO+2
SR(AC)+	SRCH3COO+	U(AC)2+	U(CH3COO)2+
SR(AC)2	SR(CH3COO)2	U(AC)3	U(CH3COO)3
BA(AC)+	BACH3COO+	EU(AC)+2	EUCH3COO+2
BA(AC)2	BA(CH3COO)2	EU(AC)2+	EU(CH3COO)2+
CU(AC)	CUCH3COO	EU(AC)3	EU(CH3COO)3
CU(AC)2-	CU(CH3COO)2-	Y(AC)+2	YCH3COO+2
RB(AC)	RBCH3COO	Y(AC)2+	Y(CH3COO)2+
RB(AC)2-	RB(CH3COO)2-	Y(AC)3	Y(CH3COO)3
TL(AC)	TLCH3COO	LU(AC)+2	LUCH3COO+2
TL(AC)2-	TL(CH3COO)2-	LU(AC)2+	LU(CH3COO)2+
CS(AC)	CSCH3COO	LU(AC)3	LU(CH3COO)3
CS(AC)2-	CS(CH3COO)2-	TB(AC)+2	TBCH3COO+2
MN(AC)2	MN(CH3COO)2	TB(AC)2+	TB(CH3COO)2+
MN(AC)3-	MN(CH3COO)3-	TB(AC)3	TB(CH3COO)3
CO(AC)+	COCH3COO+	PB(AC)3-	PB(CH3COO)3-
CO(AC)2	CO(CH3COO)2	CA(AC)2	CA(CH3COO)2
CO(AC)3-	CO(CH3COO)3-	AL(AC)+2	ALCH3COO+2

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
AL(AC)2+	AL(CH3COO)2+	C8H12O4-2	SUBERATE
CH4N2O	UREA	C9H16O4	AZELAIC-ACID
C9H18O2	N-NONANOIC-ACID	C9H15O4-	H-AZELATE
C9H17O2-	NONANOATE	C9H14O4-2	AZELATE
C10H20O2-D1	N-DECANOIC-ACID	C10H18O4	SEBACIC-ACID
C10H19O2-	DECANOATE	C10H17O4-	H-SEBACATE
C11H22O2-D3	N-UNDECANOIC-ACID	C10H16O4-2	SEBACATE
C11H21O2-	UNDECANOATE	C2H4O3-D1	GLYCOLIC-ACID
C12H24O2	N-DODECANOIC-ACID	C2H3O3-	GLYCOLATE
C12H23O2-	DODECANOATE	C3H6O3-D1	LACTIC-ACID
C7H6O2	BENZOIC-ACID	C3H5O3-	LACTATE
C7H5O2-	BENZOATE	C4H8O3	2-HYDROXYBUTANOIC
C8H8O2-D1	O-TOLUIC-ACID	C4H7O3-	2-HYDROXYBUTANOATE
O-C8H7O2-	O-TOLUATE	C5H10O3	2-HYDROXYPENTANOIC
C8H8O2-M	M-TOLUIC-ACID	C5H9O3-	2-HYDROXYPENTANOATE
M-C8H7O2-	M-TOLUATE	C6H12O3	2-HYDROXYHEXANOIC
C8H8O2-D2	P-TOLUIC-ACID	C6H11O3-	2-HYDROXYHEXANOATE
P-C8H7O2-	P-TOLUATE	C7H14O3	2-HYDROXYHEPTANOIC
C3H4O4	MALONIC-ACID	C7H13O3-	2-HYDROXYHEPTANOATE
C3H3O4-	H-MALONATE	C8H16O3	2-HYDROXYOCTANOIC
C3H2O4-2	MALONATE	C8H15O3-	2-HYDROXYOCTANOATE
C4H6O4-2	SUCCINIC-ACID	C9H18O3	2-HYDROXYNONANOIC
C4H5O4-	H-SUCCINATE	C9H17O3-	2-HYDROXYNONANOATE
C4H4O4-2	SUCCINATE	C10H20O3	2-HYDROXYDECANOIC
C5H8O4	GLUTARIC-ACID	C10H19O3-	2-HYDROXYDECANOATE
C5H7O4-	H-GLUTARATE	MG(FOR)+	MGCHO2+
C5H6O4-2	GLUTARATE	MG(FOR)2	MG(CHO2)2
C6H10O4-D1	ADIPIC-ACID	CA(FOR)+	CACHO2+
C6H9O4-	H-ADIPATE	CA(FOR)2	CA(CHO2)2
C6H8O4-2	ADIPATE	SR(FOR)+	SRCHO2+
C7H12O4-D1	PIMELIC-ACID	SR(FOR)2	SR(CHO2)2
C7H11O4-	H-PIMELATE	BA(FOR)+	BACHO2+
C7H10O4-2	PIMELATE	BA(FOR)2	BA(CHO2)2
C8H14O4-D1	SUBERIC-ACID	CU(FOR)2	CU(CHO2)2
C8H13O4-	H-SUBERATE	CD(FOR)+	CDCHO2+

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
CD(FOR)2	CD(CHO2)2	SR(PROP)2	SR(CH3CH2CO2)2
NA(FOR)	NACHO2	BA(PROP)+	BACH3CH2CO2+
NA(FOR)2-	NA(CH02)2-	BA(PROP)2	BA(CH3CH2CO2)2
K(FOR)	KCHO2	MN(PROP)+	MNCH3CH2CO2+
K(FOR)2-	K(CHO2)2-	MN(PROP)2	MN(CH3CH2CO2)2
LA(FOR)+2	LACHO2+2	FE(PROP)+	FECH3CH2CO2+
LA(FOR)2+	LA(CHO2)2+	FE(PROP)2	FE(CH3CH2CO2)2
U(FOR)+2	UCHO2+2	NI(PROP)+	NICH3CH2CO2+
U(FOR)2+	U(CHO2)2+	NI(PROP)2	NI(CH3CH2CO2)2
EU(FOR)+2	EUCHO2+2	CU(PROP)+	CUCH3CH2CO2+
EU(FOR)2+	EU(CHO2)2+	CU(PROP)2	CU(CH3CH2CO2)2
GD(FOR)+2	GDCHO2+2	ZN(PROP)+	ZNCH3CH2CO2+
GD(FOR)2+	GD(CHO2)2+	ZN(PROP)2	ZN(CH3CH2CO2)2
YB(FOR)+2	YBCHO2+2	PB(PROP)+	PBCH3CH2CO2+
YB(FOR)2+	YB(CHO2)2+	PB(PROP)2	PB(CH3CH2CO2)2
MN(FOR)+	MNCHO2+	CO(PROP)+	COCH3CH2CO2+
MN(FOR)2	MN(CHO2)2	CO(PROP)2	CO(CH3CH2CO2)2
CO(FOR)+	COCHO2+	CD(PROP)+	CDCH3CH2CO2+
CO(FOR)2	CO(CHO2)2	CD(PROP)2	CD(CH3CH2CO2)2
NI(FOR)+	NICHO2+	EU(PROP)+	EUCH3CH2CO2+
NI(FOR)2	NI(CHO2)2	EU(PROP)2	EU(CH3CH2CO2)2
ZN(FOR)+	ZNCHO2+	LA(PROP)+2	LACH3CH2CO2+2
FE(FOR)+	FECHO2+	LA(PROP)2+	LA(CH3CH2CO2)2+
FE(FOR)2	FE(CHO2)2	EU(PROP)+2	EUCH3CH2CO2+2
EU(FOR)+	EUCHO2+	EU(PROP)2+	EU(CH3CH2CO2)2+
EU(FOR)2	EU(CHO2)2	GD(PROP)+2	GDCH3CH2CO2+2
NA(PROP)	NACH3CH2CO2	GD(PROP)2+	GD(CH3CH2CO2)2+
NA(PROP)2-	NA(CH3CH2CO2)2-	YB(PROP)+2	YBCH3CH2CO2+2
K(PROP)	KCH3CH2CO2	YB(PROP)2+	YB(CH3CH2CO2)2+
K(PROP)2-	K(CH3CH2CO2)2-	U(PROP)+2	UCH3CH2CO2+2
CA(PROP)+	CACH3CH2CO2+	U(PROP)2+	U(CH3CH2CO2)2+
CA(PROP)2	CA(CH3CH2CO2)2	NA(BUT)	NACH3(CH2)2CO2
MG(PROP)+	MGCH3CH2CO2+	NA(BUT)2-	NA(CH3CH2CH2CO2)2-
MG(PROP)2	MG(CH3CH2CO2)2	K(BUT)	KCH3(CH2)2CO2
SR(PROP)+	SRCH3CH2CO2+	K(BUT)2-	K(CH3CH2CH2CO2)2-

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
CA(BUT)+	CACH3(CH2)2CO2+	U(BUT)2+	U(CH3CH2CH2CO2)2+
CA(BUT)2	CA(CH3CH2CH2CO2)2	NA(PENT)	NACH3(CH2)3CO2
MG(BUT)+	MGCH3(CH2)2CO2+	NA(PENT)2-	NA(CH3CH2CH2CH2CO2)2-
MG(BUT)2	MG(CH3CH2CH2CO2)2	K(PENT)	KCH3(CH2)3CO2
SR(BUT)+	SRCH3(CH2)2CO2+	K(PENT)2-	K(CH3CH2CH2CH2CO2)2-
SR(BUT)2	SR(CH3CH2CH2CO2)2	CA(PENT)+	CACH3(CH2)3CO2+
BA(BUT)+	BACH3(CH2)2CO2+	CA(PENT)2	CA(CH3CH2CH2CH2CO2)2
BA(BUT)2	BA(CH3CH2CH2CO2)2	MG(PENT)+	MGCH3(CH2)3CO2+1
MN(BUT)+	MNCH3(CH2)2CO2+	MG(PENT)2	MG(CH3CH2CH2CH2CO2)2
MN(BUT)2	MN(CH3CH2CH2CO2)2	SR(PENT)+	SRCH3(CH2)3CO2+
FE(BUT)+	FECH3(CH2)2CO2+	SR(PENT)2	SR(CH3CH2CH2CH2CO2)2
FE(BUT)2	FE(CH3CH2CH2CO2)2	BA(PENT)+	BACH3(CH2)3CO2+
NI(BUT)+	NICH3(CH2)2CO2+	BA(PENT)2	BA(CH3CH2CH2CH2CO2)2
NI(BUT)2	NI(CH3CH2CH2CO2)2	MN(PENT)+	MNCH3(CH2)3CO2+
CU(BUT)+	CUCH3(CH2)2CO2+	MN(PENT)2	MN(CH3CH2CH2CH2CO2)2
CU(BUT)2	CU(CH3CH2CH2CO2)2	FE(PENT)+	FECH3(CH2)3CO2+
ZN(BUT)+	ZNCH3(CH2)2CO2+	FE(PENT)2	FE(CH3CH2CH2CH2CO2)2
ZN(BUT)2	ZN(CH3CH2CH2CO2)2	NI(PENT)+	NICH3(CH2)3CO2+
PB(BUT)+	PBCH3(CH2)2CO2+	NI(PENT)2	NI(CH3CH2CH2CH2CO2)2
PB(BUT)2	PB(CH3CH2CH2CO2)2	CU(PENT)+	CUCH3(CH2)3CO2+
CO(BUT)+	COCH3(CH2)2CO2+	CU(PENT)2	CU(CH3CH2CH2CH2CO2)2
CO(BUT)2	CO(CH3CH2CH2CO2)2	ZN(PENT)+	ZNCH3(CH2)3CO2+
CD(BUT)+	CDCH3(CH2)2CO2+	ZN(PENT)2	ZN(CH3CH2CH2CH2CO2)2
CD(BUT)2	CD(CH3CH2CH2CO2)2	PB(PENT)+	PBCH3(CH2)3CO2+
EU(BUT)+	EUCH3(CH2)2CO2+	PB(PENT)2	PB(CH3CH2CH2CH2CO2)2
EU(BUT)2	EU(CH3CH2CH2CO2)2	CO(PENT)+	COCH3(CH2)3CO2+
LA(BUT)+2	LACH3(CH2)2CO2+2	CO(PENT)2	CO(CH3CH2CH2CH2CO2)2
LA(BUT)2+	LA(CH3CH2CH2CO2)2+	CD(PENT)+	CDCH3(CH2)3CO2+
EU(BUT)+2	EUCH3(CH2)2CO2+2	CD(PENT)2	CD(CH3CH2CH2CH2CO2)2
EU(BUT)2+	EU(CH3CH2CH2CO2)2+	EU(PENT)+	EUCH3(CH2)3CO2+
GD(BUT)+2	GDCH3(CH2)2CO2+2	LA(PENT)+2	LACH3(CH2)3CO2+2
GD(BUT)2+	GD(CH3CH2CH2CO2)2+	LA(PENT)2+	LA(CH3CH2CH2CH2CO2)2+
YB(BUT)+2	YBCH3(CH2)2CO2+2	EU(PENT)+2	EUCH3(CH2)3CO2+2
YB(BUT)2+	YB(CH3CH2CH2CO2)2+	EU(PENT)2+	EU(CH3CH2CH2CH2CO2)2+
U(BUT)+2	UCH3(CH2)2CO2+2	GD(PENT)+2	GDCH3(CH2)3CO2+2

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
GD(PENT)2+	GD(CH3CH2CH2CH2CO2)2+	NA(LAC)2-	NA(CH3CH2OCO2)2-
YB(PENT)+2	YBCH3(CH2)3CO2+2	K(LAC)	KCH3CH2OCO2
YB(PENT)2+	YB(CH3CH2CH2CH2CO2)2+	K(LAC)2-	K(CH3CH2OCO2)2-
U(PENT)+2	UCH3(CH2)3CO2+2	CA(LAC)+	CACH3CH2OCO2+
NA(GLYC)	NA(CH3OCO2)	CA(LAC)2	CA(CH3CH2OCO2)2
NA(GLYC)2-	NA(CH3OCO2)2-	MG(LAC)+	MGCH3CH2OCO2+
K(GLYC)	KCH3OCO2	MG(LAC)2	MG(CH3CH2OCO2)2
K(GLYC)2-	K(CH3OCO2)2-	SR(LAC)+	SRCH3CH2OCO2+
CA(GLYC)+	CACH3OCO2+	SR(LAC)2	SR(CH3CH2OCO2)2
CA(GLYC)2	CA(CH3OCO2)2	BA(LAC)+	BACH3CH2OCO2+
MG(GLYC)+	MGCH3OCO2+	BA(LAC)2	BA(CH3CH2OCO2)2
MG(GLYC)2	MG(CH3OCO2)2	MN(LAC)+	MNCH3CH2OCO2+
SR(GLYC)+	SRCH3OCO2+	MN(LAC)2	MN(CH3CH2OCO2)2
SR(GLYC)2	SR(CH3OCO2)2	FE(LAC)+	FECH3CH2OCO2+
BA(GLYC)+	BACH3OCO2+	FE(LAC)2	FE(CH3CH2OCO2)2
BA(GLYC)2	BA(CH3OCO2)2	NI(LAC)+	NICH3CH2OCO2+
MN(GLYC)+	MNCH3OCO2+	NI(LAC)2	NI(CH3CH2OCO2)2
MN(GLYC)2	MN(CH3OCO2)2	CU(LAC)+	CUCH3CH2OCO2+
FE(GLYC)+	FECH3OCO2+	CU(LAC)2	CU(CH3CH2OCO2)2
FE(GLYC)2	FE(CH3OCO2)2	ZN(LAC)+	ZNCH3CH2OCO2+
NI(GLYC)+	NICH3OCO2+	ZN(LAC)2	ZN(CH3CH2OCO2)2
NI(GLYC)2	NI(CH3OCO2)2	PB(LAC)+	PBCH3CH2OCO2+
CU(GLYC)+	CUCH3OCO2+	PB(LAC)2	PB(CH3CH2OCO2)2
CU(GLYC)2	CU(CH3OCO2)2	CO(LAC)+	COCH3CH2OCO2+
ZN(GLYC)+	ZNCH3OCO2+	CO(LAC)2	CO(CH3CH2OCO2)2
ZN(GLYC)2	ZN(CH3OCO2)2	CD(LAC)+	CDCH3CH2OCO2+
PB(GLYC)+	PBCH3OCO2+	CD(LAC)2	CD(CH3CH2OCO2)2
PB(GLYC)2	PB(CH3OCO2)2	EU(LAC)+	EU(CH3CH2OCO2)+
CO(GLYC)+	COCH3OCO2+	EU(LAC)2	EU(CH3CH2OCO2)2
CO(GLYC)2	CO(CH3OCO2)2	CA(GLY)+	CA(C2H4NO2)+
CD(GLYC)+	CDCH3OCO2+	CA(GLY)2	CA(C2H4NO2)2
CD(GLYC)2	CD(CH3OCO2)2	MG(GLY)+	MG(C2H4NO2)+
EU(GLYC)+	EUCH3OCO2+	MG(GLY)2	MG(C2H4NO2)2
EU(GLYC)2	EU(CH3OCO2)2	SR(GLY)+	SR(C2H4NO2)+
NA(LAC)	NACH3CH2OCO2	SR(GLY)2	SR(C2H4NO2)2

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
BA(GLY)+	BA(C2H4NO2)+	PB(ALA)2	PB(C3H6NO2)2
BA(GLY)2	BA(C2H4NO2)2	CO(ALA)+	CO(C3H6NO2)+
MN(GLY)+	MN(C2H4NO2)+	CO(ALA)2	CO(C3H6NO2)2
MN(GLY)2	MN(C2H4NO2)2	CD(ALA)+	CD(C3H6NO2)+
FE(GLY)+	FE(C2H4NO2)+	CD(ALA)2	CD(C3H6NO2)2
FE(GLY)2	FE(C2H4NO2)2	EU(ALA)+	EU(C3H6NO2)+
NI(GLY)+	NI(C2H4NO2)+	EU(ALA)2	EU(C3H6NO2)2
NI(GLY)2	NI(C2H4NO2)2	LACO3+	LACO3+
ZN(GLY)+	ZN(C2H4NO2)+	LAHCO3+2	LAHCO3+2
ZN(GLY)2	ZN(C2H4NO2)2	LAOH+2	LAOH+2
PB(GLY)+	PB(C2H4NO2)+	LAO+	LAO+
PB(GLY)2	PB(C2H4NO2)2	LAO2H	LAO2H,AQ
CD(GLY)+	CD(C2H4NO2)+	LAO2-	LAO2-
CD(GLY)2	CD(C2H4NO2)2	LACL+2	LACL+2
EU(GLY)+	EU(C2H4NO2)+	LACL2+	LACL2+
EU(GLY)2	EU(C2H4NO2)2	LACL3	LACL3,AQ
CA(ALA)+	CA(C3H6NO2)+	LACL4-	LACL4-
CA(ALA)2	CA(C3H6NO2)2	LANO3+2	LANO3+2
MG(ALA)+	MG(C3H6NO2)+	LAF+2	LAF+2
MG(ALA)2	MG(C3H6NO2)2	LAF2+	LAF2+
SR(ALA)+	SR(C3H6NO2)+	LAF3	LAF3,AQ
SR(ALA)2	SR(C3H6NO2)2	LAF4-	LAF4-
BA(ALA)+	BA(C3H6NO2)+	LAH2PO4+2	LAH2PO4+2
BA(ALA)2	BA(C3H6NO2)2	CECO3+	CECO3+
MN(ALA)+	MN(C3H6NO2)+	CEHCO3+2	CEHCO3+2
MN(ALA)2	MN(C3H6NO2)2	CEOH+2	CEOH+2
FE(ALA)+	FE(C3H6NO2)+	CEO+	CEO+
FE(ALA)2	FE(C3H6NO2)2	CEO2H	CEO2H,AQ
NI(ALA)+	NI(C3H6NO2)+	CEO2-	CEO2-
NI(ALA)2	NI(C3H6NO2)2	CECL2+	CECL2+
CU(ALA)+	CU(C3H6NO2)+	CECL3	CECL3,AQ
CU(ALA)2	CU(C3H6NO2)2	CECL4-	CECL4-
ZN(ALA)+	ZN(C3H6NO2)+	CEH2PO4+2	CEH2PO4+2
ZN(ALA)2	ZN(C3H6NO3)2	CENO3+2	CENO3+2
PB(ALA)+	PB(C3H6NO2)+	CEF+2	CEF+2

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
CEF2+	CEF2+	SMOH+2	SMOH+2
CEF3	CEF3,AQ	SMO+	SMO+
CEF4-	CEF4-	SMO2H	SMO2H,AQ
CEBR+2	CEBR+2	SMO2-	SMO2-
CEIO3+2	CEIO3+2	SMHCO3+2	SMHCO3+2
PRCO3+	PRCO3+	SMCL+2	SMCL+2
PRHCO3+2	PRHCO3+2	SMCL2+	SMCL2+
PRCL2+	PRCL2+	SMCL3	SMCL3,AQ
PRCL3	PRCL3,AQ	SMCL4-	SMCL4-
PRCL4-	PRCL4-	SMH2PO4+2	SMH2PO4+2
PRH2PO4+2	PRH2PO4+2	SMNO3+2	SMNO3+2
PRF+2	PRF+2	SMF+2	SMF+2
PRF2+	PRF2+	SMF2+	SMF2+
PRF3	PRF3,AQ	SMF3	SMF3,AQ
PRF4-	PRF4-	SMF4-	SMF4-
PRO+	PRO+	EUCO3+	EUCO3+
PRO2H	PRO2H,AQ	EUOH+2	EUOH+2
PRO2-	PRO2-	EUO+	EUO+
NDCO3+	NDCO3+	EUO2H	EUO2H,AQ
NDHCO3+2	NDHCO3+2	EUO2-	EUO2-
NDOH+2	NDOH+2	EUHCO3+2	EUHCO3+2
NDO+	NDO+	EUCL2+	EUCL2+
NDO2H	NDO2H,AQ	EUCL3	EUCL3,AQ
NDO2-	NDO2-	EUCL4-	EUCL4-
NDCL+2	NDCL+2	EUF+	EUF+
NDCL2+	NDCL2+	EUF2	EUF2,AQ
NDCL3	NDCL3,AQ	EUF3-	EUF3-
NDCL4-	NDCL4-	EUF4-2	EUF4-2
NDH2PO4+2	NDH2PO4+2	EUCL+	EUCL+
NDNO3+2	NDNO3+2	EUCL2	EUCL2,AQ
NDF+2	NDF+2	EUCL3-	EUCL3-
NDF2+	NDF2+	EUCL4-2	EUCL4-2
NDF3	NDF3,AQ	EUH2PO4+2	EUH2PO4+2
NDF4-	NDF4-	EUNO3+2	EUNO3+2
SMCO3+	SMCO3+	EUF+2	EUF+2

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
EUF2+	EUF2+	DYCO3+	DYCO3+
EUF3	EUF3,AQ	DYHCO3+2	DYHCO3+2
EUF4-	EUF4-	DYCL+2	DYCL+2
GDCO3+	GDCO3+	DYCL2+	DYCL2+
GDOH+2	GDOH+2	DYCL3	DYCL3,AQ
GDO+	GDO+	DYCL4-	DYCL4-
GDO2H	GDO2H,AQ	DYH2PO4+2	DYH2PO4+2
GDO2-	GDO2-	DYNO3+2	DYNO3+2
GDHCO3+2	GDHCO3+2	DYF+2	DYF+2
GDCL+2	GDCL+2	DYF2+	DYF2+
GDCL2+	GDCL2+	DYF3	DYF3,AQ
GDCL3	GDCL3,AQ	DYF4-	DYF4-
GDCL4-	GDCL4-	DYOH+2	DYOH+2
GDH2PO4+2	GDH2PO4+2	DYO+	DYO+
GDNO3+2	GDNO3+2	DYO2H	DYO2H,AQ
GDF+2	GDF+2	DYO2-	DYO2-
GDF2+	GDF2+	HOCO3+	HOCO3+
GDF3	GDF3,AQ	HOHCO3+2	HOHCO3+2
GDF4-	GDF4-	HOCL+2	HOCL+2
TBCO3+	TBCO3+	HOCL2+	HOCL2+
TBOH+2	TBOH+2	HOCL3	HOCL3,AQ
TBO+	TBO+	HOCL4-	HOCL4-
TBO2H	TBO2H,AQ	HOH2PO4+2	HOH2PO4+2
TBO2-	TBO2-	HONO3+2	HONO3+2
TBHCO3+2	TBHCO3+2	HOF+2	HOF+2
TBCL+2	TBCL+2	HOF2+	HOF2+
TBCL2+	TBCL2+	HOF3	HOF3,AQ
TBCL3	TBCL3,AQ	HOF4-	HOF4-
TBCL4-	TBCL4-	HOOH+2	HOOH+2
TBH2PO4+2	TBH2PO4+2	HOO+	HOO+
TBNO3+2	TBNO3+2	HOO2H	HOO2H,AQ
TBF+2	TBF+2	HOO2-	HOO2-
TBF2+	TBF2+	ERCO3+	ERCO3+
TBF3	TBF3,AQ	ERHCO3+2	ERHCO3+2
TBF4-	TBF4-	ERCL+2	ERCL+2

continued

Table 1.3 Components Available in the AQUEOUS Database (continued)

Alias	Component Name	Alias	Component Name
ERCL2+	ERCL2+	YBO2-	YBO2-
ERCL3	ERCL3,AQ	YBHCO3+2	YBHCO3+2
ERCL4-	ERCL4-	YBCL+2	YBCL+2
ERH2PO4+2	ERH2PO4+2	YBCL2+	YBCL2+
ERNO3+2	ERNO3+2	YBCL3	YBCL3,AQ
ERF+2	ERF+2	YBCL4-	YBCL4-
ERF2+	ERF2+	YBH2PO4+2	YBH2PO4+2
ERF3	ERF3,AQ	YBNO3+2	YBNO3+2
ERF4-	ERF4-	YBF+2	YBF+2
EROH+2	EROH+2	YBF2+	YBF2+
ERO+	ERO+	YBF3	YBF3,AQ
ERO2H	ERO2H,AQ	YBF4-	YBF4-
ERO2-	ERO2-	LUCO3+	LUCO3+
TMCO3+	TMCO3+	LUOH+2	LUOH+2
TMHCO3+2	TMHCO3+2	LUO+	LUO+
TMCL+2	TMCL+2	LUO2H	LUO2H,AQ
TMCL2+	TMCL2+	LUO2-	LUO2-
TMCL3	TMCL3,AQ	LUHCO3+2	LUHCO3+2
TMCL4-	TMCL4-	LUCL+2	LUCL+2
TMH2PO4+2	TMH2PO4+2	LUCL2+	LUCL2+
TMNO3+2	TMNO3+2	LUCL3	LUCL3,AQ
TMF+2	TMF+2	LUCL4-	LUCL4-
TMF2+	TMF2+	LUH2PO4+2	LUH2PO4+2
TMF3	TMF3,AQ	LUNO3+2	LUNO3+2
TMF4-	TMF4-	LUF+2	LUF+2
TMOH+2	TMOH+2	LUF2+	LUF2+
TMO+	TMO+	LUF3	LUF3,AQ
TMO2H	TMO2H,AQ	LUF4-	LUF4-
TMO2-	TMO2-	KOH	KOH
YBCO3+	YBCO3+	AL(OH)2+	AL(OH)2+
YBOH+2	YBOH+2	HALO2	HALO2
YBO+	YBO+	NAALO2	NAALO2
YBO2H	YBO2H,AQ	NAOH	NAOH

Table 1.3A Parameters Available in the AQU92 Databank

Parameter Name	Description
ATOMNO †	Atomic number of each atom in the compound
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 †	Number of occurences of each atom
PLXANT	Antoine liquid vapor pressure coefficients
PRADII	Pauling ion radius
S025C	Criss-Cobble absolute entropy at 25°C
VLBROC	Partial molal volume at infinite dilution

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

†† *Ideal gas at 25°C*

Table 1.3B Components Available in the AQU92 Databank

Alias	Component Name	Alias	Component Name
(CH3)2NH2+	(CH3)2NH2+	AGI2-	AGI2-
(CH3)3NH+	(CH3)3NH+	AGI3-2	AGI3--
(UO2)2OH+3	(UO2)2OH+3	AGI4-3	AGI4---
(UO2OH)2+2	(UO2OH)2++	AGNO3	SILVER-NITRATE
AG(C2H4NO2)	AG(NH2CH2COO)	AGOH	SILVER-HYDROXIDE
AG(C2H6NH)2+	AG(C2H6NH)2+	AGSCN	SILVER-THIOCYANATE
AG(CH3CO2)2-	AG(CH3COO)2-	AGSO3-	AGSO3-
AG(CH3NH2)2+	AG(CH3NH2)2+	AGSO4-	AGSO4-
AG(CN)2-	AG(CN)2-	AL(OH)4-	AL(OH)4-
AG(CN)OH-	AG(CN)OH-	AL(SO4)2-	AL(SO4)2-
AG(NH3)+	AG(NH3)+	AL+3	AL+++
AG(NH3)2+	AG(NH3)2+	ALF+2	ALF++
AG(NH3)2BR	AG(NH3)2BR	ALF2+	ALF2+
AG(NH3)2CL	AG(NH3)2CL	ALF3	ALUMINIUM-FLUORIDE
AG(NO2)2-	AG(NO2)2-	ALF4-	ALF4-
AG(OH)2-	AG(OH)2-	ALF5-2	ALF5--
AG(S2O3)2-3	AG(S2O3)2---	ALF6-3	ALF6---
AG(SCN)2-	AG(CNS)2-	ALO2-	ALO2-
AG(SCN)3-2	AG(CNS)3--	ALOH+2	ALOH++
AG(SCN)4-3	AG(CNS)4---	ALSO4+	ALSO4+
AG+	AG+	AR	ARGON
AG+2	AG++	ASO+	ASO+
AG2(CH3CO2)+	AG2(CH3COO)+	ASO2-	ASO2-
AG2SO3	AG2SO3	ASO3F-2	ASO3F--
AGBR	SILVER-BROMIDE	ASO4-3	ASO4---
AGBR2-	AGBR2-	AU(CN)2-	AU(CN)2-
AGBR3-2	AGBR3--	AU(OH)3	GOLD-HYDROXIDE
AGC2H4+	AGC2H4+	AU(SCN)2-	AU(CNS)2-
AGCH3CO2	SILVER-ACETATE	AU(SCN)4-	AU(CNS)4-
AGCL	SILVER-CHLORIDE	AU(SCN)5-2	AU(CNS)5-2
AGCL2-	AGCL2-	AU(SCN)6-3	AU(CNS)6-3
AGCL3BR-3	AGBRCL3---	AU+	AU+
AGCLBR3-3	AGBR3CL---	AUBR2-	AUBR2-
AGF	SILVER-FLUORIDE	AUBR4-	AUBR4-
AGI	SILVER-IODIDE	AUCL2-	AUCL2-

continued

Table 1.3B Components Available in the AQU92 Databank (continued)

Alias	Component Name	Alias	Component Name
AUCL4-	AUCL4-	C3H11NO	(CH3)3NHOH
AUO3-3	AUO3---	C3H6NO3-	MEACOO-
B(OH)4-	B(OH)4-	C3H9N-3	TRIMETHYL-AMINE
B4O7-2	B4O7--	C4H11NO-1	2-AMINO-2-METHYL-1-PROPANOL
BA+2	BA++	C4H12NO+	AMP+
BANO3+	BANO3+	C4H12NO2+	DEA+
BAOH+	BA(OH)+	C4H12NOO+	DGA+
BE+2	BE++	C5H10NO4-	DEACOO-
BEO2-2	BEO2--	C5H10NOO3-	DGACOO-
BF2(OH)2-	BF2(OH)2-	C5H14NO2+	MDEA+
BF3OH-	BF3OH-	CA+2	CA++
BF4-	BF4-	CACH3CO2+	CACH3CO2+
BH4-	BH4-	CACO3	CALCIUM-CARBONATE
BO2-	BO2-	CAOH+	CAOH+
BR-	BR-	CASO4	CALCIUM-SULFATE
BR2	BROMINE	CD(CH5N)2+2	CD(NH2CH3)2++
BR2CL-	BR2CL-	CD(CH5N)4+2	CD(NH2CH3)4++
BR3-	BR3-	CD(CN)4-2	CD(CN)4--
BR5-	BR5-	CD(NH3)2+2	CD(NH3)2++
BRI2-	BRI2-	CD(NH3)4+2	CD(NH3)4++
BRO-	BRO-	CD+2	CD++
BRO3-	BRO3-	CDBR+	CDBR+
BRO4-	BRO4-	CDCL+	CDCL+
C2H2O4	OXALIC-ACID	CDCL2	CADMIUM-CHLORIDE
C2H4	ETHYLENE	CDCL3-	CDCL3-
C2H4O2-1	ACETIC-ACID	CDI+	CDI+
C2H5O-	CH3CH2O-	CDI3-	CDI3-
C2H6	ETHANE	CDI4-2	CDI4--
C2H6NSO3-	NH2(CH2)2SO3-	CE(CH3CO2)2+	CE(CH3CO2)2+
C2H6O-2	ETHANOL	CE(CH3CO2)3	CERIUM-TRIACETATE
C2H7N-2	DIMETHYLAMINE	CE(SO4)2-	CE(SO4)2-
C2H7NSO3	NH2(CH2)2SO3H	CE+3	CE+++
C2H8NO+	MEA+	CE+4	CE++++
C2H9NO	(CH3)2NH2OH	CECH3CO2+2	CECH3CO2++
C2O4-2	C2O4--	CECL+2	CECL++

continued

Table 1.3B Components Available in the AQU92 Databank (continued)

Alias	Component Name	Alias	Component Name
CECLO4+2	CECLO4++	CO(NH3)6SO4+	CO(NH3)6SO4+
CEOH+3	CEOH+++	CO+2	CO++
CESO4+	CESO4+	CO+3	CO+++
CH2O2	FORMIC-ACID	CO2	CARBON-DIOXIDE
CH3CL	METHYL-CHLORIDE	CO3-2	CO3--
CH3COO-	CH3COO-	COC2H4NO2+	CONH2CH2COO+
CH3NH3+	CH3NH3+	COC2O4	COBALT-OXALATE
CH3NH3OH	CH3NH3OH	COCL+	COCL+
CH4	METHANE	CR+3	CR+++
CH4O	METHANOL	CR2O7-2	CR2O7--
CH5N	METHYL-AMINE	CRCL2+	CRCL2+
CH5N3O	NH2CONHNH2	CRO4-2	CRO4--
CHN	HYDROGEN-CYANIDE	CROH+2	CROH++
CHO2-	HCOO-	CS+	CS+
CL-	CL-	CU(C2H4NO2)+	CU(NH2CH2COO)+
CL2	CHLORINE	CU(C2H4NO2)2	CU(NH2CH2COO)2
CL2O	DICHLORINE-MONOXIDE	CU(C2O4)2-2	CU(C2O4)2--
CL3-	CL3-	CU(CH3CO2)2	COPPER-DIACETATE
CLO-	CLO-	CU(CN)2-	CU(CN)2-
CLO2	CHLORINE-DIOXIDE	CU(CN)3-2	CU(CN)3--
CLO2-	CLO2-	CU(CN)4-3	CU(CN)4---
CLO3-	CLO3-	CU(NH3)+2	CU(NH3)++
CLO4-	CLO4-	CU(NH3)2+2	CU(NH3)2++
CN-	CN-	CU(NH3)3+2	CU(NH3)3++
CO	CARBON-MONOXIDE	CU(NH3)4+2	CU(NH3)4++
CO(C2H4NO2)2	CO(NH2CH2COO)2	CU(NH3)5+2	CU(NH3)5++
CO(C2O4)2-2	CO(C2O4)2--	CU(P2O7)2-6	CU(P2O7)2-6
CO(NH3)+2	CO(NH3)++	CU(SCN)2	COPPER-THIOCYANATE
CO(NH3)5CL+2	CO(NH3)5CL++	CU(SCN)4-3	CU(CNS)4-3
CO(NH3)5NO2	CO(NH3)5NO2++	CU(SO3)2-3	CU(SO3)2---
CO(NH3)6+3	CO(NH3)6+3	CU(SO3)3-5	CU(SO3)3-5
CO(NH3)6BR+2	CO(NH3)6BR++	CU+	CU+
CO(NH3)6CL+2	CO(NH3)6CL++	CU+2	CU++
CO(NH3)6I+2	CO(NH3)6I++	CUBR+	CUBR+
CO(NH3)6N3+2	CO(NH3)6N3++	CUC2O4	COPPER-OXALATE

continued

Table 1.3B Components Available in the AQU92 Databank (continued)

Alias	Component Name	Alias	Component Name
CUCH3CO2+	CUCH3COO+	FE(OH)3	IRON-TRIHYDROXIDE
CUCHO2+	CUHCOO+	FE(OH)3-	FE(OH)3-
CUCL+	CUCL+	FE(OH)4-2	FE(OH)4--
CUCL2	COPPER-DICHLORIDE	FE(SO4)2-	FE(SO4)2-
CUCL2-	CUCL2-	FE+2	FE++
CUCL3-2	CUCL3--	FE+3	FE+++
CUF+	CUF+	FE2(OH)2+4	FE2(OH)2+4
CUN2H6P2O7-2	CU(NH3)2P2O7-2	FEBR+2	FEBR++
CUO2-2	CUO2--	FECL+2	FECL++
CUP2O7-2	CUP2O7--	FECL2	IRON-DICHLORIDE
CUSCN+	CUCNS+	FECL3	IRON-TRICHLORIDE
CUSO3-	CUSO3-	FECLO4+2	FECLO4++
CUSO4	COPPER-SULFATE	FEF+2	FEF++
DY(CH3CO2)2+	DY(CH3CO2)2+	FEF2+	FEF2+
DY(CH3CO2)3	DYSPROSIUM-TRIACETATE	FEHPO4+	FEHPO4+
DY(SO4)2-	DY(SO4)2-	FEI+2	FEI++
DY+3	DY+3	FEN3+2	FEN3++
DYCH3CO2+2	DYCH3CO2++	FENO+2	FENO++
DYSO4+	DYSO4+	FENO3+2	FENO3++
ER(CH3CO2)2+	ER(CH3CO2)2+	FEO2-2	FEO2--
ER(CH3CO2)3	ERBIUM-TRIACETATE	FEOH+	FEOH+
ER(SO4)2-	ER(SO4)2-	FEOH+2	FEOH++
ER+3	ER+3	FESCN+2	FESCN++
ERCH3CO2+2	ERCH3CO2++	FESO4+	FESO4+
ERSO4+	ERSO4+	GA+3	GA+3
EU(SO4)2-	EU(SO4)2-	GABR4-	GABR4-
EU+2	EU+2	GAF+2	GAF++
EU+3	EU+3	GAF2+	GAF2+
EUCL+2	EUCL++	GD(CH3CO2)2+	GD(CH3CO2)2+
EUSO4+	EUSO4+	GD(CH3CO2)3	GADOLINIUM-TRIACETATE
F-	F-	GD(SO4)2-	GD(SO4)2-
F6S	SULFUR-HEXAFLUORIDE	GD+3	GD+3
FE(CN)6-3	FE(CN)6-3	GDCH3CO2+2	GDCH3CO2++
FE(CN)6-4	FE(CN)6-4	GDSO4+	GDSO4+
FE(OH)2+	FE(OH)2+	GE(OH)2+2	GE(OH)2++

continued

Table 1.3B Components Available in the AQU92 Databank (continued)

Alias	Component Name	Alias	Component Name
GE(OH)3+	GE(OH)3+	H2VO4-	H2VO4-
GE(OH)4	GERMANIUM-TETRAHYDROXIDE	H2WO4	H2WO4
GE(OH)5-	GE(OH)5-	H3ASO3	H3ASO3
GE(OH)6-2	GE(OH)6--	H3ASO4	ARSENIC-ACID
GE+2	GE++	H3BO3	HYDROGEN-ORTHOBORATE
GE+4	GE+4	H3N	AMMONIA
GEF4OH-	GEF4OH-	H3O+	H3O+
GEF5-	GEF5-	H3P2O7-	H3P2O7-
GEF6-2	GEF6--	H3PO4	ORTHOPHOSPHORIC-ACID
GEOH+3	GE(OH)+++	H3SIO4-	H3SIO4-
H+	H+	H4BO5-	H2BO3.H2O2-
H2	HYDROGEN	H4N2	HYDRAZINE
H2+	H2+	H4P2O7	H4P2O7
H2ASO3-	H2ASO3-	H4SIO4	H4SIO4
H2ASO4-	H2ASO4-	H7(WO4)6-5	H7(WO4)6-5
H2AUO3-	H2AUO3-	H7SIO6-	HSI(OH)6-
H2B4O7	HYDROGEN-TETRABORATE	H8SIO6	H2(SI(OH)6)
H2CO3	CARBONIC-ACID	H9B2O10-	H2BO3.H3BO3.(H2O2)2-
H2FE(CN)6-2	H2FE(CN)6--	HASO2	ARSENOUS-ACID
H2O2	HYDROGEN-PEROXIDE	HASO3F-	HASO3F-
H2OI+	H2OI+	HASO4-2	HASO4--
H2P2O7-2	H2P2O7--	HAUO3-2	HAUO3--
H2PBO2	H2PBO2	HB4O7-	HB4O7-
H2PO3F	H2PO3F	HBR	HYDROGEN-BROMIDE
H2PO4-	H2PO4-	HBRI2	HBRI2
H2S	HYDROGEN-SULFIDE	HBRO	HYDROGEN-HYPOBROMITE
H2S2O4	H2S2O4	HBRO3	HYDROGEN-BROMATE
H2S2O8	HYDROGEN-PEROXODISULFIDE	HC2O4-	HC2O4-
H2SE	H2SE	HCL	HYDROGEN-CHLORIDE
H2SEO3	SELENIOUS-ACID	HCLO	HYDROGEN-HYPOCHLORITE
H2SIO3	H2SIO3	HCLO2	CHLOROUS-ACID
H2SIO4-2	H2SIO4--	HCLO3	CHLORIC-ACID
H2SO3	SULFUROUS-ACID	HCLO4	PERCHLORIC-ACID
H2SO4	SULFURIC-ACID	HCO3-	HCO3-
H2TEO3	TELLURIC-ACID	HCOONH4	AMMONIUM-FORMATE

continued

Table 1.3B Components Available in the AQU92 Databank (continued)

Alias	Component Name	Alias	Component Name
HCRO4-	HCRO4-	HGBR4-2	HGBR4--
HCUO2-	HCUO2-	HGBRCL	HGCLBR
HE-4	HELIUM	HGC2H4NO2+	HG(NH2CH2COO)+
HF	HYDROGEN-FLUORIDE	HGCH3COO+	HGCH3COO+
HF2-	HF2-	HGCH5N+2	HG(CH3NH2)++
HFE(CN)6-3	HFE(CN)6-3	HGCL+	HGCL+
HFEO2-	HFEO2-	HGCL2	MERCURY-DICHLORIDE
HG	MERCURY	HGCL3-	HGCL3-
HG(C2H4NO2)2	HG(NH2CH2COO)2	HGCL4-2	HGCL4--
HG(C2O4)2-2	HG(C2O4)2--	HGCLC2H4NO2	HGCL(NH2CH2COO)
HG(CH5N)2+2	HG(CH3NH2)2++	HGCN+	HGCN+
HG(CN)2	MERCURY-DICYANIDE	HGF+	HGF+
HG(CN)2CL-	HG(CN)2CL-	HGI+	HGI+
HG(CN)3-	HG(CN)3-	HGI2	MERCURY-DIIODIDE
HG(CN)3BR-2	HG(CN)3BR--	HGI2BR2-2	HGBR2I2--
HG(CN)3CL-2	HG(CN)3CL--	HGI3-	HGI3-
HG(CN)4-2	HG(CN)4--	HGI3BR-2	HGBRI3--
HG(HS)2	HG(HS)2	HGI4-2	HGI4--
HG(NH3)2+2	HG(NH3)2++	HGIBR	HGBRI
HG(NH3)3+2	HG(NH3)3++	HGIBR3-2	HGIBR3--
HG(NH3)4+2	HG(NH3)4++	HGICL	HGCLI
HG(OH)2	MERCURY-DIHYDROXIDE	HGOH+	HGOH+
HG(SCN)2	MERCURY-THIOCYANATE	HGS2-2	HGS2--
HG(SCN)3-	HG(CNS)3-	HGSC4N4-2	HG(CNS)(CN)3--
HG(SCN)4-2	HG(CNS)4-2	HGSO4	MERCURY-SULFATE
HG(SCN)BR	HG(CNS)BR	HHGO2-	HHGO2-
HG(SCN)CL	HG(CNS)CL	HI	HYDROGEN-IODIDE
HG+2	HG++	HIO	HIO
HG2+2	HG2++	HIO3	IODIC-ACID
HG2HC2O5-	HG2(OH)C2O4-	HN3	HYDROGEN-AZIDE
HG2HP2O8-2	HG2(OH)P2O7--	HNBO3	HNBO3
HG2P2O7-2	HG2P2O7--	HNO2	HYDROGEN-NITRITE
HGBR+	HGBR+	HNO2-1	NITROUS-ACID(CIS)
HGBR2	MERCURY-DIBROMIDE	HNO2-2	NITROUS-ACID(TRANS)
HGBR3-	HGBR3-	HNO3	NITRIC-ACID

continued

Table 1.3B Components Available in the AQU92 Databank (continued)

Alias	Component Name	Alias	Component Name
HO(CH3CO2)2+	HO(CH3CO2)2+	ICL	IODINE-CHLORIDE
HO(CH3CO2)3	HOLMIUM-TRIACETATE	ICL2-	ICL2-
HO(SO4)2-	HO(SO4)2-	IN(C2O4)2-	IN(C2O4)2-
HO+3	HO+3	IN(OH)2+	IN(OH)2+
HOCH3CO2+2	HOCH3CO2++	IN(SCN)2+	IN(CNS)2+
HOCN	HYDROGEN-CYANATE	IN(SCN)3	INDIUM-THIOCYANATE
HOSO4+	HOSO4+	IN+	IN+
HP2O7-3	HP2O7---	IN+2	IN++
HPBO2-	HPBO2-	IN+3	IN+++
HPO3F-	HPO3F-	INC2O4+	INC2O4+
HPO4-2	HPO4--	INOH+2	INOH++
HS-	HS-	INSCN+2	INSCN++
HS2O4-	HS2O4-	INSO4+	INSO4+
HSBO2	HSBO2	IO-	IO-
HSCN	HYDROGEN-THIOCYANATE	IO3-	IO3-
HSE-	HSE-	IO4-	IO4-
HSEO3-	HSEO3-	K+	K+
HSEO4-	HSEO4-	KP2O7-3	KP2O7-3
HSO3-	HSO3-	KR	KRYPTON
HSO4-	HSO4-	KS2O8-	KS2O8-
HTAO3	HTAO3	KSO4-	KSO4-
HVO4-2	HVO4--	LA(CH3CO2)2+	LA(CH3CO2)2+
HWO4-	HWO4-	LA(CH3CO2)3	LANTHANUM-TRIACETATE
HZNO2-	HZNO2-	LA(SO4)2-	LA(SO4)2-
I(CN)2-	I(CN)2-	LA+3	LA+3
I-	I-	LACH3CO2+2	LACH3CO2++
I2	IODINE	LASO4+	LASO4+
I2CL-	I2CL-	LI+	LI+
I2CN-	I2CN-	LIHP2O7-2	LIHP2O7--
I2O-2	I2O--	LIHPO4-	LIHPO4-
I2OH-	I2OH-	LINO3	LITHIUM-NITRATE
I3-	I3-	LIOH	LITHIUM-HYDROXIDE
IBR	IODINE-BROMIDE	LIP2O7-3	LIP2O7---
IBR2-	IBR2-	LISO4-	LISO4-
IBRCL-	IBRCL-	LU(SO4)2-	LU(SO4)2-

continued

Table 1.3B Components Available in the AQU92 Databank (continued)

Alias	Component Name	Alias	Component Name
LU+3	LU+3	NA+	NA+
LUSO4+	LUSO4+	NA2P2O7-2	NA2P2O7--
MG(C2O4)2-2	MG(C2O4)2--	NACLO	SODIUM-HYPOCHLORITE
MG+2	MG++	NACO3-	NACO3-
MGCH3CO2+	MGCH3CO2+	NAHCO3	SODIUM-HYDROGEN-CARBONATE
MGCO3	MAGNESIUM-CARBONATE	NAHP2O7-2	NAHP2O7--
MGF+	MGF+	NAS2O3-	NAS2O3-
MGHCO3+	MGHCO3+	NASO4-	NASO4-
MGIO3+	MGIO3+	NBO2+	NBO2+
MGOH+	MGOH+	NBO3-	NBO3-
MGP2O7-2	MGP2O7--	ND(CH3CO2)2+	ND(CH3CO2)2+
MGSO4	MAGNESIUM-SULFATE	ND(CH3CO2)3	NEODYMIUM-TRIACETATE
MN(C2O4)2-2	MN(C2O4)2--	ND(SO4)2-	ND(SO4)2-
MN(OH)3-	MN(OH)3-	ND+3	ND+3
MN(SCN)2	MANGANESE-THIOCYANATE	NDCH3CO2+2	NDCH3CO2++
MN+2	MN++	NDSO4+	NDSO4+
MN+3	MN+++	NE	NEON
MNC2O4	MANGANESE-OXALATE	NH2CH2COO-	NH2CH2COO-
MNCH3CO2+	MNCH3COO+	NH2CH2COOH	NH2CH2COOH
MNCL2	MANGANESE-DICHLORIDE	NH2COO-	CARBAMATE
MNCL3-	MNCL3-	NH3CH2COOH+	NH3CH2COOH+
MNHCO3+	MNHCO3+	NH4+	NH4+
MNO4-	MNO4-	NH4BR	AMMONIUM-BROMIDE
MNO4-2	MNO4--	NH4CL	AMMONIUM-CHLORIDE
MNOH+	MNOH+	NH4CL3	AMMONIUM-TRICHLORIDE
MNSCN+	MNCNS+	NH4CN	AMMONIUM-CYANIDE
MNSO4	MANGANESE-SULFATE	NH4CNO	AMMONIUM-CYANATE
MOO4-2	MOO4--	NH4F	AMMONIUM-FLUORIDE
N2	NITROGEN	NH4HF2	NH4HF2
N2H5+	N2H5+	NH4HO2	NH4HO2
N2H5BR	N2H5BR	NH4HS	NH4HS
N2H5CL	N2H5CL	NH4I	AMMONIUM-IODIDE
N2H5NO3	N2H5NO3	NH4N3	AMMONIUM-AZIDE
N2H5OH	N2H5OH	NH4NO2	AMMONIUM-NITRITE
N3-	N3-	NH4NO3	AMMONIUM-NITRATE

continued

Table 1.3B Components Available in the AQU92 Databank (continued)

Alias	Component Name	Alias	Component Name
NH4OH	AMMONIUM-HYDROXIDE	PBBRO3+	PBBRO3+
NI(CH5N)6+2	NI(CH3NH2)6++	PBCL+	PBCL+
NI(CN)4-2	NI(CN)4--	PBCL2	LEAD-DICHLORIDE
NI(NH3)2+2	NI(NH3)2++	PBCL3-	PBCL3-
NI(NH3)6+2	NI(NH3)6++	PBCLO3+	PBCLO3+
NI+2	NI++	PBF+	PBF+
NIC2O4	NICKEL-OXALATE	PBF2	LEAD-DIFLUORIDE
NIOH+	NIOH+	PBHCO2+	PBHCO2+
NIP2O7-2	NIP2O7--	PBI+	PBI+
NISCN+	NICNS+	PBI2	LEAD-DIIODIDE
NISO4	NICKEL-SULFATE	PBI3-	PBI3-
NO2-	NO2-	PBI4-2	PBI4--
NO3-	NO3-	PBNO3+	PBNO3+
NOCL	NOCL	PBOH+	PBOH+
O2	OXYGEN	PBP2O7-2	PBP2O7--
O2H-	HO2-	PBSCN+	PBCNS+
O2S	SULFUR-DIOXIDE	PD+2	PD++
O3	OZONE	PDBR4-2	PDBR4--
OCN-	CNO-	PDCL+	PDCL+
OH-	OH-	PDCL3(C2H4)-	PDCL3(C2H4)-
OSO4	OSMIUM-TETROXIDE	PH3	PHOSPHINE
P2O7-4	P2O7----	PH4+	PH4+
PB(CH3CO2)+	PB(CH3CO2)+	PH4OH	PH3.H2O
PB(CH3CO2)2	LEAD-DIACETATE	PO3F-2	PO3F--
PB(CLO3)2	PB(CLO3)2	PO4-3	PO4---
PB(HCO2)2	PB(HCO2)2	PR(CH3CO2)2+	PR(CH3CO2)2+
PB(OH)3-	PB(OH)3-	PR(CH3CO2)3	PRASEODYMIUM-TRIACETATE
PB(SCN)2	LEAD-THIOCYANATE	PR(OH)2+	PR(OH)2+
PB+2	PB++	PR(SO4)2-	PR(SO4)2-
PB3(OH)4+2	PB3(OH)4++	PR+3	PR+3
PB4(OH)4+4	PB4(OH)4+4	PRCH3CO2+2	PRCH3CO2++
PB6(OH)8+4	PB6(OH)8+4	PRCL+2	PRCL++
PBBR+	PBBR+	PRMOO4+	PRMOO4+
PBBR2	LEAD-DIBROMIDE	PRNO3+2	PRNO3+2
PBBR3-	PBBR3-	PROH+2	PROH+2

continued

Table 1.3B Components Available in the AQU92 Databank (continued)

Alias	Component Name	Alias	Component Name
PRSO4+	PRSO4+	SCN-	CNS-
PT(NH3)3CL+	PT(NH3)3CL+	SCOH+2	SCOH++
PT(NH3)4+2	PT(NH3)4++	SCSEO4+	SCSEO4+
PT(NH3)CL3-	PT(NH3)CL3-	SE-2	SE--
PT+2	PT++	SEO3-2	SEO3--
PTBR4-2	PTBR4--	SEO4-2	SEO4--
PTBR6-2	PTBR6--	SIF6-2	SIF6--
PTCL4-2	PTCL4--	SIO4-4	SIO4----
PTCL6-2	PTCL6--	SM(CH3CO2)2+	SM(CH3CO2)2+
PTI6-2	PTI6--	SM(CH3CO2)3	SAMARIUM-TRIACETATE
RA+2	RA++	SM(SO4)2-	SM(SO4)2-
RB+	RB+	SM+3	SM+3
RE-	RE-	SMCH3CO2+2	SMCH3CO2++
RECL6-2	RECL6--	SMSO4+	SMSO4+
REO4-	REO4-	SN(SO4)2	TIN-DISULFATE
RUO4	RUTHENIUM-TETROXIDE	SN+2	SN++
S-2	S--	SNF+	SNF+
S2-2	S2--	SNOH+	SNOH+
S2O3-2	S2O3--	SNOHBR	SNOHBR
S2O4-2	S2O4--	SNOHCL	SNOHCL
S2O8-2	S2O8--	SNOOH+	SNOOH+
S3-2	S3--	SNOOHF	SNO(OH)F
S4-2	S4--	SNSO4+2	SNSO4++
S4O6-2	S4O6--	SO3-2	SO3--
S5-2	S5--	SO4-2	SO4--
SB(OH)3	ANTIMONY-TRIHYDROXIDE	SR+2	SR++
SB2S4-2	SB2S4--	SROH+	SR(OH)+
SBO+	SBO+	TAO2+	TAO2+
SBO2-	SBO2-	TAO3-	TAO3-
SC(SEO4)2-	SC(SEO4)2-	TB(SO4)2-	TB(SO4)2-
SC+3	SC+3	TB+3	TB+3
SCBR+2	SCBR++	TBSO4+	TBSO4+
SCBR2+	SCBR2+	TE(OH)3+	TE(OH)3+
SCCL+2	SCCL++	TH(BRO3)2+2	TH(BRO3)2++
SCCL2+	SCCL2+	TH(C2O4)3-2	TH(C2O4)3-2

continued

Table 1.3B Components Available in the AQU92 Databank (continued)

Alias	Component Name	Alias	Component Name
TH(H2PO4)2+2	TH(H2PO4)2+2	TLBR2+	TLBR2+
TH(IO3)2+2	TH(IO3)2++	TLBR2-	TLBR2-
TH(IO3)3+	TH(IO3)3+	TLBR3	THALLIUM-TRIBROMIDE
TH(NO3)2+2	TH(NO3)2+2	TLBR4-	TLBR4-
TH(OH)2+2	TH(OH)2++	TLBRCL-	TLBRCL-
TH(SCN)2+2	TH(SCN)2++	TLCL	THALLIUM-CHLORIDE
TH(SCN)3+	TH(SCN)3+	TLCL+2	TLCL++
TH(SCN)4	TH(SCN)4	TLCL2+	TLCL2+
TH(SO4)3-2	TH(SO4)3--	TLCL2-	TLCL2-
TH(SO4)4-4	TH(SO4)4-4	TLCL3	THALLIUM-TRICHLORIDE
TH+4	TH+4	TLCL4-	TLCL4-
TH2(OH)2+6	TH2(OH)2+6	TLCLO3	THALLIUM-CHLORATE
THBRO3+3	THBRO3+3	TLCNS	THALLIUM-THIOCYANATE
THC2O4+2	THC2O4++	TLF	THALLIUM-FLUORIDE
THCH3COO+3	THCH3COO+3	TLI	THALLIUM-IODIDE
THCL+3	THCL+3	TLI2-	TLI2-
THCL2+2	THCL2++	TLI4-	TLI4-
THCL3+	THCL3+	TLIBR-	TLIBR-
THCLO3+	THCLO3+	TLNH3+	TLNH3+
THF+3	THF+3	TLNO3	THALLIUM-NITRATE
THF2+2	THF2++	TLNO3+2	TLNO3++
THF3+	THF3+	TLOH	THALLIUM-HYDROXIDE
THF4	THORIUM-TETRAFLUORIDE	TLOH+2	TLOH++
THH2PO4+3	THH2PO4+3	TLSO4-	TLSO4-
THIO3+3	THIO3+3	TM(SO4)2-	TM(SO4)2-
THNO3+3	THNO3+3	TM+3	TM+3
THOH+3	THOH+3	TMSO4+	TMSO4+
THSCN+3	THSCN+3	U(CO3)4-4	U(CO3)4-4
THSO4+2	THSO4++	U(CO3)5-6	U(CO3)5-6
TL(CN)4-	TL(CN)4-	U(NO3)2+2	U(NO3)2++
TL(OH)2+	TL(OH)2+	U(OH)4	U(OH)4
TL+	TL+	U(OH)5-	U(OH)5-
TL+3	TL+++	U(SCN)2+2	U(SCN)2++
TLBR+	TLBR+	U(SO4)2	U(SO4)2
TLBR+2	TLBR++	U+3	U+3

continued

Table 1.3B Components Available in the AQU92 Databank (continued)

Alias	Component Name	Alias	Component Name
U+4	U+4	UO2CL+	UO2CL+
U2CO7(OH)3-	U2CO7(OH)3-	UO2CL2	UO2CL2
U3O10H4+2	U3O10H4++	UO2CLO3+	UO2CLO3+
U3O11H5+	U3O11H5+	UO2CO3	UO2CO3
U3O13H7-	U3O13H7-	UO2F+	UO2F+
U3O6(CO3)6-6	U3O6(CO3)6-6	UO2F2	UO2F2
U4O15H7+	U4O15H7+	UO2F3-	UO2F3-
UBR+3	UBR+3	UO2F4-2	UO2F4--
UCL+3	UCL+3	UO2H2PO4+	UO2H2PO4+
UF+3	UF+3	UO2H3PO4+2	UO2H3PO4++
UF2+2	UF2++	UO2H5P2O8+	UO2H5P2O8+
UF3+	UF3+	UO2HPO4	UO2HPO4
UF4	UF4	UO2IO3+	UO2IO3+
UF5-	UF5-	UO2N3+	UO2N3+
UF6-2	UF6--	UO2NO3+	UO2NO3+
UI+3	UI+3	UO2OH+	UO2OH+
UNO3+3	UNO3+3	UO2PO4-	UO2PO4-
UO2(CO3)2-2	UO2(CO3)2--	UO2S2O3	UO2S2O3
UO2(CO3)3-4	UO2(CO3)3-4	UO2SCN+	UO2SCN+
UO2(CO3)3-5	UO2(CO3)3-5	UO2SO3	UO2SO3
UO2(H2PO4)2	UO2(H2PO4)2	UO2SO4	UO2SO4
UO2(IO3)2	UO2(IO3)2	UOH+3	UOH+3
UO2(N3)2	UO2(N3)2	USCN+3	USCN+3
UO2(N3)3-	UO2(N3)3-	USO4+2	USO4++
UO2(N3)4-2	UO2(N3)4--	V+2	V++
UO2(OH)2	UO2(OH)2	V+3	V+++
UO2(OH)3-	UO2(OH)3-	VO+2	VO++
UO2(OH)4-2	UO2(OH)4--	VO2+	VO2+
UO2(SCN)2	UO2(SCN)2	VO3-	VO3-
UO2(SCN)3-	UO2(SCN)3-	VOSCN+	VOSCN+
UO2(SO4)2-2	UO2(SO4)2--	WO4-2	WO4--
UO2+	UO2+	XE	XENON
UO2+2	UO2++	Y(C2O4)2-	Y(C2O4)2-
UO2BR+	UO2BR+	Y(C2O4)3-3	Y(C2O4)3-3
UO2BRO3+	UO2BRO3+	Y(SO4)2-	Y(SO4)2-

continued

Table 1.3B Components Available in the AQU92 Databank (continued)

Alias	Component Name	Alias	Component Name
Y+3	Y+3	ZN(SCN)4-2	ZN(CNS)4--
Y2(OH)2+4	Y2(OH)2+4	ZN+2	ZN++
YB(CH3CO2)2+	YB(CH3CO2)2+	ZNBR+	ZNBR+
YB(CH3CO2)3	YTTERBIUM-TRIACETATE	ZNBR2	ZINC-DIBROMIDE
YB(SO4)2-	YB(SO4)2-	ZNBR3-	ZNBR3-
YB+3	YB+3	ZNC2O4	ZINC-OXALATE
YBCH3CO2+2	YBCH3CO2++	ZNCL+	ZNCL+
YBR+2	YBR++	ZNCL2	ZINC-DICHLORIDE
YBSO4+	YBSO4+	ZNCL3-	ZNCL3-
YC2O4+	YC2O4+	ZNCL4-2	ZNCL4--
YCL+2	YCL++	ZNCLO4+	ZNCLO4+
YNO3+2	YNO3++	ZNF+	ZNF+
YOH+2	YOH++	ZNI+	ZNI+
YSCN+2	YCNS++	ZNI2	ZINC-DIIODIDE
YSO4+	YSO4+	ZNI3-	ZNI3-
ZN(C2O4)2-2	ZN(C2O4)2--	ZNI4-2	ZNI4--
ZN(CHO2)2	ZINC-FORMATE	ZNN2H4+2	ZNN2H4++
ZN(CHO2)3-	ZN(CHO2)3-	ZNN3+	ZNN3+
ZN(CHO2)4-2	ZN(CHO2)4--	ZNN6	ZN(N3)2
ZN(CN)4-2	ZN(CN)4--	ZNNH3+2	ZNNH3++
ZN(N2H4)2+2	ZN(N2H4)2++	ZNO2-2	ZNO2--
ZN(N2H4)3+2	ZN(N2H4)3++	ZNOH+	ZNOH+
ZN(N2H4)4+2	ZN(N2H4)4++	ZNSO4	ZINC-SULFATE
ZN(NH3)2+2	ZN(NH3)2++	ZR(OH)2+2	ZR(OH)2++
ZN(NH3)3+2	ZN(NH3)3++	ZR(OH)3+	ZR(OH)3+
ZN(NH3)4+2	ZN(NH3)4++	ZR(OH)4	ZIRCONIUM-TETRAHYDROXIDE
ZN(OH)2	ZINC-DIHYDROXIDE	ZR(SO4)2	ZIRCONIUM-DISULFATE
ZN(OH)3-	ZN(OH)3-	ZR(SO4)3-2	ZR(SO4)3--
ZN(OH)4-2	ZN(OH)4--	ZR+4	ZR+4
ZN(OH)CL	ZN(OH)CL	ZROH+3	ZR(OH)+++
ZN(SCN)2	ZINC-THIOCYANATE	ZRSO4+2	ZRSO4++

Table 1.4 Parameters Available in ASPENPCD Databank

Parameter Name	Description
API	Standard API gravity at 60°F
CPDIEC	Dielectric constant
CPIG	Ideal gas heat capacity coefficients
DELTA	Solubility parameter at 25°C
DGFORM†	Standard free energy of formation
DHFORM†	Standard heat of formation
DHLCVT	Cavett enthalpy departure parameter
DHVLB	Heat of vaporization at TB
DHVLWT	Watson heat of vaporization parameters
GMUQQ	UNIQUAC area parameter
GMUQR	UNIQUAC volume parameter
MULAND	Andrade liquid viscosity coefficients
MUP	Dipole moment
MW	Molecular weight
NATOM	Vector containing numbers of C, H, O, N, S, F, Cl, Br, I,
NTHA	Nothnagel parameters
OMEGA	Pitzer acentric factor
OMGCTD	Acentric factor for the COSTALD model
PC	Critical pressure
PLCAVT	Cavett vapor pressure coefficients
PLXANT	Extended Antoine vapor pressure coefficients
RGYR	Radius of gyration
RKTZRA	Rackett parameter
SG	Standard specific gravity at 60°F
TB	Normal boiling point
TC	Critical temperature
TFP	Normal freezing point
UFGRP††	UNIFAC functional group data
VB	Liquid molar volume at TB
VC	Critical volume
VLCVT1	Scatchard-Hildebrand characteristic volume parameter
VLSTD	Standard liquid volume at 60°F
VSTCTD	Characteristic volume for the COSTALD model
WATSOL	Water solubility coefficients
ZC	Critical compressibility factor

† *Ideal gas at 25°C*

†† *Contains UNIFAC functional group number and number of occurences of each group*

Table 1.5 Components Available in the ASPENPCD Databank

Alias	Component Name	Alias	Component Name
AR	ARGON	CBRF3	TRIFLUOROBROMOMETHANE
BCL3	BORON-TRICHLORIDE	CCLF3	CHLOROTRIFLUOROMETHANE
BF3	BORON-TRIFLUORIDE	CCL2F2	DICHLORODIFLUOROMETHANE
BR2	BROMINE	CCL2O	PHOSGENE
CLNO	NITROSYL-CHLORIDE	CCL3F	TRICHLOROFLUOROMETHANE
CL2	CHLORINE	CCL4	CARBON-TETRACHLORIDE
CL3P	PHOSPHORUS-TRICHLORIDE	CF4	CARBON-TETRAFLUORIDE
CL4SI	SILICON-TETRACHLORIDE	CO	CARBON-MONOXIDE
D2	DEUTERIUM	COS	CARBONYL-SULFIDE
D2O	DEUTERIUM-OXIDE	CO2	CARBON-DIOXIDE
F2	FLUORINE	CS2	CARBON-DISULFIDE
F3N	NITROGEN-TRIFLUORIDE	CHCLF2	CHLORODIFLUOROMETHANE
F4SI	SILICON-TETRAFLUORIDE	CHCL2F	DICHLOROMONOFLUOROMETHAN
F6S	SULFUR-HEXAFLUORIDE	CHCL3	CHLOROFORM
HBR	HYDROGEN-BROMIDE	CHN	HYDROGEN-CYANIDE
HCL	HYDROGEN-CHLORIDE	CH2BR2	DIBROMOMETHANE
HF	HYDROGEN-FLUORIDE	CH2CL2	DICHLOROMETHANE
HI	HYDROGEN-IODIDE	CH2O	FORMALDEHYDE
H2	HYDROGEN	CH2O2	FORMIC-ACID
H2O	WATER	CH3BR	METHYL-BROMIDE
H2S	HYDROGEN-SULFIDE	CH3CL	METHYL-CHLORIDE
H3N	AMMONIA	CH3F	METHYL-FLUORIDE
H4N2	HYDRAZINE	CH3I	METHYL-IODIDE
HE-4	HELIUM-4	CH3NO2	NITROMETHANE
I2	IODINE	CH4	METHANE
KR	KRYPTON	CH4O	METHANOL
NO	NITRIC-OXIDE	CH4S	METHYL-MERCAPTAN
NO2	NITROGEN-DIOXIDE	CH5N	METHYL-AMINE
N2	NITROGEN	CH6N2	METHYL-HYDRAZINE
N2O	NITROUS-OXIDE	C2CLF5	CHLOROPENTAFLUOROETHANE
NE	NEON	C2CL2F4-1	1,1-DICHLORO-1,2,2,2-
O2	OXYGEN	C2CL2F4-2	1,2-DICHLORO-1,1,2,2-
O2S	SULFUR-DIOXIDE	C2CL3F3	1,2,2-TRICHLORO-1,1,2-
O3	OZONE	C2CL4	TETRACHLOROETHYLENE
O3S	SULFUR-TRIOXIDE	C2CL4F2	1,1,2,2-TETRACHLORO-1,2-
XE	XENON	C2F4	PERFLUOROETHENE

continued

Table 1.5 Components Available in the ASPENPCD Databank (continued)

Alias	Component Name	Alias	Component Name
C2F6	PERFLUOROETHANE	C2H8N2	ETHYLENEDIAMINE
C2N2	CYANOGEN	C3H3N	ACRYLONITRILE
C2HCL3	TRICHLOROETHYLENE	C3H4-1	PROPADIENE
C2HF3O2	TRIFLUOROACETIC-ACID	C3H4-2	METHYL-ACETYLENE
C2H2	ACETYLENE	C3H4O	ACROLEIN
C2H2F2	1,1-DIFLUOROETHYLENE	C3H4O2-1	ACRYLIC-ACID
C2H2O	KETENE	C3H4O2-2	VINYL-FORMATE
C2H3CL	VINYL-CHLORIDE	C3H5CL	ALLYL-CHLORIDE
C2H3CLF2	1-CHLORO-1,1-DIFLUOROETHANE	C3H5CL3	1,2,3-TRICHLOROPROPANE
C2H3CLO	ACETYL-CHLORIDE	C3H5N	PROPIONITRILE
C2H3CL3	1,1,2-TRICHLOROETHANE	C3H6-1	CYCLOPROPANE
C2H3F	VINYL-FLUORIDE	C3H6-2	PROPYLENE
C2H3F3	1,1,1-TRIFLUOROETHANE	C3H6CL2	1,2-DICHLOROPROPANE
C2H3N	ACETONITRILE	C3H6O-1	ACETONE
C2H3NO	METHYL-ISOCYANATE	C3H6O-2	ALLYL-ALCOHOL
C2H4	ETHYLENE	C3H6O-3	N-PROPIONALDEHYDE
C2H4CL2-1	1,1-DICHLOROETHANE	C3H6O-4	PROPYLENE-OXIDE
C2H4CL2-2	1,2-DICHLOROETHANE	C3H6O-5	VINYL-METHYL-ETHER
C2H4F2	1,1-DIFLUOROETHANE	C3H6O2-1	PROPIONIC-ACID
C2H4O-1	ACETALDEHYDE	C3H6O2-2	ETHYL-FORMATE
C2H4O-2	ETHYLENE-OXIDE	C3H6O2-3	METHYL-ACETATE
C2H4O2-1	ACETIC-ACID	C3H7CL-1	PROPYL-CHLORIDE
C2H4O2-2	METHYL-FORMATE	C3H7CL-2	ISOPROPYL-CHLORIDE
C2H5BR	ETHYL-BROMIDE	C3H8	PROPANE
C2H5CL	ETHYL-CHLORIDE	C3H8O-1	1-PROPANOL
C2H5F	ETHYL-FLUORIDE	C3H8O-2	ISOPROPYL-ALCOHOL
C2H5N	ETHYLENE-IMINE	C3H8O-3	METHYL-ETHYL-ETHER
C2H6	ETHANE	C3H8O2-1	METHYLAL
C2H6O-1	DIMETHYL-ETHER	C3H8O2-2	PROPANEDIOL-1,2
C2H6O-2	ETHANOL	C3H8O2-3	1,3-PROPANEDIOL
C2H6O2	ETHYLENE-GLYCOL	C3H8O3	GLYCEROL
C2H6S-1	ETHYL-MERCAPTAN	C3H8S	METHYL-ETHYL-SULFIDE
C2H6S-2	DIMETHYL-SULFIDE	C3H9N-1	N-PROPYL-AMINE
C2H7N-1	ETHYL-AMINE	C3H9N-2	ISOPROPYL-AMINE
C2H7N-2	DIMETHYLAMINE	C3H9N-3	TRIMETHYL-AMINE
C2H7NO	MONOETHANOLAMINE	C4H2O3	MALEIC-ANHYDRIDE

continued

Table 1.5 Components Available in the ASPENPCD Databank (continued)

Alias	Component Name	Alias	Component Name
C4H4	VINYLACETYLENE	C4H10-1	N-BUTANE
C4H4O	FURAN	C4H10-2	ISOBUTANE
C4H4S	THIOPHENE	C4H10O-1	N-BUTANOL
C4H5N-1	ALLYL-CYANIDE	C4H10O-2	2-BUTANOL
C4H5N-2	PYRROLE	C4H10O-3	ISOBUTANOL
C4H6-1	1-BUTYNE	C4H10O-4	TERT-BUTYL-ALCOHOL
C4H6-2	2-BUTYNE	C4H10O-5	DIETHYL-ETHER
C4H6-3	1,2-BUTADIENE	C4H10O2	1,2-DIMETHOXYETHANE
C4H6-4	1,3-BUTADIENE	C4H10O3	DIETHYLENE-GLYCOL
C4H6O2-1	VINYL-ACETATE	C4H10S	DIETHYL-SULFIDE
C4H6O2-2	METHYL-ACRYLATE	C4H10S2	DIETHYL-DISULFIDE
C4H6O3	ACETIC-ANHYDRIDE	C4H11N-1	N-BUTYL-AMINE
C4H6O4-1	DIMETHYL-OXALATE	C4H11N-2	ISOBUTYL-AMINE
C4H6O4-2	SUCCINIC-ACID	C4H11N-3	DIETHYL-AMINE
C4H7N	BUTYRONITRILE	C5H5N	PYRIDINE
C4H8-1	1-BUTENE	C5H8-1	CYCLOPENTENE
C4H8-2	CIS-2-BUTENE	C5H8-2	1,2-PENTADIENE
C4H8-3	TRANS-2-BUTENE	C5H8-3	1-TRANS-3-PENTADIENE
C4H8-4	CYCLOBUTANE	C5H8-4	1,4-PENTADIENE
C4H8-5	ISOBUTYLENE	C5H8-5	1-PENTYNE
C4H8O-1	N-BUTYRALDEHYDE	C5H8-6	2-METHYL-1,3-BUTADIENE
C4H8O-2	ISOBUTYRALDEHYDE	C5H8-7	3-METHYL-1,2-BUTADIENE
C4H8O-3	METHYL-ETHYL-KETONE	C5H8O	CYCLOPENTANONE
C4H8O-4	TETRAHYDROFURAN	C5H8O2	ETHYL-ACRYLATE
C4H8O-5	VINYL-ETHYL-ETHER	C5H10-1	CYCLOPENTANE
C4H8O2-1	N-BUTYRIC-ACID	C5H10-2	1-PENTENE
C4H8O2-2	1,4-DIOXANE	C5H10-3	CIS-2-PENTENE
C4H8O2-3	ETHYL-ACETATE	C5H10-4	TRANS-2-PENTENE
C4H8O2-4	ISOBUTYRIC-ACID	C5H10-5	2-METHYL-1-BUTENE
C4H8O2-5	METHYL-PROPIONATE	C5H10-6	2-METHYL-2-BUTENE
C4H8O2-6	N-PROPYL-FORMATE	C5H10-7	3-METHYL-1-BUTENE
C4H9CL-1	1-CHLOROBUTANE	C5H10O-1	VALERALDEHYDE
C4H9CL-2	2-CHLOROBUTANE	C5H10O-2	METHYL-N-PROPYL-KETONE
C4H9CL-3	TERT-BUTYL-CHLORIDE	C5H10O-3	METHYL-ISOPROPYL-KETONE
C4H9N	PYRROLIDINE	C5H10O-4	DIETHYL-KETONE
C4H9NO	MORPHOLINE	C5H10O2-1	N-VALERIC-ACID

continued

Table 1.5 Components Available in the ASPENPCD Databank (continued)

Alias	Component Name	Alias	Component Name
C5H10O2-2	ISOBUTYL-FORMATE	C6H12-5	TRANS-2-HEXENE
C5H10O2-3	N-PROPYL-ACETATE	C6H12-6	CIS-3-HEXENE
C5H10O2-4	ETHYL-PROPIONATE	C6H12-7	TRANS-3-HEXENE
C5H10O2-5	METHYL-BUTYRATE	C6H12-8	2-METHYL-2-PENTENE
C5H10O2-6	METHYL-ISOBUTYRATE	C6H12-9	3-METHYL-CIS-2-PENTENE
C5H11N	PIPERIDINE	C6H12-10	3-METHYL-TRANS-2-PENTENE
C5H12-1	N-PENTANE	C6H12-11	4-METHYL-CIS-2-PENTENE
C5H12-2	2-METHYL-BUTANE	C6H12-12	4-METHYL-TRANS-2-PENTENE
C5H12-3	2,2-DIMETHYL-PROPANE	C6H12-13	2,3-DIMETHYL-1-BUTENE
C5H12O-1	1-PENTANOL	C6H12-14	2,3-DIMETHYL-2-BUTENE
C5H12O-2	2-METHYL-1-BUTANOL	C6H12-15	3,3-DIMETHYL-1-BUTENE
C5H12O-3	3-METHYL-1-BUTANOL	C6H12O-1	CYCLOHEXANOL
C5H12O-4	2-METHYL-2-BUTANOL	C6H12O-2	METHYL-ISOBUTYL-KETONE
C5H12O-5	2,2-DIMETHYL-1-PROPANOL	C6H12O2-1	N-BUTYL-ACETATE
C5H12O-6	ETHYL-PROPYL-ETHER	C6H12O2-2	ISOBUTYL-ACETATE
C6F6	PERFLUOROBENZENE	C6H12O2-3	ETHYL-BUTYRATE
C6F12	PERFLUOROCYCLOHEXANE	C6H12O2-4	ETHYL-ISOBUTYRATE
C6F14	PERFLUORO-N-HEXANE	C6H12O2-5	N-PROPYL-PROPIONATE
C6H4CL2-1	O-DICHLOROBENZENE	C6H14-1	N-HEXANE
C6H4CL2-2	M-DICHLOROBENZENE	C6H14-2	2-METHYL-PENTANE
C6H4CL2-3	P-DICHLOROBENZENE	C6H14-3	3-METHYL-PENTANE
C6H5BR	BROMOBENZENE	C6H14-4	2,2-DIMETHYL-BUTANE
C6H5CL	CHLOROBENZENE	C6H14-5	2,3-DIMETHYL-BUTANE
C6H5F	FLUOROBENZENE	C6H14O-1	1-HEXANOL
C6H5I	IODOBENZENE	C6H14O-2	ETHYL-BUTYL-ETHER
C6H6	BENZENE	C6H14O-3	DIISOPROPYL-ETHER
C6H6O	PHENOL	C6H15N-1	DIPROPYLAMINE
C6H7N-1	ANILINE	C6H15N-2	TRIETHYLAMINE
C6H7N-2	4-METHYLPYRIDINE	C7F14	PERFLUOROMETHYLCYCLOHEXA
C6H10-1	1,5-HEXADIENE	C7F16	PERFLUORO-N-HEPTANE
C6H10-2	CYCLOHEXENE	C7H5N	BENZONITRILE
C6H10O	CYCLOHEXANONE	C7H6O	BENZALDEHYDE
C6H12-1	CYCLOHEXANE	C7H6O2	BENZOIC-ACID
C6H12-2	METHYLCYCLOPENTANE	C7H8	TOLUENE
C6H12-3	1-HEXENE	C7H8O-1	METHYL-PHENYL-ETHER
C6H12-4	CIS-2-HEXENE	C7H8O-2	BENZYL-ALCOHOL

continued

Table 1.5 Components Available in the ASPENPCD Databank (continued)

Alias	Component Name	Alias	Component Name
C7H8O-3	O-CRESOL	C8H10-4	ETHYLBENZENE
C7H8O-4	M-CRESOL	C8H10O-1	O-ETHYLPHENOL
C7H8O-5	P-CRESOL	C8H10O-2	M-ETHYLPHENOL
C7H9N-1	2,3-DIMETHYLPYRIDINE	C8H10O-3	P-ETHYLPHENOL
C7H9N-2	2,5-DIMETHYLPYRIDINE	C8H10O-4	PHENETOLE
C7H9N-3	3,4-DIMETHYLPYRIDINE	C8H10O-5	2,3-XYLENOL
C7H9N-4	3,5-DIMETHYLPYRIDINE	C8H10O-6	2,4-XYLENOL
C7H9N-5	METHYLPHENYLAMINE	C8H10O-7	2,5-XYLENOL
C7H9N-6	O-TOLUIDINE	C8H10O-8	2,6-XYLENOL
C7H9N-7	M-TOLUIDINE	C8H10O-9	3,4-XYLENOL
C7H9N-8	P-TOLUIDINE	C8H10O-10	3,5-XYLENOL
C7H14-1	CYCLOHEPTANE	C8H11N	N,N-DIMETHYLANILINE
C7H14-2	1,1-DIMETHYLCYCLOPENTANE	C8H16-1	1,1-DIMETHYLCYCLOHEXANE
C7H14-3	CIS-1,2-DIMETHYLCYCLOPENTANE	C8H16-2	CIS-1,2-DIMETHYLCYCLOHEXANE
C7H14-4	TRANS-1,2-	C8H16-3	TRANS-1,2-
C7H14-5	ETHYLCYCLOPENTANE	C8H16-4	CIS-1,3-DIMETHYLCYCLOHEXANE
C7H14-6	METHYLCYCLOHEXANE	C8H16-5	TRANS-1,3-DIMETHYL-
C7H14-7	1-HEPTENE	C8H16-6	CIS-1,4-DIMETHYLCYCLOHEXANE
C7H14-8	2,3,3-TRIMETHYL-1-BUTENE	C8H16-7	TRANS-1,4-DIMETHYL-
C7H16-1	N-HEPTANE	C8H16-8	ETHYLCYCLOHEXANE
C7H16-2	2-METHYLHEXANE	C8H16-9	1,1,2-TRIMETHYLCYCLOPENTANE
C7H16-3	3-METHYLHEXANE	C8H16-10	1,1,3-TRIMETHYLCYCLOPENTANE
C7H16-4	2,2-DIMETHYLPENTANE	C8H16-11	CIS,CIS,TRANS-1,2,4-
C7H16-5	2,3-DIMETHYLPENTANE	C8H16-12	CIS,TRANS,CIS-1,2,4-
C7H16-6	2,4-DIMETHYLPENTANE	C8H16-13	1-METHYL-1-
C7H16-7	3,3-DIMETHYLPENTANE	C8H16-14	N-PROPYLCYCLOPENTANE
C7H16-8	3-ETHYLPENTANE	C8H16-15	ISOPROPYLCYCLOPENTANE
C7H16-9	2,2,3-TRIMETHYLBUTANE	C8H16-16	1-OCTENE
C7H16O	1-HEPTANOL	C8H16-17	TRANS-2-OCTENE
C8H4O3	PHTHALIC-ANHYDRIDE	C8H18-1	N-OCTANE
C8H8	STYRENE	C8H18-2	2-METHYLHEPTANE
C8H8O	METHYL-PHENYL-KETONE	C8H18-3	3-METHYLHEPTANE
C8H8O2	METHYL-BENZOATE	C8H18-4	4-METHYLHEPTANE
C8H10-1	O-XYLENE	C8H18-5	2,2-DIMETHYLHEXANE
C8H10-2	M-XYLENE	C8H18-6	2,3-DIMETHYLHEXANE
C8H10-3	P-XYLENE	C8H18-7	2,4-DIMETHYLHEXANE

continued

Table 1.5 Components Available in the ASPENPCD Databank (continued)

Alias	Component Name	Alias	Component Name
C8H18-8	2,5-DIMETHYLHEXANE	C9H20-9	2,3,3,4-TETRAMETHYLPENTANE
C8H18-9	3,3-DIMETHYLHEXANE	C10H8	NAPHTHALENE
C8H18-10	3,4-DIMETHYLHEXANE	C10H12	1,2,3,4-TETRAHYDRO-
C8H18-11	3-ETHYLHEXANE	C10H14-1	N-BUTYLBENZENE
C8H18-12	2,2,3-TRIMETHYLPENTANE	C10H14-2	ISOBUTYLBENZENE
C8H18-13	2,2,4-TRIMETHYLPENTANE	C10H14-3	SEC-BUTYLBENZENE
C8H18-14	2,3,3-TRIMETHYLPENTANE	C10H14-4	TERT-BUTYLBENZENE
C8H18-15	2,3,4-TRIMETHYLPENTANE	C10H14-5	1-METHYL-2-ISOPROPYLBENZENE
C8H18-16	2-METHYL-3-ETHYLPENTANE	C10H14-6	1-METHYL-3-ISOPROPYLBENZENE
C8H18-17	3-METHYL-3-ETHYLPENTANE	C10H14-7	1-METHYL-4-ISOPROPYLBENZENE
C8H18O-1	1-OCTANOL	C10H14-8	1,4-DIETHYLBENZENE
C8H18O-2	2-OCTANOL	C10H14-9	1,2,4,5-TETRAMETHYLBENZENE
C8H18O-3	2-ETHYLHEXANOL	C10H15N	N-BUTYLANILINE
C8H18O-4	BUTYL-ETHER	C10H18-1	CIS-DECALIN
C8H19N	DIBUTYLAMINE	C10H18-2	TRANS-DECALIN
C9H10	ALPHA-METHYL-STYRENE	C10H19N	CAPRYLONITRILE
C9H10O2	ETHYL-BENZOATE	C10H20-1	N-BUTYLCYCLOHEXANE
C9H12-1	N-PROPYLBENZENE	C10H20-2	ISOBUTYLCYCLOHEXANE
C9H12-2	ISOPROPYLBENZENE	C10H20-3	SEC-BUTYLCYCLOHEXANE
C9H12-3	1-METHYL-2-ETHYLBENZENE	C10H20-4	TERT-BUTYLCYCLOHEXANE
C9H12-4	1-METHYL-3-ETHYLBENZENE	C10H20-5	1-DECENE
C9H12-5	1-METHYL-4-ETHYLBENZENE	C10H22-1	N-DECANE
C9H12-6	1,2,3-TRIMETHYLBENZENE	C10H22-2	3,3,5-TRIMETHYLHEPTANE
C9H12-7	1,2,4-TRIMETHYLBENZENE	C10H22-3	2,2,3,3-TETRAMETHYLHEXANE
C9H12-8	1,3,5-TRIMETHYLBENZENE	C10H22-4	2,2,5,5-TETRAMETHYLHEXANE
C9H18-1	N-PROPYLCYCLOHEXANE	C10H22O	1-DECANOL
C9H18-2	ISOPROPYLCYCLOHEXANE	C11H10-1	1-METHYLNAPHTHALENE
C9H18-3	1-NONENE	C11H10-2	2-METHYLNAPHTHALENE
C9H20-1	N-NONANE	C11H14O2	BUTYL-BENZOATE
C9H20-2	2,2,3-TRIMETHYLHEXANE	C11H22-1	N-HEXYLCYCLOPENTANE
C9H20-3	2,2,4-TRIMETHYLHEXANE	C11H22-2	1-UNDECENE
C9H20-4	2,2,5-TRIMETHYLHEXANE	C11H24	N-UNDECANE
C9H20-5	3,3-DIETHYLPENTANE	C12H10	DIPHENYL
C9H20-6	2,2,3,3-TETRAMETHYLPENTANE	C12H10O	DIPHENYL-ETHER
C9H20-7	2,2,3,4-TETRAMETHYLPENTANE	C12H24-1	N-HEPTYLCYCLOPENTANE
C9H20-8	2,2,4,4-TETRAMETHYLPENTANE	C12H24-2	1-DODECENE

continued

Table 1.5 Components Available in the ASPENPCD Databank (continued)

Alias	Component Name	Alias	Component Name
C12H26	N-DODECANE	C17H34	N-DODECYLCYCLOPENTANE
C12H26O-1	DIHEXYLETHER	C17H36O	HEPTADECANOL
C12H26O-2	DODECANOL	C17H36	N-HEPTADECANE
C12H27N	TRIBUTYLAMINE	C18H14-1	O-TERPHENYL
C13H12	DIPHENYLMETHANE	C18H14-2	M-TERPHENYL
C13H26-1	N-OCTYLCYCLOPENTANE	C18H14-3	P-TERPHENYL
C13H26-2	1-TRIDECENE	C18H36-1	1-OCTADECENE
C13H28	N-TRIDECANE	C18H36-2	N-TRIDECYLCYCLOPENTANE
C14H10-1	ANTHRACENE	C18H38	N-OCTADECANE
C14H10-2	PHENANTHRENE	C18H38O	1-OCTADECANOL
C14H28-1	N-NONYLCYCLOPENTANE	C19H38	N-TETRADECYLCYCLOPENTANE
C14H28-2	1-TETRADECENE	C19H40	N-NONADECANE
C14H30	N-TETRADECANE	C20H40	N-PENTADECYLCYCLOPENTANE
C15H30-1	N-DECYLCYCLOPENTANE	C20H42	N-EICOSANE
C15H30-2	1-PENTADECENE	C20H42O	1-EICOSANOL
C15H32	N-PENTADECANE	C21H42	N-HEXADECYLCYCLOPENTANE
C16H22O4	DIBUTYL-O-PHTHALATE	C4H11NO2-1	DIETHANOLAMINE
C16H32-1	N-DECYLCYCLOHEXANE	C6H15NO2	DIISOPROPANOLAMINE
C16H32-2	1-HEXADECENE	C4H11NO2-2	DIGLYCOLAMINE
C16H34	N-HEXADECANE		

Table 1.6 Parameters Available in the INORGANIC Databank

Parameter Name †	Description
ATOMNO ††	Atomic number of each atom in the compound
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
CPXSP4	Solid property parameters range 4
CPXSP5	Solid property parameters range 5
CPXSP6	Solid property parameters range 6
CPSXP7	Solid property parameters range 7
MW	Molecular weight
NOATOM ††	Number of occurrences of each atom
TB	Normal boiling temperature
TFP	Normal freezing temperature
VSPOLY	Molar volume parameters of solid

† *The properties are enthalpy, entropy, Gibbs free energy and heat capacity.*

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

Table 1.7 Components Available in the INORGANIC Databank

Alias	Component Name	Alias	Component Name
(NH4)2SO4	AMMONIUM-SULFATE	AGF	SILVER-FLUORIDE
1/2-H2	1/2-HYDROGEN	AGI	SILVER-IODIDE
1/2-N2	1/2-NITROGEN	AGI:A	SILVER-IODIDE:SOL-A
1/2-O2	1/2-OXYGEN	AGI:B	SILVER-IODIDE:SOL-B
1/2-P2	1/2-PHOSPHORUS-P2	AGNO3	SILVER-NITRATE
1/2-S2	1/2-SULFUR-S2	AGNO3:A	SILVER-NITRATE:SOL-A
1/4-P4	1/4-PHOSPHORUS-P4	AGNO3:B	SILVER-NITRATE:SOL-B
2PBO*PBSO4	TRILEAD-DIOXIDE-SULFATE	AGP2	SILVER-DIPHOSPHIDE
3PBO*PBSO4	TETRALEAD-TRIOXIDE-SULFATE	AGP3	SILVER-TRIPHOSPHIDE
4PBO*PBSO4	PENTALEAD-TETRAOXIDE-	AL	ALUMINIUM
AG	SILVER	AL(OH)3	ALUMINIUM-HYDROXIDE-
AG2CO3	SILVER-CARBONATE	AL18B4O33	18-ALUMINIUM-4-BORON-33-
AG2CRO4	SILVER-CHROMATE	AL2(SO4)3	ALUMINIUM-SULFATE
AG2O	SILVER-OXIDE	AL2BR6	DIALUMINIUM-HEXABROMIDE-
AG2S	SILVER-SULFIDE	AL2CA	2-ALUMINIUM-CALCIUM
AG2S:A	SILVER-SULFIDE:SOL-A	AL2CE	2-ALUMINIUM-CERIUM
AG2S:B	SILVER-SULFIDE:SOL-B	AL2CL6	DIALUMINIUM-HEXACHLORIDE-
AG2S:C	SILVER-SULFIDE:SOL-C	AL2F6	DIALUMINIUM-HEXAFLUORIDE-
AG2SE	SILVER-SELENIDE	AL2I6	DIALUMINIUM-HEXAIODIDE-GAS
AG2SE:A	SILVER-SELENIDE:SOL-A	AL2LA	2-ALUMINIUM-LANTHANUM
AG2SE:B	SILVER-SELENIDE:SOL-B	AL2O	DIALUMINIUM-OXIDE-GAS
AG2SE:C	SILVER-SELENIDE:SOL-C	AL2O2	DIALUMINIUM-DIOXIDE-GAS
AG2SO4	SILVER-SULFATE	AL2O3	ALUMINIUM-OXIDE-ALPHA-
AG2SO4:A	SILVER-SULFATE:SOL-A	AL2O3*3H2O	GIBBSITE
AG2SO4:B	SILVER-SULFATE:SOL-B	AL2O3*H2O	DIASPORE
AG2TE	SILVER-TELLURIDE	AL2O3*H2O-B	BOEHMITE
AG2TE:A	SILVER-TELLURIDE:SOL-A	AL2O3-C	ALUMINIUM-OXIDE-GAMMA
AG2TE:B	SILVER-TELLURIDE:SOL-B	AL2O3-D	ALUMINUIM-OXIDE-DELTA
AG2WO4	SILVER-TUNGSTATE	AL2O3-K	ALUMINIUM-OXIDE-KAPPA
AG3ASO4	SILVER-ARSENATE	AL2S3	ALUMINIUM-SULFIDE
AGBR	SILVER-BROMIDE	AL2SE2	DIALUMINIUM-DISELENIDE-GAS
AGBRO3	SILVER-BROMATE	AL2SE3	ALUMINIUM-SELENIDE
AGCL	SILVER-CHLORIDE	AL2SIO5	ALUMINIUM-SILICATE-KYANITE
AGCLO3	SILVER-CHLORATE	AL2SIO5-A	ALUMINIUM-SILICATE-
AGCN	SILVER-CYANIDE	AL2SIO5-S	ALUMINIUM-SILICATE-

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
AL2TE3	ALUMINIUM-TELLURIDE	ALN	ALUMINIUM-NITRIDE
AL2TIO5	DIALUMINIUM-TITANIUM-	ALNI	ALUMINIUM-NICKEL
AL2U	2-ALUMINIUM-URANIUM	ALNI3	ALUMINIUM-3-NICKEL
AL3NI	3-ALUMINIUM-NICKEL	ALO	ALUMINIUM-MONOXIDE-GAS
AL3NI2	3-ALUMINIUM-2-NICKEL	ALO2	ALUMINIUM-DIOXIDE-GAS
AL3TH	3-ALUMINIUM-THORIUM	ALOCL	ALUMINIUM-CHLORIDE-OXIDE
AL3TI	3-ALUMINIUM-TITANIUM	ALOF	ALUMINIUM-FLUORIDE-OXIDE-
AL3U	3-ALUMINIUM-URANIUM	ALOF2	ALUMINIUM-DIFLUORIDE-OXIDE-
AL4B2O9	4-ALUMINIUM-2-BORON-9-OXIDE	ALP	ALUMINIUM-PHOSPHIDE
AL4C3	TETRAALUMINIUM-TRICARBIDE	ALPO4	ALUMINIUM-PHOSPHATE
AL4CA	4-ALUMINIUM-CALCIUM	ALPO4:A	ALUMINIUM-PHOSPHATE:SOL-A
AL4CE	4-ALUMINIUM-CERIUM	ALPO4:B	ALUMINIUM-PHOSPHATE:SOL-B
AL4MG2SI5O18	CORDIERITE	ALPO4:C	ALUMINIUM-PHOSPHATE:SOL-C
AL4U	4-ALUMINIUM-URANIUM	ALS	ALUMINIUM-MONOSULFIDE-GAS
AL5CO2	5-ALUMINIUM-2-COBALT	ALSB	ALUMINIUM-ANTIMONY
AL6SI2O13	MULLITE	ALTE	ALUMINIUM-MONOTELLURIDE-
ALAS	ALUMINIUM-ARSENIDE	ALTI	ALUMINIUM-TITANIUM
ALASO4	ALUMINIUM-ARSENATE	AM	AMERICIUM
ALB12	ALUMINIUM-DODECABORIDE	AM:A	AMERICIUM:SOL-A
ALB2	ALUMINIUM-DIBORIDE	AM:B	AMERICIUM:SOL-B
ALBR	ALUMINIUM-MONOBROMIDE-GAS	AM:C	AMERICIUM:SOL-C
ALBR3	ALUMINIUM-BROMIDE	ANALCITE	NAALSI2O6*H2O
ALCL	ALUMINIUM-MONOCHLORIDE-GAS	ANTHOPHYLLIT	ANTHOPHYLLITE
ALCL2	ALUMINIUM-DICHLORIDE-GAS	AR	ARGON
ALCL3	ALUMINIUM-CHLORIDE	AS	ARSENIC
ALCL3*6H2O	ALUMINIUM-CHLORIDE-	AS-2	ARSENIC-DIATOMIC
ALCO	ALUMINIUM-COBALT	AS-3	ARSENIC-TRIATOMIC
ALF	ALUMINIUM-MONOFLUORIDE-GAS	AS-4	ARSENIC-4-ATOMIC
ALF2	ALUMINIUM-DIFLUORIDE-GAS	AS2O3	ARSENIC-OXIDE-CLAUDETITE
ALF3	ALUMINIUM-FLUORIDE	AS2O3-A	ARSENIC-OXIDE-ARSENOLITE
ALF3:A	ALUMINIUM-FLUORIDE:SOL-A	AS2O5	DIARSENIC-PENTAOXIDE
ALF3:B	ALUMINIUM-FLUORIDE:SOL-B	AS2S2	DIARSENIC-DISULFIDE
ALH3	ALUMINIUM-HYDRIDE-	AS2S3	ARSENIC-SULFIDE
ALI3	ALUMINIUM-IODIDE	AS2S3:1	ARSENIC-SULFIDE:SOL-1
ALLI	ALUMINIUM-LITHIUM	AS2S3:2	ARSENIC-SULFIDE:SOL-2

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
AS2SE3	ARSENIC-SELENIDE	AUSE	GOLD-MONOSELENIDE-ALPHA
AS2TE3	ARSENIC-TELLURIDE	AUSE-B	GOLD-MONOSELENIDE-BETA
AS4O6	TETRAARSENIC-HEXAOXIDE-GAS	AUSN	GOLD-TIN
AS4S4	TETRAARSENIC-TETRASULFIDE	AUSN2	GOLD-2-TIN
AS4S4-R	TETRAARSENIC-TETRASULFIDE-	AUSN4	GOLD-4-TIN
ASBR3	ARSENIC-BROMIDE-GAS	AUTE2	GOLD-DITELLURIDE
ASCL3	ARSENIC-CHLORIDE	B	BORON-BETA
ASF3	ARSENIC-FLUORIDE	B-GL	BORON-GLASS
ASF5	ARSENIC-PENTAFLUORIDE-GAS	B-I	BORON-MONOIODIDE-GAS
ASH3	ARSENIC-HYDRIDE	B-I2	BORON-DIIODIDE-GAS
ASI3	ARSENIC-IODIDE	B-I3	BORON-TRIIODIDE-GAS
ASO	ARSENIC-MONOXIDE-GAS	B2H6	DIBORANE
ASS	ARSENIC-MONOSULFIDE-GAS	B2O3	BORON-OXIDE
ASSE	ARSENIC-MONOSELENIDE-GAS	B2O3-GL	BORON-OXIDE-GLASS
ASTE	ARSENIC-MONOTELLURIDE-GAS	B2S3	DIBORON-TRISULFIDE
AU	GOLD	B4C	TETRABORON-MONOCARBIDE
AU(OH)3	GOLD-TRIHYDROXIDE-	BA	BARIUM
AU2O3	DIGOLD-TRIOXIDE	BA(NO3)2	BARIUM-NITRATE
AU2P3	DIGOLD-TRIPHOSPHIDE	BA(OH)2	BARIUM-HYDROXIDE
AU3ASO4	TRIGOLD-ARSENATE	BA(OH)2:A	BARIUM-HYDROXIDE:SOL-A
AUBR	GOLD-MONOBROMIDE	BA(OH)2:B	BARIUM-HYDROXIDE:SOL-B
AUCD	GOLD-CADMIUM	BA2SI3O8	DIBARIUM-TRISILICATE
AUCL	GOLD-MONOCHLORIDE	BA2SIO4	BARIUM-ORTHOSILICATE
AUCL3	GOLD-TRICHLORIDE	BA2SN	2-BARIUM-TIN
AUCU	GOLD-COPPER	BA2TIO4	DIBARIUM-TITANIUM-TETRAOXIDE
AUCU3	GOLD-3-COPPER	BA3(ASO4)2	BARIUM-ARSENATE
AUCU3:11	GOLD-3-COPPER:SA-11	BA3AL2O6	TRIBARIUM-DIALUMINIUM-
AUCU3:A	GOLD-3-COPPER:SOL-A	BA3N2	TRIBARIUM-DINITRIDE
AUCU:12	GOLD-COPPER:SA-12	BAAL2O4	BARIUM-DIALUMINIUM-
AUCU:22	GOLD-COPPER:SA-22	BABR2	BARIUM-BROMIDE
AUCU:A	GOLD-COPPER:SOL-A	BAC2	BARIUM-DICARBIDE
AUF3	GOLD-TRIFLUORIDE	BACL	BARIUM-MONOCHLORIDE-GAS
AUI	GOLD-MONOIODIDE	BACL2	BARIUM-CHLORIDE
AUS	GOLD-MONOSULFIDE-GAS	BACL2:1	BARIUM-CHLORIDE:SOL-1
AUSB2	GOLD-2-ANTIMONY	BACL2:2	BARIUM-CHLORIDE:SOL-2

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
BACO3	BARIUM-CARBONATE	BBR2	BORON-DIBROMIDE-GAS
BACO3:A	BARIUM-CARBONATE:SOL-A	BBR3	BORON-TRIBROMIDE
BACO3:B	BARIUM-CARBONATE:SOL-B	BCL	BORON-MONOCHLORIDE-GAS
BACO3:C	BARIUM-CARBONATE:SOL-C	BCL2	BORON-DICHLORIDE-GAS
BACRO4	BARIUM-CHROMATE	BCL3	BORON-TRICHLORIDE
BAF	BARIUM-MONOFLUORIDE-GAS	BE	BERYLLIUM
BAF2	BARIUM-FLUORIDE	BE(OH)2	BERYLLIUM-HYDROXIDE-ALPHA
BAF2:A	BARIUM-FLUORIDE:SOL-A	BE(OH)2-B	BERYLLIUM-HYDROXIDE-BETA
BAF2:B	BARIUM-FLUORIDE:SOL-B	BE2C	DIBERYLLIUM-CARBIDE
BAF2:C	BARIUM-FLUORIDE:SOL-C	BE2CL4	DIBERYLLIUM-TETRACHLORIDE-
BAH	BARIUM-MONOHYDRIDE-GAS	BE2SIO4	BERYLLIUM-SILICATE-PHENACITE
BAH2	BARIUM-HYDRIDE	BE3(ASO4)2	BERYLLIUM-ARSENATE
BAH2:1	BARIUM-HYDRIDE:SOL-1	BE3B2O6	TRIBERYLLIUM-DIBORATE
BAH2:2	BARIUM-HYDRIDE:SOL-2	BE3N2	ALPHA-BERYLLIUM-NITRIDE
BAHFO3	BARIUM-HAFNIUM-TRIOXIDE	BEAL2O4	BERYLLIUM-DIALUMINIUM-
BAI	BARIUM-MONOIODIDE-GAS	BEAL6O10	BERYLLIUM-HEXAALUMINIUM-
BAI2	BARIUM-IODIDE	BEBR	BERYLLIUM-MONOBROMIDE-GAS
BAMOO4	BARIUM-MOLYBDATE	BEBR2	BERYLLIUM-BROMIDE
BAO	BARIUM-OXIDE	BECL	BERYLLIUM-MONOCHLORIDE-GAS
BAO2	BARIUM-PEROXIDE	BECL2	BERYLLIUM-CHLORIDE
BAS	BARIUM-SULFIDE	BECL2:A	BERYLLIUM-CHLORIDE:SOL-A
BASI2O5	BARIUM-DISILICATE	BECL2:B	BERYLLIUM-CHLORIDE:SOL-B
BASIO3	BARIUM-METASILICATE	BEF	BERYLLIUM-MONOFLUORIDE-GAS
BASO4	BARIUM-SULFATE	BEF2	BERYLLIUM-FLUORIDE
BASO4:1	BARIUM-SULFATE:SOL-1	BEF2:2	BERYLLIUM-FLUORIDE:SOL-2
BASO4:2	BARIUM-SULFATE:SOL-2	BEF2:A	BERYLLIUM-FLUORIDE:SOL-A
BATE	BARIUM-TELLURIDE	BEH	BERYLLIUM-MONOHYDRIDE-GAS
BATIO3	BARIUM-TITANIUM-TRIOXIDE	BEI	BERYLLIUM-MONOIODIDE-GAS
BATIO3:1	BARIUM-TITANIUM-TRIOXIDE:SOL-	BEI2	BERYLLIUM-IODIDE
BATIO3:2	BARIUM-TITANIUM-TRIOXIDE:SOL-	BEO	BERYLLIUM-OXIDE
BATIO3:3	BARIUM-TITANIUM-TRIOXIDE:SOL-	BEO:A	BERYLLIUM-OXIDE:SOL-A
BAUO4	BARIUM-URANATE	BEO:B	BERYLLIUM-OXIDE:SOL-B
BAWO4	BARIUM-TUNGSTATE	BEOH	BERYLLIUM-MONOHYDROXIDE-
BAZRO3	BARIUM-ZIRCONIUM-TRIOXIDE	BES	BERYLLIUM-SULFIDE
BBR	BORON-MONOBROMIDE-GAS	BESO4	BERYLLIUM-SULFATE

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
BESO4*2H2O	BERYLLIUM-SULFATE-DIHYDRATE	BIK3:A	BISMUTH-3-POTASSIUM:SOL-A
BESO4*4H2O	BERYLLIUM-SULFATE-	BIK3:B	BISMUTH-3-POTASSIUM:SOL-B
BESO4:A	BERYLLIUM-SULFATE:SOL-A	BIMN	BISMUTH-MANGANESE
BESO4:B	BERYLLIUM-SULFATE:SOL-B	BINI	BISMUTH-NICKEL
BESO4:C	BERYLLIUM-SULFATE:SOL-C	BIOCL	BISMUTH-CHLORIDE-OXIDE
BEWO4	BERYLLIUM-TUNGSTATE	BIU	BISMUTH-URANIUM
BF	BORON-MONOFLUORIDE-GAS	BN	BORON-NITRIDE
BF2	BORON-DIFLUORIDE-GAS	BOCL	BORON-CHLORIDE-OXIDE-GAS
BF3	BORON-TRIFLUORIDE	BP	BORON-MONOPHOSPHIDE
BH	BORON-MONOHYDRIDE-GAS	BR	BROMINE-MONATOMIC-GAS
BI	BISMUTH	BR2	BROMINE
BI2	BISMUTH-DIATOMIC-GAS	BS	BORON-MONOSULFIDE-GAS
BI2(SO4)3	BISMUTH-SULFATE	C	CARBON-GRAPHITE
BI2O3	BISMUTH-OXIDE	C-2	CARBON-DIATOMIC-GAS
BI2O3:A	BISMUTH-OXIDE:SOL-A	C-3	CARBON-TRIATOMIC-GAS
BI2O3:B	BISMUTH-OXIDE:SOL-B	C-D	CARBON-DIAMOND
BI2S3	BISMUTH-SULFIDE	C2CL4	TETRACHLOROETHYLENE
BI2SE3	BISMUTH-SELENIDE	C2CL6	HEXACHLOROETHANE
BI2TE3	BISMUTH-TELLURIDE	C2F4	PERFLUOROETHENE
BI2U	2-BISMUTH-URANIUM	C2F6	PERFLUOROETHANE
BI4U3	4-BISMUTH-3-URANIUM	C2H2	ACETYLENE
BIASO4	BISMUTH-ARSENATE	C2H2O	KETENE
BIBR	BISMUTH-MONOBROMIDE-GAS	C2H3CL	VINYL-CHLORIDE
BIBR3	BISMUTH-BROMIDE	C2H4	ETHYLENE
BIBR3:A	BISMUTH-BROMIDE:SOL-A	C2H4O-1	ACETALDEHYDE
BIBR3:B	BISMUTH-BROMIDE:SOL-B	C2H5CL	ETHYL-CHLORIDE
BICL	BISMUTH-MONOCHLORIDE-GAS	C2H6	ETHANE
BICL3	BISMUTH-CHLORIDE	C2N2	ETHANEDINITRILE
BIF	BISMUTH-MONOFLUORIDE-GAS	C3H4-1	PROPADIENE
BIF3	BISMUTH-FLUORIDE	C3H4-2	METHYL-ACETYLENE
BII	BISMUTH-MONOIODIDE	C3H6-1	CYCLOPROPANE
BII3	BISMUTH-IODIDE	C3H6-2	PROPYLENE
BII:A	BISMUTH-MONOIODIDE:SOL-A	C3H8	PROPANE
BII:B	BISMUTH-MONOIODIDE:SOL-B	C4H10-1	N-BUTANE
BIK3	BISMUTH-3-POTASSIUM	C4H6-1	1-BUTYNE

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
C4H8-4	CYCLOBUTANE	CA2SN	2-CALCIUM-TIN
C4H8-5	ISOBUTYLENE	CA2V2O7	CALCIUM-PYROVANADATE
C5H10-1	CYCLOPENTANE	CA3(ASO4)2	CALCIUM-ARSENATE
C5H12-1	N-PENTANE	CA3(PO4)2	CALCIUM-PHOSPHATE
C5H8-1	CYCLOPENTENE	CA3(VO4)2	CALCIUM-ORTHOVANADATE
C5H8-2	1-2-PENTADIENE	CA3AL2O6	3-CALCIUM-2-ALUMINIUM-6-OXIDE
C6H6O	PHENOL	CA3AL2O6*6W	3-CALCIUM-2-ALUMINIUM-6-OXIDE-
C8H14	OCT-1-YNE	CA3AL2SI3O12	GROSSULAR
C9H16	NON-1-YNE	CA3B2O6	TRICALCIUM-DIBORATE
CA	CALCIUM	CA3MGSI2O8	MERWINITE
CA(NO3)2	CALCIUM-NITRATE	CA3N2	TRICALCIUM-DINITRIDE
CA(OCL)CL	CALCIUM-CHLORIDE-	CA3P2	TRICALCIUM-DIPHOSPHIDE
CA(OH)2	CALCIUM-HYDROXIDE	CA3PO4-2:1	CALCIUM-PHOSPHATE:SOL-1
CA(VO3)2	CALCIUM-METAVANADATE	CA3PO4-2:A	CALCIUM-PHOSPHATE:SOL-A
CA12AL14O33	12-CALCIUM-14-ALUMINIUM-33-	CA3PO4-2:B	CALCIUM-PHOSPHATE:SOL-B
CA2AL2O5	2-CALCIUM-2-ALUMINIUM-5-OXIDE	CA3SB2	3-CALCIUM-2-ANTIMONY
CA2AL2SIO7	GEHLENITE	CA3SI2O7	TRICALCIUM-DISILICATE-
CA2B2O5	DICALCIUM-DIBORATE	CA3SI2O7*3W	TRICALCIUM-DISILICATE-
CA2B2O5:A	DICALCIUM-DIBORATE:SOL-A	CA3SIO5	TRICALCIUM-SILICATE
CA2B2O5:B	DICALCIUM-DIBORATE:SOL-B	CA3TI2O7	3-CALCIUM-2-TITANIUM-7-OXIDE
CA2FE2O5	DICALCIUM-DIIRON-PENTAOXIDE	CA3WO6	CALCIUM-ORTHOTUNGSTATE
CA2MGSI2O7	AKERMANITE	CA4SI3*3:2W	4-CALCIUM-3-SILICATE-3:2-
CA2P2O7	CALCIUM-PYROPHOSPHATE	CA4TI3O10	4-CALCIUM-3-TITANIUM-10-OXIDE
CA2P2O7:A	CALCIUM-PYROPHOSPHATE:SOL-	CA5SI6*11:2W	5-CALCIUM-6-SILICATE-5.5-HYDRA
CA2P2O7:B	CALCIUM-PYROPHOSPHATE:SOL-	CA5SI6*21:2W	5-CALCIUM-6-SILICATE-10.5-HYDR
CA2P2O7:C	CALCIUM-PYROPHOSPHATE:SOL-	CA5SI6O17*3W	5-CALCIUM-6-SILICATE-3-HYDRATE
CA2PB	2-CALCIUM-LEAD	CA6SI6O18*W	6-CALCIUM-6-SILICATE-HYDRATE
CA2SI	2-CALCIUM-SILICON	CA:A	CALCIUM:SOL-A
CA2SI3*5:2W	2-CALCIUM-3-SILICATE-5:2-	CA:B	CALCIUM:SOL-B
CA2SIO4	OLIVINE	CAAL2O4	CALCIUM-2-ALUMINIUM-4-OXIDE
CA2SIO4*7:6W	CALCIUM-ORTHOSILICATE-7:6-	CAAL2SI2O8	ANORTHITE
CA2SIO4-B	LARNITE	CAAL2SIO6	PYROXENE
CA2SIO4:A	OLIVINE:SOL-A	CAAL4O7	CALCIUM-4-ALUMINIUM-7-OXIDE
CA2SIO4:A1	OLIVINE:SOL-A1	CAB2O4	CALCIUM-DIBORATE
CA2SIO4:C	OLIVINE:SOL-C	CAB4O7	CALCIUM-TETRABORATE

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
CABR	CALCIUM-MONOBROMIDE-GAS	CAOH	CALCIUM-MONOHYDROXIDE-GAS
CABR2	CALCIUM-BROMIDE	CAPB	CALCIUM-LEAD
CAC2	CALCIUM-DICARBIDE	CAS	CALCIUM-SULFIDE
CAC2:A	CALCIUM-DICARBIDE:SOL-A	CASE	CALCIUM-SELENIDE
CAC2:B	CALCIUM-DICARBIDE:SOL-B	CASI	CALCIUM-SILICON
CACL	CALCIUM-MONOCHLORIDE-GAS	CASI2	CALCIUM-2-SILICON
CACL2	CALCIUM-CHLORIDE	CASI2O5*2H2O	CALCIUM-2-SILICATE-2-HYDRATE
CACN2	CALCIUM-CYANAMIDE	CASIO3	WOLLASTONITE
CACO3	CALCIUM-CARBONATE-CALCITE	CASIO3-B	PSEUDOWOLLASTONITE
CACO3-A	CALCIUM-CARBONATE-	CASN	CALCIUM-TIN
CAF	CALCIUM-MONOFLUORIDE-GAS	CASO3	CALCIUM-SULFITE
CAF2	CALCIUM-FLUORIDE	CASO3*1:2W	CALCIUM-SULFITE-HEMIHYDRATE
CAF2:A	CALCIUM-FLUORIDE:SOL-A	CASO4	CALCIUM-SULFATE
CAF2:B	CALCIUM-FLUORIDE:SOL-B	CASO4*1:2W:A	CALCIUM-SULFATE-
CAFE2O4	CALCIUM-DIIRON-TETRAOXIDE	CASO4*2H2O	CALCIUM-SULFATE-DIHYDRATE-
CAH	CALCIUM-MONOHYDRIDE-GAS	CASO4:1	CALCIUM-SULFATE:SOL-1
CAH2	CALCIUM-HYDRIDE	CASO4:2	CALCIUM-SULFATE:SOL-2
CAH2:A	CALCIUM-HYDRIDE:SOL-A	CATE	CALCIUM-TELLURIDE
CAH2:B	CALCIUM-HYDRIDE:SOL-B	CATIO3	CALCIUM-TITANIUM-TRIOXIDE-
CAHFO3	CALCIUM-HAFNIUM-TRIOXIDE	CATIO3:A	PEROVSKITE:SOL-A
CAHPO4	CALCIUM-HYDROGEN-	CATIO3:B	PEROVSKITE:SOL-B
CAHPO4*2H2O	CALCIUM-HYDROGEN-	CATISIO5	SPHENE
CAI	CALCIUM-MONOIODIDE-GAS	CAUO4	CALCIUM-URANATE
CAI2	CALCIUM-IODIDE	CAUO4:A	CALCIUM-URANATE:SOL-A
CAMG(CO3)2	DOLOMITE	CAUO4:B	CALCIUM-URANATE:SOL-B
CAMG2	CALCIUM-2-MAGNESIUM	CAWO4	CALCIUM-TUNGSTATE
CAMGO2	CALCIUM-MAGNESIUM-DIOXIDE	CAZN	CALCIUM-ZINC
CAMGSI2O6	DIOPSIDE	CAZN2	CALCIUM-2-ZINC
CAMGSIO4	MONTICELLITE	CAZRO3	CALCIUM-ZIRCONIUM-TRIOXIDE
CAMOO4	CALCIUM-MOLYBDATE	CBR	BROMOMETHYLIDYNE-GAS
CANO3*2*2H2O	CALCIUM-NITRATE-DIHYDRATE	CBR4	TETRABROMOMETHANE-GAS
CANO3*2*3H2O	CALCIUM-NITRATE-TRIHYDRATE	CCL	CHLOROMETHYLIDYNE-GAS
CANO3*2*4H2O	CALCIUM-NITRATE-	CCL2	DICHLOROMETHYLENE-GAS
CAO	CALCIUM-OXIDE	CCL2O	PHOSGENE
CAO2	CALCIUM-PEROXIDE	CCL3	TRICHLOROMETHYL-GAS

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
CD	CADMIUM	CEALO3	CERIUM-ALUMINIUM-TRIOXIDE
CD(OH)2	CADMIUM-HYDROXIDE	CEB6	CERIUM-HEXABORIDE
CD11U	11-CADMIUM-URANIUM	CEBR3	CERIUM-BROMIDE
CD3(ASO4)2	CADMIUM-ARSENATE	CEC2	CERIUM-DICARBIDE
CD3AS2	CADMIUM-ARSENIDE	CECL3	CERIUM-CHLORIDE
CDAL2O4	CADMIUM-DIALUMINIUM-	CECRO3	CERIUM-CHROMIUM-TRIOXIDE
CDBR2	CADMIUM-BROMIDE	CEF3	CERIUM-FLUORIDE
CDCL2	CADMIUM-CHLORIDE	CEH2	CERIUM-DIHYDRIDE
CDCO3	CADMIUM-CARBONATE	CEI3	CERIUM-IODIDE
CDF2	CADMIUM-FLUORIDE	CEMG	CERIUM-MAGNESIUM
CDGA2O4	CADMIUM-DIGALLIUM-	CEN	CERIUM-NITRIDE
CDI2	CADMIUM-IODIDE	CEO	CERIUM-MONOXIDE-GAS
CDO	CADMIUM-OXIDE	CEO2	CERIUM-DIOXIDE
CDS	CADMIUM-SULFIDE	CES	CERIUM-MONOSULFIDE
CDSB	CADMIUM-ANTIMONY	CESIUM	CESIUM
CDSE	CADMIUM-SELENIDE	CETE	CERIUM-MONOTELLURIDE-GAS
CDSEO3	CADMIUM-SELENITE	CF	FLUOROMETHYLIDYNE-GAS
CDSIO3	CADMIUM-METASILICATE	CF2	DIFLUOROMETHYLENE-GAS
CDSO4	CADMIUM-SULFATE	CF3	TRIFLUOROMETHYL-GAS
CDSO4:1	CADMIUM-SULFATE:SOL-1	CF4	CARBON-TETRAFLUORIDE
CDSO4:A	CADMIUM-SULFATE:SOL-A	CH	METHYLIDYNE-GAS
CDSO4:B	CADMIUM-SULFATE:SOL-B	CH2	METHYLENE-GAS
CDTE	CADMIUM-TELLURIDE	CH2CL2	DICHLOROMETHANE
CDTIO3	CADMIUM-TITANIUM-TRIOXIDE	CH2O	FORMALDEHYDE
CDTIO3:A	CADMIUM-TITANIUM-	CH3	METHYL-GAS
CDTIO3:B	CADMIUM-TITANIUM-	CH3CL	METHYL-CHLORIDE
CDWO4	CADMIUM-TUNGSTATE	CH4	METHANE
CE	CERIUM	CHCL3	CHLOROFORM
CE2(SO4)3	CERIUM-SULFATE	CHN	HYDROGEN-CYANIDE
CE2C3	DICERIUM-TRICARBIDE	CHO	OXOMETHYL-GAS
CE2O3	CERIUM-OXIDE	CHRYSOTILE	MG3SI2O5(OH)4
CE2S3	CERIUM-SULFIDE	CL	CHLORINE-MONATOMIC-GAS
CE3S4	TRICERIUM-TETRASULFIDE	CL2	CHLORINE
CE:C	CERIUM:SOL-C	CL2O	DICHLORINE-MONOXIDE-GAS
CE:D	CERIUM:SOL-D	CLF	CHLORINE-MONOFLUORIDE-GAS

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
CLF3	CHLORINE-TRIFLUORIDE-GAS	COFE2O4:11	COBALT-DIIRON-
CLO	CHLORINE-MONOXIDE-GAS	COI2	COBALT-DIIODIDE
CN	CYANOGEN-GAS	COO	COBALT-MONOXIDE
CN2	CARBON-NITRIDE-NCN-RADICAL-	COP	COBALT-MONOPHOSPHIDE
CO	CARBON-MONOXIDE	COP3	COBALT-TRIPHOSPHIDE
CO(OH)2	COBALT-HYDROXIDE-	COS	CARBONYL-SULFIDE
CO-CL	COBALT-MONOCHLORIDE-GAS	COS0.89	COBALT-0.89-SULFIDE
CO-CL2	COBALT-DICHLORIDE	COS2	COBALT-DISULFIDE
CO-F2	COBALT-DIFLUORIDE	COSB0.98	COBALT-0.98-ANTIMONY
CO2	CARBON-DIOXIDE	COSB2	COBALT-2-ANTIMONY
CO2B	DICOBALT-BORIDE	COSB3	COBALT-3-ANTIMONY
CO2CL4	DICOBALT-TETRACHLORIDE-GAS	COSEO3	COBALT-SELENITE
CO2P	DICOBALT-PHOSPHIDE	COSN	COBALT-TIN
CO2SIO4	DICOBALT-SILICATE	COSO4	COBALT-SULFATE
CO2TIO4	DICOBALT-TITANIUM-TETRAOXIDE	COSO4:A	COBALT-SULFATE:SOL-A
CO3(ASO4)2	COBALT-ARSENATE	COSO4:B	COBALT-SULFATE:SOL-B
CO3N	TRICOBALT-NITRIDE	COTIO3	COBALT-TITANIUM-TRIOXIDE
CO3O4	TRICOBALT-TETRAOXIDE	COWO4	COBALT-TUNGSTATE
CO3S4	TRICOBALT-TETRASULFIDE	COWO4:A	COBALT-TUNGSTATE:SOL-A
CO:A	COBALT:SOL-A	COWO4:B	COBALT-TUNGSTATE:SOL-B
CO:B	COBALT:SOL-B	CR	CHROMIUM
COB	COBALT-MONOBORIDE	CR(CO)6	CHROMIUM-HEXACARBONYL
COBALT	COBALT	CR2(SO4)3	CHROMIUM-SULFATE
COBR2	COBALT-DIBROMIDE	CR23C6	23-CHROMIUM-6-CARBIDE
COBR2:1	COBALT-DIBROMIDE:SOL-1	CR2FEO4	DICHROMIUM-IRON-TETRAOXIDE
COBR2:21	COBALT-DIBROMIDE:SOL-21	CR2MGO4	DICHROMIUM-MAGNESIUM-
COCL	CARBONYL-CHLORIDE-GAS	CR2N	DICHROMIUM-NITRIDE
COCL3	COBALT-TRICHLORIDE-GAS	CR2NB	2-CHROMIUM-NIOBIUM
COCO3	COBALT-CARBONATE	CR2NIO4	DICHROMIUM-NICKEL-
COCR2O4	COBALT-DICHROMIUM-	CR2O3	DICHROMIUM-TRIOXIDE
COF	CARBONYL-FLUORIDE-GAS	CR2TA	2-CHROMIUM-TANTALUM
COF2	CARBONIC-DIFLUORIDE-GAS	CR3(ASO4)2	TRICHROMIUM-ARSENATE
COF3	COBALT-TRIFLUORIDE	CR3C2	3-CHROMIUM-2-CARBIDE
COFE2O4	COBALT-DIIRON-TETRAOXIDE	CR3SI	3-CHROMIUM-SILICON
COFE2O4:1	COBALT-DIIRON-	CR5SI3	5-CHROMIUM-3-SILICON

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
CR7C3	7-CHROMIUM-3-CARBIDE	CS2CO3	CESIUM-CARBONATE
CRASO4	CHROMIUM-ARSENATE	CS2F2	DICESIUM-DIFLUORIDE-GAS
CRB	CHROMIUM-MONOBORIDE	CS2O	CESIUM-OXIDE
CRB2	CHROMIUM-DIBORIDE	CS2O3	DICESIUM-TRIOXIDE
CRBR2	CHROMIUM-DIBROMIDE	CS2SO4	CESIUM-SULFATE
CRBR3	CHROMIUM-TRIBROMIDE	CS2SO4:A	CESIUM-SULFATE:SOL-A
CRBR4	CHROMIUM-TETRABROMIDE-GAS	CS2SO4:B	CESIUM-SULFATE:SOL-B
CRCL2	CHROMIUM-DICHLORIDE	CS3ASO4	CESIUM-ARSENATE
CRCL3	CHROMIUM-TRICHLORIDE	CSBR	CESIUM-BROMIDE
CRCL4	CHROMIUM-TETRACHLORIDE-GAS	CSCL	CESIUM-CHLORIDE
CRF2	CHROMIUM-DIFLUORIDE	CSCL:A	CESIUM-CHLORIDE:SOL-A
CRF3	CHROMIUM-TRIFLUORIDE	CSCL:B	CESIUM-CHLORIDE:SOL-B
CRF4	CHROMIUM-TETRAFLUORIDE	CSF	CESIUM-FLUORIDE
CRI2	CHROMIUM-DIIODIDE	CSI	CESIUM-IODIDE
CRI3	CHROMIUM-TRIIODIDE	CSO	CESIUM-MONOXIDE-GAS
CRN	CHROMIUM-NITRIDE	CSO2	CESIUM-DIOXIDE
CRNAO2	CHROMIUM-SODIUM-DIOXIDE	CSOH	CESIUM-HYDROXIDE
CRO	CHROMIUM-MONOXIDE-GAS	CSOH:A	CESIUM-HYDROXIDE:SOL-A
CRO2	CHROMIUM-DIOXIDE	CSOH:B	CESIUM-HYDROXIDE:SOL-B
CRO2CL2	CHROMIUM-DICHLORIDE-DIOXIDE-	CSOH:C	CESIUM-HYDROXIDE:SOL-C
CRO3	CHROMIUM-TRIOXIDE	CU	COPPER
CRS	CHROMIUM-MONOSULFIDE	CU(OH)2	COPPER-HYDROXIDE
CRS1.17	CHROMIUM-1.17-SULFIDE	CU2MG	2-COPPER-1-MAGNESIUM
CRS1.17:A	CHROMIUM-1.17-SULFIDE:SOL-A	CU2O	DICOPPER-OXIDE
CRS1.17:B	CHROMIUM-1.17-SULFIDE:SOL-B	CU2OSO4	DICOPPER-OXIDE-SULFATE
CRS1.17:C	CHROMIUM-1.17-SULFIDE:SOL-C	CU2S	DICOPPER-SULFIDE
CRS:1	CHROMIUM-MONOSULFIDE:SOL-1	CU2S:A	DICOPPER-SULFIDE:SOL-A
CRS:2	CHROMIUM-MONOSULFIDE:SOL-2	CU2S:B	DICOPPER-SULFIDE:SOL-B
CRSI	CHROMIUM-SILICON	CU2S:C	DICOPPER-SULFIDE:SOL-C
CRSI2	CHROMIUM-2-SILICON	CU2SB	2-COPPER-ANTIMONY
CS	CARBON-MONOSULFIDE-GAS	CU2SB:1	2-COPPER-ANTIMONY:SOL-1
CS-2	CESIUM-DIATOMIC-GAS	CU2SB:11	2-COPPER-ANTIMONY:SOL-11
CS2	CARBON-DISULFIDE	CU2SE	DICOPPER-SELENIDE
CS2(OH)2	DICESIUM-DIHYDROXIDE-GAS	CU2SE:A	DICOPPER-SELENIDE:SOL-A
CS2CL2	DICESIUM-DICHLORIDE-GAS	CU2SE:B	DICOPPER-SELENIDE:SOL-B

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
CU2SO4	DICOPPER-SULFATE	CUFE2O4:B	COPPER-DIIRON-
CU2TE	DICOPPER-TELLURIDE	CUFE2O4:C	COPPER-DIIRON-
CU2TE:A	DICOPPER-TELLURIDE:SOL-A	CUFEO2	COPPER-IRON-DIOXIDE
CU2TE:B	DICOPPER-TELLURIDE:SOL-B	CUFEO2:A	COPPER-IRON-DIOXIDE:SOL-A
CU2TE:C	DICOPPER-TELLURIDE:SOL-C	CUFEO2:B	COPPER-IRON-DIOXIDE:SOL-B
CU2TE:D	DICOPPER-TELLURIDE:SOL-D	CUFES2	COPPER-IRON-DISULFIDE
CU2TE:E	DICOPPER-TELLURIDE:SOL-E	CUFES2:A	COPPER-IRON-DISULFIDE:SOL-A
CU2TE:Z	DICOPPER-TELLURIDE:SOL-Z	CUFES2:B	COPPER-IRON-DISULFIDE:SOL-B
CU3(ASO4)2	TRICOPPER-DIARSENATE	CUFES2:C	COPPER-IRON-DISULFIDE:SOL-C
CU3AS	TRICOPPER-ARSENIDE	CUI	COPPER-MONOIODIDE
CU3ASO4	TRICOPPER-ARSENATE	CUI:A	COPPER-MONOIODIDE:SOL-A
CU3BR3	TRICOPPER-TRIBROMIDE-GAS	CUI:B	COPPER-MONOIODIDE:SOL-B
CU3CL3	TRICOPPER-TRICHLORIDE-GAS	CUI:C	COPPER-MONOIODIDE:SOL-C
CU3I3	TRICOPPER-TRIIODIDE-GAS	CUMG2	1-COPPER-2-MAGNESIUM
CU3P	TRICOPPER-PHOSPHIDE	CUMOO4	COPPER-MOLYBDATE
CU5FES4	PENTACOPPER-IRON-	CUO	COPPER-MONOXIDE
CU5FES4:A	PENTACOPPER-IRON-	CUP2	COPPER-DIPHOSPHIDE
CU5FES4:B	PENTACOPPER-IRON-	CUS	COPPER-SULFIDE
CU5FES4:C	PENTACOPPER-IRON-	CUSE	COPPER-SELENIDE
CUBR	COPPER-MONOBROMIDE	CUSE:B	COPPER-SELENIDE:SOL-B
CUBR2	COPPER-DIBROMIDE	CUSE:O	COPPER-SELENIDE:SOL-O
CUBR:A	COPPER-MONOBROMIDE:SOL-A	CUSEO3	COPPER-SELENITE
CUBR:B	COPPER-MONOBROMIDE:SOL-B	CUSO4	COPPER-SULFATE
CUBR:C	COPPER-MONOBROMIDE:SOL-C	CUSO4*3H2O	COPPER-SULFATE-TRIHYDRATE
CUCL	COPPER-MONOCHLORIDE	CUSO4*5H2O	COPPER-SULFATE-
CUCL2	COPPER-DICHLORIDE	CUSO4*H2O	COPPER-SULFATE-
CUCL2:A	COPPER-DICHLORIDE:SOL-A	CUTE	COPPER-TELLURIDE
CUCL2:B	COPPER-DICHLORIDE:SOL-B	D	DEUTERIUM-MONATOMIC-GAS
CUCL:A	COPPER-MONOCHLORIDE:SOL-A	D2	DEUTERIUM
CUCL:B	COPPER-MONOCHLORIDE:SOL-B	D2O	WATER-D2
CUCN	COPPER-CYANIDE	D2S	HYDROGEN-SULFIDE-D2-GAS
CUF	COPPER-MONOFLUORIDE	DCL	HYDROGEN-CHLORIDE-D1-GAS
CUF2	COPPER-DIFLUORIDE	DF	HYDROGEN-FLUORIDE-D1-GAS
CUFE2O4	COPPER-DIIRON-TETRAOXIDE	DH	HYDROGEN-D1-GAS
CUFE2O4:A	COPPER-DIIRON-	DICKITE	AL2SI2O7*2H2O-D

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
DS	HYDROGEN-MONOSULFIDE-D1-	FE	IRON
DY	DYSPROSIUM	FE(CO)5	IRON-PENTACARBONYL
DY2O3	DYSPROSIUM-OXIDE	FE(OH)2	IRON-DIHYDROXIDE
DY:A	DYSPROSIUM:SOL-A	FE(OH)3	IRON-TRIHYDROXIDE
DY:B	DYSPROSIUM:SOL-B	FE(VO3)2	IRON-VANADATE
DYBR3	DYSPROSIUM-BROMIDE-GAS	FE0.877S	PYRRHOTITE
DYCL3	DYSPROSIUM-CHLORIDE	FE0.877S:A	PYRRHOTITE:SOL-A
DYCL3*6H2O	DYSPROSIUM-CHLORIDE-	FE0.877S:B	PYRRHOTITE:SOL-B
DYF3	DYSPROSIUM-FLUORIDE	FE0.947O	WUESTITE
DYI3	DYSPROSIUM-IODIDE-GAS	FE2(SO4)3	DIIRON-TRISULFATE
E-	ELECTRON-GAS	FE2B	DIIRON-BORIDE
ER	ERBIUM	FE2BR4	DIIRON-TETRABROMIDE-GAS
ER2O3	ERBIUM-OXIDE-CUBIC	FE2CL4	DIIRON-TETRACHLORIDE-GAS
ERBR3	ERBIUM-BROMIDE-GAS	FE2CL6	DIIRON-HEXACHLORIDE-GAS
ERCL3	ERBIUM-CHLORIDE	FE2I4	DIIRON-TETRAIODIDE-GAS
ERCL3*6H2O	ERBIUM-CHLORIDE-	FE2MGO4	DIIRON-MAGNESIUM-TETRAOXIDE
ERF3	ERBIUM-FLUORIDE	FE2MNO4	DIIRON-MANGANESE-TETRAOXIDE
ERF3:A	ERBIUM-FLUORIDE:SOL-A	FE2MNO4:1	DIIRON-MANGANESE-
ERF3:B	ERBIUM-FLUORIDE:SOL-B	FE2MNO4:2	DIIRON-MANGANESE-
ERI3	ERBIUM-IODIDE-GAS	FE2NIO4	DIIRON-NICKEL-TETRAOXIDE
EU	EUROPIUM	FE2NIO4:A	DIIRON-NICKEL-TETRAOXIDE:SOL-
EU2O3	EUROPIUM-OXIDE-CUBIC	FE2NIO4:B	DIIRON-NICKEL-TETRAOXIDE:SOL-
EU2O3-M	EUROPIUM-OXIDE-MONOCLINIC	FE2O3	HEMATITE
EU2O3-M:M1	EUROPIUM-OXIDE-	FE2O3*H2O	IRON-TRIOXIDE-HYDRATE-
EU2O3-M:M2	EUROPIUM-OXIDE-	FE2O3:A	HEMATITE:SOL-A
EUBR2	EUROPIUM-DIBROMIDE	FE2O3:B	HEMATITE:SOL-B
EUBR3	EUROPIUM-BROMIDE	FE2SIO4	IRON-ORTHOSILICATE-FAYALITE
EUCL3	EUROPIUM-CHLORIDE	FE2TA	2-IRON-TANTALUM
EUCL3*6H2O	EUROPIUM-CHLORIDE-	FE2TIO4	DIIRON-TITANIUM-TETROXIDE
EUF3	EUROPIUM-FLUORIDE	FE2U	2-IRON-URANIUM
EUF3:A	EUROPIUM-FLUORIDE:SOL-A	FE2ZNO4	DIIRON-ZINC-TETRAOXIDE
EUF3:B	EUROPIUM-FLUORIDE:SOL-B	FE3(ASO4)2	TRIIRON-DIARSENATE
EUS	EUROPIUM-MONOSULFIDE	FE3C	TRIIRON-CARBIDE
F	FLUORINE-MONATOMIC-GAS	FE3C:A	TRIIRON-CARBIDE:SOL-A
F2	FLUORINE	FE3C:B	TRIIRON-CARBIDE:SOL-B

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
FE3MO2	3-IRON-2-MOLYBDENUM	FES2	IRON-DISULFIDE
FE3O4	MAGNETITE	FES:A	IRON-MONOSULFIDE:SOL-A
FE3O4:A	MAGNETITE:SOL-A	FES:B	IRON-MONOSULFIDE:SOL-B
FE3O4:B	MAGNETITE:SOL-B	FES:C	IRON-MONOSULFIDE:SOL-C
FE4N	TETRAIRON-NITRIDE	FESE0.96	IRON-0.96-SELENIDE
FE4N:A	TETRAIRON-NITRIDE:SOL-A	FESE0.96:A	IRON-0.96-SELENIDE:SOL-A
FE4N:B	TETRAIRON-NITRIDE:SOL-B	FESE0.96:B	IRON-0.96-SELENIDE:SOL-B
FE:A	IRON:SOL-A	FESI	IRON-SILICON
FE:B	IRON:SOL-B	FESI2	LEBOITE-BETA
FE:C	IRON:SOL-C	FESI2.33	LEBOITE-ALPHA
FE:D	IRON:SOL-D	FESIO3	IRON-METASILICATE
FEAL2O4	IRON-DIALUMINIUM-TETRAOXIDE	FESO4	IRON-SULFATE
FEASO4	IRON-ARSENATE	FETE0.9	IRON-0.9-TELLURIDE
FEASO4:A	IRON-ARSENATE:SOL-A	FETE2	IRON-DITELLURIDE
FEASO4:B	IRON-ARSENATE:SOL-B	FETI	IRON-TITANIUM
FEASO4:C	IRON-ARSENATE:SOL-C	FETIO3	IRON-TITANIUM-TRIOXIDE-
FEB	IRON-MONOBORIDE	FEV2O4	IRON-DIVANADIUM-TETRAOXIDE
FEBR2	IRON-DIBROMIDE	FEWO4	IRON-TUNGSTATE
FEBR2:1	IRON-DIBROMIDE:SOL-1	GA	GALLIUM
FEBR2:2	IRON-DIBROMIDE:SOL-2	GA2(SEO4)3	GALLIUM-SELENATE
FEBR3	IRON-TRIBROMIDE	GA2CL6	DIGALLIUM-HEXACHLORIDE-GAS
FECL	IRON-MONOCHLORIDE-GAS	GA2O	DIGALLIUM-OXIDE-GAS
FECL2	IRON-DICHLORIDE	GA2O3	GALLIUM-OXIDE
FECL3	IRON-TRICHLORIDE	GA2S	DIGALLIUM-SULFIDE-GAS
FECO3	IRON-CARBONATE	GA2S3	DIGALLIUM-TRISULFIDE
FEF2	IRON-DIFLUORIDE	GA2SE3	DIGALLIUM-TRISELENIDE
FEF3	IRON-TRIFLUORIDE	GA2TE3	DIGALLIUM-TRITELLURIDE
FEI2	IRON-DIIODIDE	GAAS	GALLIUM-ARSENIDE
FEI2:1	IRON-DIIODIDE:SOL-1	GAASO4	GALLIUM-ARSENATE
FEI2:2	IRON-DIIODIDE:SOL-2	GABR3	GALLIUM-BROMIDE
FEMOO4	IRON-MOLYBDATE	GACL	GALLIUM-MONOCHLORIDE-GAS
FENAO2	IRON-SODIUM-DIOXIDE	GACL2	GALLIUM-DICHLORIDE-GAS
FEO	IRON-MONOXIDE	GACL3	GALLIUM-CHLORIDE
FEOCL	IRON-CHLORIDE-OXIDE	GAF	GALLIUM-MONOFLUORIDE-GAS
FES	IRON-MONOSULFIDE	GAF2	GALLIUM-DIFLUORIDE-GAS

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
GAF3	GALLIUM-FLUORIDE	GEF3	GERMANIUM-TRIFLUORIDE-GAS
GAI3	GALLIUM-IODIDE	GEF4	GERMANIUM-TETRAFLUORIDE-
GAN	GALLIUM-NITRIDE	GEH4	GERMANIUM-TETRAHYDRIDE
GAO	GALLIUM-MONOXIDE-GAS	GEI4	GERMANIUM-TETRAIODIDE-GAS
GAP	GALLIUM-PHOSPHIDE	GEMG2	GERMANIUM-2-MAGNESIUM
GAS	GALLIUM-MONOSULFIDE	GENI2	GERMANIUM-2-NICKEL
GASB	GALLIUM-ANTIMONY	GEO	GERMANIUM-MONOXIDE-GAS
GASE	GALLIUM-MONOSELENIDE	GEO2	GERMANIUM-DIOXIDE
GATE	GALLIUM-MONOTELLURIDE	GEO2:A	GERMANIUM-DIOXIDE:SOL-A
GD	GADOLINIUM	GEO2:B	GERMANIUM-DIOXIDE:SOL-B
GD2O3	GADOLINIUM-OXIDE-CUBIC	GEP	GERMANIUM-PHOSPHIDE
GD2O3-M	GADOLINIUM-OXIDE-MONOCLINIC	GES	GERMANIUM-MONOSULFIDE
GD:A	GADOLINIUM:SOL-A	GES2	GERMANIUM-DISULFIDE
GD:B	GADOLINIUM:SOL-B	GESE	GERMANIUM-MONOSELENIDE
GDBR3	GADOLINIUM-BROMIDE	GESE2	GERMANIUM-DISELENIDE
GDCL3	GADOLINIUM-CHLORIDE	GETE	GERMANIUM-MONOTELLURIDE
GDF3	GADOLINIUM-FLUORIDE	GEU	GERMANIUM-URANIUM
GDF3:A	GADOLINIUM-FLUORIDE:SOL-A	H	HYDROGEN-MONATOMIC-GAS
GDF3:B	GADOLINIUM-FLUORIDE:SOL-B	H2	HYDROGEN
GDI3	GADOLINIUM-IODIDE	H2O	WATER
GDI3:A	GADOLINIUM-IODIDE:SOL-A	H2O2	HYDROGEN-PEROXIDE
GDI3:B	GADOLINIUM-IODIDE:SOL-B	H2S	HYDROGEN-SULFIDE
GDOCL	GADOLINIUM-CHLORIDE-OXIDE	H2S2	DIHYDROGEN-DISULFIDE-GAS
GE	GERMANIUM	H2SE	HYDROGEN-SELENIDE-GAS
GE2U	2-GERMANIUM-URANIUM	H2SO4	SULFURIC-ACID
GE3U	3-GERMANIUM-URANIUM	H2TE	HYDROGEN-TELLURIDE-GAS
GE3U5	3-GERMANIUM-5-URANIUM	H2WO4	TUNGSTIC-ACID
GE5U3	5-GERMANIUM-3-URANIUM	H3BO3	BORIC-ACID
GEBR4	GERMANIUM-TETRABROMIDE-GAS	H3N	AMMONIA
GECL	GERMANIUM-MONOCHLORIDE-	H3PO4	PHOSPHORIC-ACID
GECL2	GERMANIUM-DICHLORIDE-GAS	H4N2	HYDRAZINE
GECL3	GERMANIUM-TRICHLORIDE-GAS	HAFNIUM	HAFNIUM
GECL4	GERMANIUM-TETRACHLORIDE-	HALLOYSITE	AL2SI2O7*2H2O-H
GEF	GERMANIUM-MONOFLUORIDE-	HBO2	METABORIC-ACID
GEF2	GERMANIUM-DIFLUORIDE-GAS	HBR	HYDROGEN-BROMIDE

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
HCL	HYDROGEN-CHLORIDE	HGI2:A	MERCURY-DIIODIDE:SOL-A
HDO	WATER-D1-GAS	HGI2:B	MERCURY-DIIODIDE:SOL-B
HE	HELIUM	HGO	MERCURY-OXIDE-RED
HF	HYDROGEN-FLUORIDE	HGS	MERCURY-SULFIDE-RED
HF:A	HAFNIUM:SOL-A	HGS:B	MERCURY-SULFIDE-RED:SOL-B
HF:B	HAFNIUM:SOL-B	HGS:R	MERCURY-SULFIDE-RED:SOL-R
HFB2	HAFNIUM-DIBORIDE	HGSE	MERCURY-SELENIDE
HFBR4	HAFNIUM-TETRABROMIDE	HGSEO3	MERCURY-SELENITE
HFC	HAFNIUM-CARBIDE	HGSO4	MERCURY-SULFATE
HFCL2	HAFNIUM-DICHLORIDE-GAS	HGTE	MERCURY-TELLURIDE
HFCL3	HAFNIUM-TRICHLORIDE-GAS	HI	HYDROGEN-IODIDE
HFCL4	HAFNIUM-TETRACHLORIDE	HNCO	ISOCYANIC-ACID-GAS
HFF4	HAFNIUM-TETRAFLUORIDE	HNO3	NITRIC-ACID
HFI4	HAFNIUM-TETRAIODIDE	HO	HOLMIUM
HFN	HAFNIUM-NITRIDE	HO2O3	HOLMIUM-OXIDE
HFO2	HAFNIUM-DIOXIDE	HO:A	HOLMIUM:SOL-A
HFO2:A	HAFNIUM-DIOXIDE:SOL-A	HO:B	HOLMIUM:SOL-B
HFO2:B	HAFNIUM-DIOXIDE:SOL-B	HOBR3	HOLMIUM-BROMIDE
HFSRO3	HAFNIUM-STRONTIUM-TRIOXIDE	HOCL3	HOLMIUM-CHLORIDE
HG	MERCURY	HOCL3*6H2O	HOLMIUM-CHLORIDE-
HG2BR2	DIMERCURY-DIBROMIDE	HOF3	HOLMIUM-FLUORIDE
HG2CL2	DIMERCURY-DICHLORIDE	HOF3:A	HOLMIUM-FLUORIDE:SOL-A
HG2F2	DIMERCURY-DIFLUORIDE	HOF3:B	HOLMIUM-FLUORIDE:SOL-B
HG2I2	DIMERCURY-DIIODIDE	HS	HYDROGEN-MONOSULFIDE-GAS
HG2SO4	DIMERCURY-SULFATE	I	IODINE-MONATOMIC-GAS
HG3(ASO4)2	TRIMERCURY-DIARSENATE	I2	IODINE
HGBR	MERCURY-MONOBROMIDE-GAS	IN	INDIUM
HGBR2	MERCURY-DIBROMIDE	IN2(SO4)3	DIINDIUM-TRISULFATE
HGCL	MERCURY-MONOCHLORIDE-GAS	IN2CL6	DIINDIUM-HEXACHLORIDE-GAS
HGCL2	MERCURY-DICHLORIDE	IN2O	DIINDIUM-OXIDE-GAS
HGF	MERCURY-MONOFLUORIDE-GAS	IN2O3	DIINDIUM-TRIOXIDE
HGF2	MERCURY-DIFLUORIDE	IN2S3	DIINDIUM-TRISULFIDE
HGH	MERCURY-MONOHYDRIDE-GAS	IN2S3:A	DIINDIUM-TRISULFIDE:SOL-A
HGI	MERCURY-MONOIODIDE-GAS	IN2S3:B	DIINDIUM-TRISULFIDE:SOL-B
HGI2	MERCURY-DIIODIDE	IN2S3:C	DIINDIUM-TRISULFIDE:SOL-C

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
IN2SE3	DIINDIUM-TRISELENIDE	IRBR3	IRIDIUM-TRIBROMIDE
IN2SE3:A	DIINDIUM-TRISELENIDE:SOL-A	IRCL3	IRIDIUM-TRICHLORIDE
IN2SE3:B	DIINDIUM-TRISELENIDE:SOL-B	IRF6	IRIDIUM-HEXAFLUORIDE-GAS
IN2TE	DIINDIUM-TELLURIDE	IRI	IRIDIUM-MONOIODIDE
IN2TE3	DIINDIUM-TRITELLURIDE	IRI2	IRIDIUM-DIIODIDE
IN2TE3:A	DIINDIUM-TRITELLURIDE:SOL-A	IRO2	IRIDIUM-DIOXIDE
IN2TE3:B	DIINDIUM-TRITELLURIDE:SOL-B	IRO3	IRIDIUM-TRIOXIDE-GAS
IN5S6	PENTAINDIUM-HEXASULFIDE	IRS2	IRIDIUM-DISULFIDE
INAS	INDIUM-ARSENIDE	K	POTASSIUM
INASO4	INDIUM-ARSENATE	K2	POTASSIUM-DIATOMIC-GAS
INBR	INDIUM-MONOBROMIDE	K2(CN)2	DIPOTASSIUM-DICYANIDE-GAS
INBR3	INDIUM-TRIBROMIDE	K2(OH)2	DIPOTASSIUM-DIHYDROXIDE-GAS
INCL	INDIUM-MONOCHLORIDE	K2B407	DIPOTASSIUM-TETRABORATE
INCL2	INDIUM-DICHLORIDE	K2B6O10	DIPOTASSIUM-HEXABORATE
INCL2:1	INDIUM-DICHLORIDE:SOL-1	K2B8O13	DIPOTASSIUM-OCTABORATE
INCL2:2	INDIUM-DICHLORIDE:SOL-2	K2BR2	DIPOTASSIUM-DIBROMIDE-GAS
INCL3	INDIUM-TRICHLORIDE	K2CL2	DIPOTASSIUM-DICHLORIDE-GAS
INCL:A	INDIUM-MONOCHLORIDE:SOL-A	K2CO3	POTASSIUM-CARBONATE
INCL:B	INDIUM-MONOCHLORIDE:SOL-B	K2CRO4	POTASSIUM-CHROMATE
INF	INDIUM-MONOFLUORIDE-GAS	K2CRO4:A	POTASSIUM-CHROMATE:SOL-A
INF2	INDIUM-DIFLUORIDE-GAS	K2CRO4:B	POTASSIUM-CHROMATE:SOL-B
INF3	INDIUM-TRIFLUORIDE	K2F2	DIPOTASSIUM-DIFLUORIDE-GAS
INI	INDIUM-MONOIODIDE	K2HPO4	DIPOTASSIUM-HYDROGEN-
INI2	INDIUM-DIIODIDE-GAS	K2I2	DIPOTASSIUM-DIIODIDE-GAS
INI3	INDIUM-TRIIODIDE	K2O	POTASSIUM-OXIDE
INN	INDIUM-NITRIDE	K2O2	DIPOTASSIUM-PEROXIDE
INP	INDIUM-PHOSPHIDE	K2S	POTASSIUM-SULFIDE
INP:A	INDIUM-PHOSPHIDE:SOL-A	K2S:1	POTASSIUM-SULFIDE:SOL-1
INP:B	INDIUM-PHOSPHIDE:SOL-B	K2S:2	POTASSIUM-SULFIDE:SOL-2
INS	INDIUM-MONOSULFIDE	K2SI2O5	POTASSIUM-DISILICATE
INSB	INDIUM-ANTIMONY	K2SI2O5:B	POTASSIUM-DISILICATE:SOL-B
INSE	INDIUM-MONOSELENIDE	K2SI2O5:C	POTASSIUM-DISILICATE:SOL-C
INTE	INDIUM-MONOTELLURIDE	K2SI4O9	POTASSIUM-TETRASILICATE
IR	IRIDIUM	K2SI4O9:A	POTASSIUM-TETRASILICATE:SOL-
IR2S3	DIIRIDIUM-TRISULFIDE	K2SI4O9:B	POTASSIUM-TETRASILICATE:SOL-

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
K2SIO3	POTASSIUM-METASILICATE	KO	POTASSIUM-MONOXIDE-GAS
K2SO3	POTASSIUM-SULFITE	KO2	POTASSIUM-DIOXIDE
K2SO4	POTASSIUM-SULFATE	KOH	POTASSIUM-HYDROXIDE
K2SO4:A	POTASSIUM-SULFATE:SOL-A	KOH:A	POTASSIUM-HYDROXIDE:SOL-A
K2SO4:B	POTASSIUM-SULFATE:SOL-B	KOH:B	POTASSIUM-HYDROXIDE:SOL-B
K3ALCL6	TRIPOTASSIUM-	KR	KRYPTON
K3ALF6	TRIPOTASSIUM-	LA	LANTHANUM
K3ASO4	POTASSIUM-ARSENATE	LA2O3	LANTHANUM-OXIDE
K3PO4	POTASSIUM-PHOSPHATE	LA2S3	LANTHANUM-SULFIDE
KAL(SO4)2	POTASSIUM-ALUMINIUM-SULFATE	LA2SE3	LANTHANUM-SELENIDE
KALCL4	POTASSIUM-	LA2TE3	LANTHANUM-TELLURIDE
KALSI2O6	LEUCITE	LA:A	LANTHANUM:SOL-A
KALSI3O8	SANIDINE	LA:B	LANTHANUM:SOL-B
KALSI3O8-A	ADULARIA	LA:C	LANTHANUM:SOL-C
KALSI3O8-M	MICROCLINE	LAASO4	LANTHANUM-ARSENATE
KALSIO4	KALIOPHILITE	LABR3	LANTHANUM-BROMIDE
KALSO4*2*12W	POTASSIUM-ALUMINIUM-SULFATE-	LACL3	LANTHANUM-CHLORIDE
KALSO4*2*3W	POTASSIUM-ALUMINIUM-SULFATE-	LAF3	LANTHANUM-FLUORIDE
KAOLINITE	AL2SI2O7*2H2O	LAH2	LANTHANUM-DIHYDRIDE
KBO2	POTASSIUM-METABORATE	LAI3	LANTHANUM-IODIDE
KBR	POTASSIUM-BROMIDE	LAMG	LANTHANUM-MAGNESIUM
KCL	POTASSIUM-CHLORIDE	LAN	LANTHANUM-NITRIDE
KCLO4	POTASSIUM-PERCHLORATE	LAO	LANTHANUM-MONOXIDE-GAS
KCLO4:1	POTASSIUM-PERCHLORATE:SOL-1	LAOCL	LANTHANUM-CHLORIDE-OXIDE
KCLO4:2	POTASSIUM-PERCHLORATE:SOL-2	LAS	LANTHANUM-MONOSULFIDE
KCN	POTASSIUM-CYANIDE	LASE	LANTHANUM-MONOSELENIDE
KF	POTASSIUM-FLUORIDE	LAWSONITE	CAAL2SI2O8*2H2O
KH	POTASSIUM-HYDRIDE	LI	LITHIUM
KH2PO4	POTASSIUM-DIHYDROGEN-	LI2	LITHIUM-DIATOMIC-GAS
KH2PO4:1	POTASSIUM-DIHYDROGEN-	LI2(OH)2	DILITHIUM-DIHYDROXIDE-GAS
KH2PO4:2	POTASSIUM-DIHYDROGEN-	LI2B4O7	DILITHIUM-TETRABORATE
KI	POTASSIUM-IODIDE	LI2B6O10	DILITHIUM-HEXABORATE
KNO3	POTASSIUM-NITRATE	LI2BEF4	DILITHIUM-
KNO3:A	POTASSIUM-NITRATE:SOL-A	LI2BR2	DILITHIUM-DIBROMIDE-GAS
KNO3:B	POTASSIUM-NITRATE:SOL-B	LI2CL2	DILITHIUM-DICHLORIDE-GAS

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
LI2CO3	LITHIUM-CARBONATE	LIALSIO4	EUCRYPTITE
LI2CO3:A	LITHIUM-CARBONATE:SOL-A	LIALSIO4:B	EUCRYPTITE:SOL-B
LI2CO3:B	LITHIUM-CARBONATE:SOL-B	LIALSIO4:C	EUCRYPTITE:SOL-C
LI2CO3:C	LITHIUM-CARBONATE:SOL-C	LIBEF3	LITHIUM-TRIFLUOROBERYLLATE
LI2F2	DILITHIUM-DIFLUORIDE-GAS	LIBO2	LITHIUM-METABORATE
LI2I2	DILITHIUM-DIIODIDE-GAS	LIBR	LITHIUM-BROMIDE
LI2O	LITHIUM-OXIDE	LICL	LITHIUM-CHLORIDE
LI2O2	DILITHIUM-PEROXIDE	LICLO	LITHIUM-HYPOCHLORITE-GAS
LI2S	LITHIUM-SULFIDE	LICLO4	LITHIUM-PERCHLORATE
LI2SE	LITHIUM-SELENIDE	LIF	LITHIUM-FLUORIDE
LI2SI2O5	LITHIUM-DISILICATE	LIFEO2	LITHIUM-IRON-DIOXIDE
LI2SI2O5:A	LITHIUM-DISILICATE:SOL-A	LIFO	LITHIUM-HYPOFLUORITE-GAS
LI2SI2O5:B	LITHIUM-DISILICATE:SOL-B	LIH	LITHIUM-HYDRIDE
LI2SIO3	LITHIUM-METASILICATE	LII	LITHIUM-IODIDE
LI2SO4	LITHIUM-SULFATE	LIO	LITHIUM-MONOXIDE-GAS
LI2SO4:A	LITHIUM-SULFATE:SOL-A	LIOH	LITHIUM-HYDROXIDE
LI2SO4:B	LITHIUM-SULFATE:SOL-B	LU	LUTETIUM
LI2TE	LITHIUM-TELLURIDE	LU2O3	LUTETIUM-OXIDE
LI2TIO3	DILITHIUM-TITANIUM-TRIOXIDE	MG	MAGNESIUM
LI2TIO3:A	DILITHIUM-TITANIUM-TRIOXIDE:S-A	MG(NO3)2	MAGNESIUM-NITRATE
LI2TIO3:B	DILITHIUM-TITANIUM-TRIOXIDE:S-B	MG(OH)2	MAGNESIUM-HYDROXIDE
LI2ZRO3	DILITHIUM-ZIRCONIUM-TRIOXIDE	MG(OH)CL	MAGNESIUM-CHLORIDE-
LI3ALF6	TRILITHIUM-	MG(VO3)2	MAGNESIUM-METAVANADATE
LI3ALF6:B	TRILITHIUM-6-	MG2BR4	DIMAGNESIUM-TETRABROMIDE-
LI3ALF6:C	TRILITHIUM-6-	MG2C3	DIMAGNESIUM-TRICARBIDE
LI3ALF6:D	TRILITHIUM-6-	MG2F4	DIMAGNESIUM-TETRAFLUORIDE-
LI3ALF6:E	TRILITHIUM-6-	MG2PB	2-MAGNESIUM-LEAD
LI3ASO4	LITHIUM-ARSENATE	MG2SI	2-MAGNESIUM-SILICON
LI3F3	TRILITHIUM-TRIFLUORIDE-GAS	MG2SIO4	MAGNESIUM-ORTHOSILICATE
LI3N	TRILITHIUM-NITRIDE	MG2TH	2-MAGNESIUM-THORIUM
LI4SIO4	LITHIUM-ORTHOSILICATE	MG2TIO4	DIMAGNESIUM-TITANIUM-
LIALF4	LITHIUM-	MG2V2O7	MAGNESIUM-PYROVANADATE
LIALO2	LITHIUM-ALUMINATE	MG3(ASO4)2	MAGNESIUM-ARSENATE
LIALSI2O6	ALPHA-SPODUMENE	MG3(PO4)2	MAGNESIUM-ORTHOPHOSPHATE
LIALSI2O6-B	BETA-SPODUMENE	MG3N2	TRIMAGNESIUM-DINITRIDE

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
MG3N2:A	TRIMAGNESIUM-DINITRIDE:SOL-A	MN2O3	DIMANGANESE-TRIOXIDE
MG3N2:B	TRIMAGNESIUM-DINITRIDE:SOL-B	MN2P	DIMANGANESE-PHOSPHIDE
MG3N2:C	TRIMAGNESIUM-DINITRIDE:SOL-C	MN2SB	2-MANGANESE-ANTIMONY
MGAL2O4	MAGNESIUM-DIALUMINIUM-	MN2SB:1	2-MANGANESE-ANTIMONY:SOL-1
MGB2	MAGNESIUM-DIBORIDE	MN2SB:2	2-MANGANESE-ANTIMONY:SOL-2
MGB4	MAGNESIUM-TETRABORIDE	MN2SIO4	TEPHROITE
MGBR	MAGNESIUM-MONOBROMIDE-GAS	MN2TIO4	DIMANGANESE-TITANIUM-
MGBR2	MAGNESIUM-BROMIDE	MN3(ASO4)2	MANGANESE-ARSENATE
MGC2	MAGNESIUM-DICARBIDE	MN3C	TRIMANGANESE-CARBIDE
MGCL	MAGNESIUM-MONOCHLORIDE-	MN3O4	TRIMANGANESE-TETRAOXIDE
MGCL2	MAGNESIUM-CHLORIDE	MN3O4:A	TRIMANGANESE-
MGCO3	MAGNESIUM-CARBONATE	MN3O4:B	TRIMANGANESE-
MGF	MAGNESIUM-MONOFLUORIDE-	MN3SI	3-MANGANESE-SILICON
MGF2	MAGNESIUM-FLUORIDE	MN3SI:1	3-MANGANESE-SILICON:SOL-1
MGH2	MAGNESIUM-HYDRIDE	MN3SI:2	3-MANGANESE-SILICON:SOL-2
MGI	MAGNESIUM-MONOIODIDE-GAS	MN4N	TETRAMANGANESE-
MGI2	MAGNESIUM-IODIDE	MN5N2	PENTAMANGANESE-DINITRIDE
MGMOO4	MAGNESIUM-MOLYBDATE	MN5SI3	5-MANGANESE-3-SILICON
MGNI2	MAGNESIUM-2-NICKEL	MN7C3	HEPTAMANGANESE-TRICARBIDE
MGO	MAGNESIUM-OXIDE	MN:A	MANGANESE:SOL-A
MGOH	MAGNESIUM-MONOHYDROXIDE-	MN:B	MANGANESE:SOL-B
MGS	MAGNESIUM-SULFIDE	MN:C	MANGANESE:SOL-C
MGSE	MAGNESIUM-SELENIDE	MN:D	MANGANESE:SOL-D
MGSEO3	MAGNESIUM-SELENITE	MNAL2O4	MANGANESE-DIALUMINIUM-
MGSIO3	MAGNESIUM-METASILICATE	MNAS	MANGANESE-ARSENIDE
MGSIO3:1	MAGNESIUM-METASILICATE:SOL-1	MNAS:1	MANGANESE-ARSENIDE:SOL-1
MGSIO3:2	MAGNESIUM-METASILICATE:SOL-2	MNAS:2	MANGANESE-ARSENIDE:SOL-2
MGSIO3:3	MAGNESIUM-METASILICATE:SOL-3	MNAS:3	MANGANESE-ARSENIDE:SOL-3
MGSO4	MAGNESIUM-SULFATE	MNB	MANGANESE-MONOBORIDE
MGTE	MAGNESIUM-TELLURIDE	MNB2	MANGANESE-DIBORIDE
MGTI2O5	MAGNESIUM-DITITANIUM-	MNBR2	MANGANESE-DIBROMIDE
MGTIO3	MAGNESIUM-TITANIUM-TRIOXIDE	MNCL2	MANGANESE-DICHLORIDE
MGWO4	MAGNESIUM-TUNGSTATE	MNCO3	MANGANESE-CARBONATE
MN	MANGANESE	MNF2	MANGANESE-DIFLUORIDE
MN15C4	15-MANGANESE-4-CARBID	MNF2:A	MANGANESE-DIFLUORIDE:SOL-A

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
MNF2:B	MANGANESE-DIFLUORIDE:SOL-B	MOO3	MOLYBDENUM-TRIOXIDE
MNF3	MANGANESE-TRIFLUORIDE	MOS2	MOLYBDENUM-DISULFIDE
MNI2	MANGANESE-DIIODIDE	MOS3	MOLYBDENUM-TRISULFIDE
MNMOO4	MANGANESE-MOLYBDATE	MOSI2	MOLYBDENUM-2-SILICON
MNO	MANGANESE-OXIDE	MUSCOVITE	KAL3SI3O10(OH)2
MNO2	MANGANESE-DIOXIDE	N	NITROGEN-MONATOMIC-GAS
MNP	MANGANESE-MONOPHOSPHIDE	N-D	IMIDOGEN-D1-GAS
MNP3	MANGANESE-TRIPHOSPHIDE	N2	NITROGEN
MNS	MANGANESE-MONOSULFIDE-	N2O	DINITROGEN-OXIDE
MNS2	MANGANESE-DISULFIDE	N2O3	DINITROGEN-TRIOXIDE
MNSB	MANGANESE-ANTIMONY	N2O5	DINITROGEN-PENTAOXIDE
MNSE	MANGANESE-SELENIDE	NA	SODIUM
MNSI	MANGANESE-SILICON	NA2	SODIUM-DIATOMIC-GAS
MNSI1.7	MANGANESE-1.7-SILICON	NA2(CN)2	DISODIUM-DICYANIDE-GAS
MNSIO3	RHODONITE	NA2(OH)2	DISODIUM-DIHYDROXIDE-GAS
MNSN2	MANGANESE-2-TIN	NA2B4O7	DISODIUM-TETRABORATE
MNSO4	MANGANESE-SULFATE	NA2BR2	DISODIUM-DIBROMIDE-GAS
MNTE	MANGANESE-TELLURIDE	NA2CL2	DISODIUM-DICHLORIDE-GAS
MNTE2	MANGANESE-DITELLURIDE	NA2CO3	SODIUM-CARBONATE
MNTE:A	MANGANESE-TELLURIDE:SOL-A	NA2CO3:1	SODIUM-CARBONATE:SOL-1
MNTE:B	MANGANESE-TELLURIDE:SOL-B	NA2CO3:2	SODIUM-CARBONATE:SOL-2
MNTIO3	MANGANESE-TITANIUM-TRIOXIDE	NA2CRO4	SODIUM-CHROMATE
MNWO4	MANGANESE-TUNGSTATE	NA2CRO4:A	SODIUM-CHROMATE:SOL-A
MO	MOLYBDENUM	NA2CRO4:B	SODIUM-CHROMATE:SOL-B
MO(CO)6	MOLYBDENUM-HEXACARBONYL	NA2F2	DISODIUM-DIFLUORIDE-GAS
MO2C	DIMOLYBDENUM-CARBIDE	NA2MOO4	SODIUM-MOLYBDATE
MO2N	DIMOLYBDENUM-NITRIDE	NA2MOO4:A	SODIUM-MOLYBDATE:SOL-A
MO2S3	MOLYBDENUM-SESQUISULFIDE	NA2MOO4:B	SODIUM-MOLYBDATE:SOL-B
MO3SI	3-MOLYBDENUM-SILICON	NA2MOO4:C	SODIUM-MOLYBDATE:SOL-C
MO5SI3	5-MOLYBDENUM-3-SILICON	NA2MOO4:D	SODIUM-MOLYBDATE:SOL-D
MOASO4	MOLYBDENUM-ARSENATE	NA2O	SODIUM-OXIDE
MOC	MOLYBDENUM-MONOCARBIDE-	NA2O2	DISODIUM-PEROXIDE
MOO	MOLYBDENUM-MONOXIDE-GAS	NA2O2:A	DISODIUM-PEROXIDE:SOL-A
MOO2	MOLYBDENUM-DIOXIDE	NA2O2:B	DISODIUM-PEROXIDE:SOL-B
MOO2CL2	MOLYBDENUM-DICHLORIDE-	NA2O:A	SODIUM-OXIDE:SOL-A

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
NA2O:B	SODIUM-OXIDE:SOL-B	NA3PO4	SODIUM-PHOSPHATE
NA2O:C	SODIUM-OXIDE:SOL-C	NA3VO4	SODIUM-ORTHOVANADATE
NA2S	SODIUM-SULFIDE	NA4SIO4	SODIUM-ORTHOSILICATE
NA2S2	DISODIUM-DISULFIDE	NA4V2O7	SODIUM-PYROVANADATE
NA2S3	DISODIUM-TRISULFIDE	NA6SI2O7	HEXASODIUM-DISILICON-
NA2S4	DISODIUM-TETRASULFIDE	NAALCL4	SODIUM-
NA2S:1	SODIUM-SULFIDE:SOL-1	NAALO2	SODIUM-ALUMINATE
NA2S:2	SODIUM-SULFIDE:SOL-2	NAALO2:A	SODIUM-ALUMINATE:SOL-A
NA2SI2O5	SODIUM-DISILICATE	NAALO2:B	SODIUM-ALUMINATE:SOL-B
NA2SI2O5:A	SODIUM-DISILICATE:SOL-A	NAALSI2O6	JADEITE
NA2SI2O5:B	SODIUM-DISILICATE:SOL-B	NAALSI2O6-D	DEHYDRATED-ANALCITE
NA2SI2O5:C	SODIUM-DISILICATE:SOL-C	NAALSI3O8	ALBITE
NA2SIO3	SODIUM-METASILICATE	NAALSI3O8-A	ANALBITE
NA2SO3	SODIUM-SULFITE	NAALSIO4	NEPHELINE
NA2SO4	SODIUM-SULFATE	NAALSIO4:A	NEPHELINE:SOL-A
NA2SO4-III	SODIUM-SULFATE-III	NAALSIO4:B	NEPHELINE:SOL-B
NA2SO4:1	SODIUM-SULFATE:SOL-1	NAALSIO4:C	NEPHELINE:SOL-C
NA2SO4:4	SODIUM-SULFATE:SOL-4	NAB3O5	SODIUM-TRIBORATE
NA2SO4:5	SODIUM-SULFATE:SOL-5	NABO2	SODIUM-METABORATE
NA2TE	SODIUM-TELLURIDE	NABR	SODIUM-BROMIDE
NA2TI2O5	DISODIUM-DITITANIUM-	NACL	SODIUM-CHLORIDE
NA2TI3O7	DISODIUM-TRITITANIUM-	NACLO4	SODIUM-PERCHLORATE
NA2TIO3	DISODIUM-TITANIUM-TRIOXIDE	NACLO4:A	SODIUM-PERCHLORATE:SOL-A
NA2TIO3:A	DISODIUM-TITANIUM-	NACLO4:B	SODIUM-PERCHLORATE:SOL-B
NA2TIO3:B	DISODIUM-TITANIUM-	NACN	SODIUM-CYANIDE
NA2WO4	SODIUM-TUNGSTATE	NAF	SODIUM-FLUORIDE
NA2WO4:1	SODIUM-TUNGSTATE:SOL-1	NAH	SODIUM-HYDRIDE
NA2WO4:2	SODIUM-TUNGSTATE:SOL-2	NAHCO3	SODIUM-HYDROGEN-CARBONATE
NA3ALCL6	TRISODIUM-	NAI	SODIUM-IODIDE
NA3ALF6	CRYOLITE	NANO2	SODIUM-NITRITE
NA3ALF6:A	CRYOLITE:SOL-A	NANO3	SODIUM-NITRATE
NA3ALF6:B	CRYOLITE:SOL-B	NANO3:1	SODIUM-NITRATE:SOL-1
NA3ALF6:C	CRYOLITE:SOL-C	NANO3:2	SODIUM-NITRATE:SOL-2
NA3AS	TRISODIUM-ARSENIDE	NAO	SODIUM-MONOXIDE-GAS
NA3ASO4	SODIUM-ARSENATE	NAO2	SODIUM-SUPEROXIDE

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
NAOH	SODIUM-HYDROXIDE	NBO2:C	NIOBIUM-DIOXIDE:SOL-C
NAOH:A	SODIUM-HYDROXIDE:SOL-A	NBO2CL	NIOBIUM-CHLORIDE-DIOXIDE
NAOH:B	SODIUM-HYDROXIDE:SOL-B	NBOCL2	NIOBIUM-DICHLORIDE-OXIDE
NATE	SODIUM-TELLURIDE	NBOCL3	NIOBIUM-TRICHLORIDE-OXIDE
NATE3	SODIUM-TRITELLURIDE	NBSI2	NIOBIUM-2-SILICON
NAVO3	SODIUM-METAVANADATE	NCO	NCO-RADICAL-GAS
NAVO3:1	SODIUM-METAVANADATE:SOL-1	ND	NEODYMIUM
NAVO3:2	SODIUM-METAVANADATE:SOL-2	ND2	AMIDOGEN-D2-GAS
NB	NIOBIUM	ND2(SO4)3	NEODYMIUM-SULFATE
NB2C	DINIOBIUM-CARBIDE	ND2O3	NEODYMIUM-OXIDE
NB2N	DINIOBIUM-NITRIDE	ND2O3:A	NEODYMIUM-OXIDE:SOL-A
NB2O5	DINIOBIUM-PENTAOXIDE	ND2O3:B	NEODYMIUM-OXIDE:SOL-B
NB5SI3	5-NIOBIUM-3-SILICON	ND2S3	NEODYMIUM-SULFIDE
NBB2	NIOBIUM-DIBORIDE	ND2SE3	NEODYMIUM-SELENIDE
NBBR5	NIOBIUM-PENTABROMIDE	ND2TE3	NEODYMIUM-TELLURIDE
NBC	NIOBIUM-CARBIDE	ND2ZR2O7	NEODYMIUM-ZIRCONIUM-
NBC0.702	NIOBIUM-0.702-CARBIDE	ND3	AMMONIA-D3-GAS
NBC0.825	NIOBIUM-0.825-CARBIDE	ND:A	NEODYMIUM:SOL-A
NBCL2	NIOBIUM-DICHLORIDE	ND:B	NEODYMIUM:SOL-B
NBCL2.33	NIOBIUM-2.33-CHLORIDE	NDBR3	NEODYMIUM-BROMIDE
NBCL2.67	NIOBIUM-2.67-CHLORIDE	NDCL3	NEODYMIUM-CHLORIDE
NBCL3	NIOBIUM-TRICHLORIDE	NDF3	NEODYMIUM-FLUORIDE
NBCL3.13	NIOBIUM-3.13-CHLORIDE	NDH2	NEODYMIUM-DIHYDRIDE
NBCL4	NIOBIUM-TETRACHLORIDE	NDI3	NEODYMIUM-IODIDE
NBCL5	NIOBIUM-PENTACHLORIDE	NDI3:A	NEODYMIUM-IODIDE:SOL-A
NBF5	NIOBIUM-PENTAFLUORIDE	NDI3:B	NEODYMIUM-IODIDE:SOL-B
NBFE2	NIOBIUM-2-IRON	NDOCL	NEODYMIUM-CHLORIDE-OXIDE
NBI5	NIOBIUM-PENTAIODIDE	NDS	NEODYMIUM-MONOSULFIDE
NBN	NIOBIUM-NITRIDE	NDSE	NEODYMIUM-MONOSELENIDE
NBN:A	NIOBIUM-NITRIDE:SOL-A	NDTE	NEODYMIUM-MONOTELLURIDE
NBN:B	NIOBIUM-NITRIDE:SOL-B	NE	NEON-MONATOMIC
NBO	NIOBIUM-MONOXIDE	NH	IMIDOGEN-GAS
NBO2	NIOBIUM-DIOXIDE	NH2	AMIDOGEN-GAS
NBO2:A	NIOBIUM-DIOXIDE:SOL-A	NH4CL	AMMONIUM-CHLORIDE
NBO2:B	NIOBIUM-DIOXIDE:SOL-B	NH4CL:1	AMMONIUM-CHLORIDE:SOL-1

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
NH4CL:2	AMMONIUM-CHLORIDE:SOL-2	NIO:A	NICKEL-OXIDE:SOL-A
NH4CLO4	AMMONIUM-PERCHLORATE	NIO:B	NICKEL-OXIDE:SOL-B
NH4I	AMMONIUM-IODIDE	NIO:C	NICKEL-OXIDE:SOL-C
NI	NICKEL	NIS	NICKEL-SULFIDE
NI(CO)4	NICKEL-TETRACARBONYL-GAS	NIS0.84	NICKEL-0.84-SULFIDE
NI11AS8	11-NICKEL-8-ARSENIDE	NIS2	NICKEL-DISULFIDE
NI2P	DINICKEL-PHOSPHIDE	NIS:A	NICKEL-SULFIDE:SOL-A
NI2SIO4	DINICKEL-ORTHOSILICATE	NIS:B	NICKEL-SULFIDE:SOL-B
NI3(ASO4)2	NICKEL-ARSENATE	NISB	NICKEL-ANTIMONY
NI3C	TRINICKEL-CARBIDE	NISE1.05	NICKEL-1.05-SELENIDE
NI3P	TRINICKEL-PHOSPHIDE	NISE1.143	NICKEL-1.143-SELENIDE
NI3S2	TRINICKEL-DISULFIDE	NISE1.25	NICKEL-1.25-SELENIDE
NI3S2:1	TRINICKEL-DISULFIDE:SOL-1	NISE1.25:A	NICKEL-1.25-SELENIDE:SOL-A
NI3S2:2	TRINICKEL-DISULFIDE:SOL-2	NISE1.25:B	NICKEL-1.25-SELENIDE:SOL-B
NI3S4	TRINICKEL-TETRASULFIDE	NISE1.25:C	NICKEL-1.25-SELENIDE:SOL-C
NI3SN	3-NICKEL-TIN	NISE2	NICKEL-DISELENIDE
NI3SN2	3-NICKEL-2-TIN	NISEO3	NICKEL-SELENITE
NI3TI	3-NICKEL-TITANIUM	NISI	NICKEL-SILICON
NI4B3	TETRANICKEL-TRIBORIDE	NISO4	NICKEL-SULFATE
NI5AS2	5-NICKEL-2-ARSENIDE	NITE1.1	NICKEL-1.1-TELLURIDE
NI5P2	PENTANICKEL-DIPHOSPHIDE	NITI	NICKEL-TITANIUM
NI7SI13	7-NICKEL-13-SILICON	NITI2	NICKEL-2-TITANIUM
NIAL2O4	NICKEL-DIALUMINIUM-	NITIO3	NICKEL-TITANIUM-TRIOXIDE
NIAS	NICKEL-ARSENIDE	NIWO4	NICKEL-TUNGSTATE
NIB	NICKEL-MONOBORIDE	NO	NITRIC-OXIDE
NIBR	NICKEL-MONOBROMIDE-GAS	NO2	NITROGEN-DIOXIDE
NIBR2	NICKEL-BROMIDE	NO2CL	NITRYL-CHLORIDE-GAS
NICL	NICKEL-MONOCHLORIDE-GAS	NO3	NITROGEN-TRIOXIDE-GAS
NICL2	NICKEL-CHLORIDE	NOBR	NITROSYL-BROMIDE-GAS
NICO3	NICKEL-CARBONATE	NOCL	NITROSYL-CHLORIDE-GAS
NIF	NICKEL-MONOFLUORIDE-GAS	NOF	NITROSYL-FLUORIDE-GAS
NIF2	NICKEL-FLUORIDE	NP	NEPTUNIUM
NII	NICKEL-MONOIODIDE-GAS	NP:A	NEPTUNIUM:SOL-A
NII2	NICKEL-IODIDE	NP:B	NEPTUNIUM:SOL-B
NIO	NICKEL-OXIDE	NP:C	NEPTUNIUM:SOL-C

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
NPCL3	NEPTUNIUM-TRICHLORIDE	PA	PROTACTINIUM
NPCL4	NEPTUNIUM-TETRACHLORIDE	PA:A	PROTACTINIUM:SOL-A
NPF3	NEPTUNIUM-TRIFLUORIDE	PA:B	PROTACTINIUM:SOL-B
NPF6	NEPTUNIUM-HEXAFLUORIDE	PB	LEAD
NPO2	NEPTUNIUM-DIOXIDE	PB2	LEAD-DIATOMIC-GAS
NPO3*H2O	NEPTUNIUM-TRIOXIDE-HYDRATE	PB2I4	DILEAD-TETRAIODIDE-GAS
NPOCL2	NEPTUNIUM-DICHLORIDE-OXIDE	PB2SIO4	DILEAD-ORTHOSILICATE
O	OXYGEN-MONATOMIC-GAS	PB3(ASO4)2	LEAD-ARSENATE
O2	OXYGEN	PB3O4	TRILEAD-TETRAOXIDE
O2S	SULFUR-DIOXIDE	PB4SIO6	TETRALEAD-SILICATE
O3	OZONE	PBB2O4	LEAD-DIBORATE
O3S	SULFUR-TRIOXIDE	PBB4O7	LEAD-TETRABORATE
OD	HYDROXYL-D1-GAS	PBBR	LEAD-MONOBROMIDE-GAS
OF2	OXYGEN-DIFLUORIDE-GAS	PBBR2	LEAD-DIBROMIDE
OH	HYDROXYL-GAS	PBBR4	LEAD-TETRABROMIDE-GAS
OS	OSMIUM	PBCL	LEAD-MONOCHLORIDE-GAS
OSO2	OSMIUM-DIOXIDE	PBCL2	LEAD-DICHLORIDE
OSO4	OSMIUM-TETRAOXIDE-YELLOW	PBCL4	LEAD-TETRACHLORIDE-GAS
OSP2	OSMIUM-DIPHOSPHIDE	PBCO3	LEAD-CARBONATE
OSS2	OSMIUM-DISULFIDE	PBF	LEAD-MONOFLUORIDE-GAS
OSSE2	OSMIUM-DISELENIDE	PBF2	LEAD-DIFLUORIDE
P	PHOSPHORUS-WHITE	PBF2:A	LEAD-DIFLUORIDE:SOL-A
P-R	PHOSPHORUS-RED	PBF2:B	LEAD-DIFLUORIDE:SOL-B
P2	PHOSPHORUS-DIATOMIC-GAS	PBF4	LEAD-TETRAFLUORIDE-GAS
P2O5	DIPHOSPHORUS-PENTAOXIDE-	PBH	LEAD-MONOHYDRIDE-GAS
P4	PHOSPHORUS-4-ATOMIC-GAS	PBI	LEAD-MONOIODIDE-GAS
P4O10	TETRAPHOSPHORUS-DECAOXIDE	PBI2	LEAD-DIIODIDE
P4O6	TETRAPHOSPHORUS-HEXAOXIDE-	PBI4	LEAD-TETRAIODIDE-GAS
P4S10	TETRAPHOSPHORUS-	PBMOO4	LEAD-MOLYBDATE
P4S3	TETRAPHOSPHORUS-TRISULFIDE	PBO*PBCO3	DILEAD-OXIDE-CARBONATE
P4S3:A	TETRAPHOSPHORUS-	PBO*PBSO4	DILEAD-OXIDE-SULFATE
P4S3:B	TETRAPHOSPHORUS-	PBO-R	LEAD-OXIDE-RED
P4S5	TETRAPHOSPHORUS-	PBO-Y	LEAD-OXIDE-YELLOW-MASSICOT
P4S6	TETRAPHOSPHORUS-	PBO2	LEAD-DIOXIDE
P4S7	TETRAPHOSPHORUS-	PBR3	PHOSPHORUS-TRIBROMIDE-GAS

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
PBS	LEAD-SULFIDE	PR	PRASEODYMIUM
PBSE	LEAD-SELENIDE	PR2O3	PRASEODYMIUM-OXIDE
PBSEO3	LEAD-SELENITE	PR3S4	TRIPRASEODYMIUM-
PBSEO4	LEAD-SELENATE	PR7O12	7-PRASEODYMIUM-12-OXIDE
PBSIO3	LEAD-METASILICATE	PR:A	PRASEODYMIUM:SOL-A
PBSO4	LEAD-SULFATE	PR:B	PRASEODYMIUM:SOL-B
PBSO4:A	LEAD-SULFATE:SOL-A	PRBR3	PRASEODYMIUM-BROMIDE
PBSO4:B	LEAD-SULFATE:SOL-B	PRCL3	PRASEODYMIUM-CHLORIDE
PBTE	LEAD-TELLURIDE	PRF3	PRASEODYMIUM-FLUORIDE
PBTIO3	LEAD-TITANIUM-TRIOXIDE	PRH2	PRASEODYMIUM-DIHYDRIDE
PBTIO3:A	LEAD-TITANIUM-TRIOXIDE:SOL-A	PRI3	PRASEODYMIUM-IODIDE
PBTIO3:B	LEAD-TITANIUM-TRIOXIDE:SOL-B	PRO1.833	PRASEODYMIUM-1.833-OXIDE
PBWO4	LEAD-TUNGSTATE	PRO1.833:A	PRASEODYMIUM-1.833-
PCL3	PHOSPHORUS-TRICHLORIDE-GAS	PRO1.833:B	PRASEODYMIUM-1.833-
PCL5	PHOSPHORUS-PENTACHLORIDE-	PRO2	PRASEODYMIUM-DIOXIDE
PD	PALLADIUM	PRS	PRASEODYMIUM-MONOSULFIDE
PD4S	TETRAPALLADIUM-SULFIDE	PS	PHOSPHORUS-MONOSULFIDE-
PDCL2	PALLADIUM-CHLORIDE	PT	PLATINUM
PDF2	PALLADIUM-FLUORIDE	PT5SE4	PENTAPLATINUM-TETRASELENIDE
PDI2	PALLADIUM-IODIDE	PTBR2	PLATINUM-DIBROMIDE
PDI2:A	PALLADIUM-IODIDE:SOL-A	PTBR3	PLATINUM-TRIBROMIDE
PDI2:B	PALLADIUM-IODIDE:SOL-B	PTBR4	PLATINUM-TETRABROMIDE
PDO	PALLADIUM-OXIDE	PTCL2	PLATINUM-DICHLORIDE
PDS	PALLADIUM-SULFIDE	PTCL3	PLATINUM-TRICHLORIDE
PDS2	PALLADIUM-DISULFIDE	PTCL4	PLATINUM-TETRACHLORIDE
PDTE	PALLADIUM-TELLURIDE	PTI4	PLATINUM-TETRAIODIDE
PF3	PHOSPHORUS-TRIFLUORIDE-GAS	PTO2	PLATINUM-DIOXIDE-GAS
PF5	PHOSPHORUS-PENTAFLUORIDE-	PTS	PLATINUM-MONOSULFIDE
PH3	PHOSPHINE	PTS2	PLATINUM-DISULFIDE
PI3	PHOSPHORUS-TRIIODIDE-GAS	PU	PLUTONIUM
PN	PHOSPHORUS-MONONITRIDE-	PU(SO4)2	PLUTONIUM-DISULFATE
PO	PHOSPHORUS-MONOXIDE-GAS	PU2C3	DIPLUTONIUM-TRICARBIDE
PO2	PHOSPHORUS-DIOXIDE-GAS	PU2O3	DIPLUTONIUM-TRIOXIDE-ALPHA
POBR3	PHOSPHORUS-TRIBROMIDE-	PU2O3-B	DIPLUTONIUM-TRIOXIDE-BETA
POCL3	PHOSPHORUS-TRICHLORIDE-	PU2S3	DIPLUTONIUM-TRISULFIDE

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
PU:A	PLUTONIUM:SOL-A	RB2SI2O5	RUBIDIUM-DISILICATE
PU:B	PLUTONIUM:SOL-B	RB2SI4O9	RUBIDIUM-TETRASILICATE
PU:C	PLUTONIUM:SOL-C	RB2SIO3	RUBIDIUM-METASILICATE
PU:D	PLUTONIUM:SOL-D	RB2SO4	RUBIDIUM-SULFATE
PU:D1	PLUTONIUM:S.-D1	RB2SO4:A	RUBIDIUM-SULFATE:SOL-A
PU:E	PLUTONIUM:SOL-E	RB2SO4:B	RUBIDIUM-SULFATE:SOL-B
PUBR3	PLUTONIUM-TRIBROMIDE	RB3ASO4	RUBIDIUM-ARSENATE
PUC0.88	PLUTONIUM-0.88-CARBIDE	RBBR	RUBIDIUM-BROMIDE
PUC2	PLUTONIUM-DICARBIDE	RBCL	RUBIDIUM-CHLORIDE
PUCL3	PLUTONIUM-TRICHLORIDE	RBF	RUBIDIUM-FLUORIDE
PUF3	PLUTONIUM-TRIFLUORIDE	RBI	RUBIDIUM-IODIDE
PUF4	PLUTONIUM-TETRAFLUORIDE	RBO2	RUBIDIUM-PEROXIDE
PUF6	PLUTONIUM-HEXAFLUORIDE	RE	RHENIUM
PUH2	PLUTONIUM-DIHYDRIDE	RE2O7	DIRHENIUM-HEPTAOXIDE
PUH3	PLUTONIUM-TRIHYDRIDE	RE2O7:A	DIRHENIUM-HEPTAOXIDE:SOL-A
PUI3	PLUTONIUM-TRIIODIDE	RE2O7:B	DIRHENIUM-HEPTAOXIDE:SOL-B
PUN	PLUTONIUM-NITRIDE	RE2S7	DIRHENIUM-HEPTASULFIDE
PUO	PLUTONIUM-OXIDE	RE2TE5	DIRHENIUM-PENTATELLURIDE
PUO2	PLUTONIUM-DIOXIDE	RE2Y	2-RHENIUM-YTTRIUM
PUOBR	PLUTONIUM-BROMIDE-OXIDE	RE3AS7	TRIRHENIUM-HEPTAARSENIDE
PUOCL	PLUTONIUM-CHLORIDE-OXIDE	RE5SI3	5-RHENIUM-3-SILICON
PUOF	PLUTONIUM-FLUORIDE-OXIDE	REASO4	RHENIUM-ARSENATE
PUOI	PLUTONIUM-IODIDE-OXIDE	REBR3	RHENIUM-TRIBROMIDE
PUS	PLUTONIUM-MONOSULFIDE	RECL3	RHENIUM-TRICHLORIDE
RB	RUBIDIUM	REO2	RHENIUM-DIOXIDE
RB2	RUBIDIUM-DIATOMIC-GAS	REO3	RHENIUM-TRIOXIDE
RB2CL2	DIRUBIDIUM-DICHLORIDE-GAS	RES2	RHENIUM-DISULFIDE
RB2CO3	RUBIDIUM-CARBONATE	RESI	RHENIUM-SILICON
RB2CO3:1	RUBIDIUM-CARBONATE:SOL-1	RESI2	RHENIUM-2-SILICON
RB2CO3:2	RUBIDIUM-CARBONATE:SOL-2	RH	RHODIUM
RB2F2	DIRUBIDIUM-DIFLUORIDE-GAS	RH2O3	DIRHODIUM-TRIOXIDE
RB2O	RUBIDIUM-OXIDE	RH3U	3-RHODIUM-URANIUM
RB2O:A	RUBIDIUM-OXIDE:SOL-A	RHCL2	RHODIUM-DICHLORIDE-GAS
RB2O:B	RUBIDIUM-OXIDE:SOL-B	RHCL3	RHODIUM-TRICHLORIDE
RB2O:C	RUBIDIUM-OXIDE:SOL-C	RHO2	RHODIUM-DIOXIDE-GAS

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
RN	RADON-MONATOMIC-GAS	SB2O5	DIANTIMONY-PENTAOXIDE
RU	RUTHENIUM	SB2S3	DIANTIMONY-TRISULFIDE-BLACK
RU3U	3-RUTHENIUM-URANIUM	SB2S4	DIANTIMONY-TETRASULFIDE-GAS
RUCL3	RUTHENIUM-TRICHLORIDE	SB2SE3	DIANTIMONY-TRISELENIDE
RUCL4	RUTHENIUM-TETRACHLORIDE-	SB2TE3	DIANTIMONY-TRITELLURIDE
RUF5	RUTHENIUM-PENTAFLUORIDE	SB3S2	TRIANTIMONY-DISULFIDE-GAS
RUO2	RUTHENIUM-DIOXIDE	SB4	ANTIMONY-4-ATOMIC-GAS
RUO3	RUTHENIUM-TRIOXIDE-GAS	SB4O6	TETRAANTIMONY-HEXAOXIDE-
RUO4	RUTHENIUM-TETROXIDE-GAS	SB4S3	TETRAANTIMONY-TRISULFIDE-
RUS2	RUTHENIUM-DISULFIDE	SBBR3	ANTIMONY-TRIBROMIDE
RUSE2	RUTHENIUM-DISELENIDE	SBCL	ANTIMONY-MONOCHLORIDE-GAS
S	SULFUR-RHOMBIC-MONOCLINIC	SBCL3	ANTIMONY-TRICHLORIDE
S-N	SULFUR-MONONITRIDE-GAS	SBCL5	ANTIMONY-PENTACHLORIDE-GAS
S2	SULFUR-DIATOMIC-GAS	SBF	ANTIMONY-MONOFLUORIDE-GAS
S2BR2	DISULFUR-DIBROMIDE-GAS	SBF3	ANTIMONY-TRIFLUORIDE
S2CL	DISULFUR-CHLORIDE-RADICAL-	SBH3	ANTIMONY-TRIHYDRIDE-GAS
S2CL2	DISULFUR-DICHLORIDE	SBI3	ANTIMONY-TRIIODIDE
S2F10	DISULFUR-DECAFLUORIDE-GAS	SBO	ANTIMONY-OXIDE-GAS
S2O	DISULFUR-OXIDE-GAS	SBOCL	ANTIMONY-CHLORIDE-OXIDE
S3	SULFUR-TRIATOMIC-GAS	SBR2	SULFUR-DIBROMIDE-GAS
S4	SULFUR-4-ATOMIC-GAS	SBS	ANTIMONY-SULFIDE-GAS
S5	SULFUR-5-ATOMIC-GAS	SBSE	ANTIMONY-SELENIDE-GAS
S6	SULFUR-6-ATOMIC-GAS	SBZN	ANTIMONY-ZINC
S7	SULFUR-7-ATOMIC-GAS	SC	SCANDIUM
S8	SULFUR-8-ATOMIC-GAS	SC2O3	SCANDIUM-OXIDE
S:MO	SULFUR-RHOMBIC-	SC:A	SCANDIUM:SOL-A
S:RH	SULFUR-RHOMBIC-	SC:B	SCANDIUM:SOL-B
SB	ANTIMONY	SCASO4	SCANDIUM-ARSENATE
SB2	ANTIMONY-DIATOMIC-GAS	SCBR3	SCANDIUM-BROMIDE
SB2(SO4)3	DIANTIMONY-TRISULFATE	SCCL3	SCANDIUM-CHLORIDE
SB2O3	DIANTIMONY-TRIOXIDE-CUBIC	SCF3	SCANDIUM-FLUORIDE
SB2O3-O	DIANTIMONY-TRIOXIDE-	SCL	SULFUR-MONOCHLORIDE-GAS
SB2O3:A	DIANTIMONY-TRIOXIDE-	SCL2	SULFUR-DICHLORIDE-GAS
SB2O3:B	DIANTIMONY-TRIOXIDE-	SCN	SCANDIUM-NITRIDE
SB2O4	DIANTIMONY-TETRAOXIDE	SE	SELENIUM

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
SE2	SELENIUM-DIATOMIC-GAS	SI2W	2-SILICON-TUNGSTEN
SE2BR2	DISELENIUM-DIBROMIDE-GAS	SI2ZR	2-SILICON-ZIRCONIUM
SE2CL2	DISELENIUM-DICHLORIDE	SI3	SILICON-TRIATOMIC-GAS
SE3	SELENIUM-TRIATOMIC-GAS	SI3N4	TRISILICON-TETRANITRIDE-ALPHA
SE4	SELENIUM-4-ATOMIC-GAS	SI3TA5	3-SILICON-5-TANTALUM
SE5	SELENIUM-5-ATOMIC-GAS	SI3TI5	3-SILICON-5-TITANIUM
SE6	SELENIUM-6-ATOMIC-GAS	SI3U	3-SILICON-URANIUM
SE7	SELENIUM-7-ATOMIC-GAS	SI3V5	3-SILICON-5-VANADIUM
SE8	SELENIUM-8-ATOMIC-GAS	SI3W5	3-SILICON-5-TUNGSTEN
SEBR2	SELENIUM-DIBROMIDE-GAS	SI3ZR5	3-SILICON-5-ZIRCONIUM
SECL2	SELENIUM-DICHLORIDE-GAS	SI5TH3	5-SILICON-3-THORIUM
SECL4	SELENIUM-TETRACHLORIDE	SI5U3	5-SILICON-3-URANIUM
SEF	SELENIUM-FLUORIDE-GAS	SIBR	SILICON-MONOBROMIDE-GAS
SEF2	SELENIUM-DIFLUORIDE-GAS	SIBR2	SILICON-DIBROMIDE-GAS
SEF4	SELENIUM-TETRAFLUORIDE-GAS	SIBR3	SILICON-TRIBROMIDE-GAS
SEF5	SELENIUM-PENTAFLUORIDE-GAS	SIBR4	SILICON-TETRABROMIDE
SEF6	SELENIUM-HEXAFLUORIDE-GAS	SIC	SILICON-CARBIDE-CUBIC
SEO	SELENIUM-OXIDE-GAS	SICL	SILICON-CHLORIDE-GAS
SEO2	SELENIUM-DIOXIDE	SICL2	SILICON-DICHLORIDE-GAS
SF	SULFUR-MONOFLUORIDE-GAS	SICL3	SILICON-TRICHLORIDE-GAS
SF2	SULFUR-DIFLUORIDE-GAS	SICL4	SILICON-TETRACHLORIDE-GAS
SF3	SULFUR-TRIFLUORIDE-GAS	SIF	SILICON-FLUORIDE-GAS
SF4	SULFUR-TETRAFLUORIDE-GAS	SIF2	SILICON-DIFLUORIDE-GAS
SF5	SULFUR-PENTAFLUORIDE-GAS	SIF3	SILICON-TRIFLUORIDE-GAS
SF6	SULFUR-HEXAFLUORIDE-GAS	SIF4	SILICON-TETRAFLUORIDE-GAS
SI	SILICON	SIH	SILICON-HYDRIDE-GAS
SI2	SILICON-DIATOMIC-GAS	SIH4	SILANE-GAS
SI2H6	DISILANE-GAS	SII	SILICON-IODIDE-GAS
SI2TA	2-SILICON-TANTALUM	SII2	SILICON-DIIODIDE-GAS
SI2TH	2-SILICON-THORIUM	SII3	SILICON-TRIIODIDE-GAS
SI2TH3	2-SILICON-3-THORIUM	SII4	SILICON-TETRAIODIDE
SI2TI	2-SILICON-TITANIUM	SIO	SILICON-OXIDE-GAS
SI2U	2-SILICON-URANIUM	SIO2	SILICON-DIOXIDE
SI2U3	2-SILICON-3-URANIUM	SIO2-CR	SILICON-DIOXIDE-CRISTOBALITE
SI2V	2-SILICON-VANADIUM	SIO2:HC	SILICON-DIOXIDE:S-HC

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
SIO2:HQ	SILICON-DIOXIDE:S-HQ	SN3(ASO4)2	TRITIN-ARSENATE
SIO2:LQ	SILICON-DIOXIDE:S-LQ	SN3S4	TRITIN-TETRASULFIDE
SIOF2	SILICON-DIFLUORIDE-OXIDE-GAS	SNBR2	TIN-DIBROMIDE
SIP	SILICON-PHOSPHIDE	SNBR4	TIN-TETRABROMIDE
SIS	SILICON-SULFIDE-GAS	SNCL	TIN-MONOCHLORIDE-GAS
SIS2	SILICON-DISULFIDE	SNCL2	TIN-DICHLORIDE
SISE	SILICON-SELENIDE-GAS	SNCL4	TIN-TETRACHLORIDE
SITA2	SILICON-2-TANTALUM	SNF	TIN-MONOFLUORIDE-GAS
SITH	SILICON-THORIUM	SNF2	TIN-DIFLUORIDE
SITI	SILICON-TITANIUM	SNH4	TIN-TETRAHYDRIDE-GAS
SIU	SILICON-URANIUM	SNI2	TIN-DIIODIDE
SIU3	SILICON-3-URANIUM	SNI4	TIN-TETRAIODIDE
SIV3	SILICON-3-VANADIUM	SNO	TIN-MONOXIDE
SIZR	SILICON-ZIRCONIUM	SNO2	TIN-DIOXIDE
SIZR2	SILICON-2-ZIRCONIUM	SNS	TIN-MONOSULFIDE
SM	SAMARIUM	SNS2	TIN-DISULFIDE
SM2O3	DISAMARIUM-TRIOXIDE-CUBIC	SNS:A	TIN-MONOSULFIDE:SOL-A
SM2O3-M	DISAMARIUM-TRIOXIDE-	SNS:B	TIN-MONOSULFIDE:SOL-B
SM2O3-M:M1	DISAMARIUM-3-OXIDE-	SNSE	TIN-MONOSELENIDE
SM2O3-M:M2	DISAMARIUM-3-OXIDE-	SNSE2	TIN-DISELENIDE
SM2ZR2O7	DISAMARIUM-DIZIRCONIUM-	SNSO4	TIN-MONOSULFATE
SM:A	SAMARIUM:SOL-A	SNTE	TIN-MONOTELLURIDE
SM:B	SAMARIUM:SOL-B	SO	SULFUR-MONOXIDE-GAS
SMC2	SAMARIUM-DICARBIDE	SO2CL2	SULFONYL-DICHLORIDE-GAS
SMC2:A	SAMARIUM-DICARBIDE:SOL-A	SO2F2	SULFONYL-DIFLUORIDE-GAS
SMC2:B	SAMARIUM-DICARBIDE:SOL-B	SOCL2	SULFINYL-DICHLORIDE-GAS
SMCL2	SAMARIUM-DICHLORIDE	SOF2	SULFINYL-DIFLUORIDE-GAS
SMCL3	SAMARIUM-TRICHLORIDE	SR	STRONTIUM
SMOF	SAMARIUM-FLUORIDE-OXIDE	SR(OH)2	STRONTIUM-HYDROXIDE
SMOF:A	SAMARIUM-FLUORIDE-OXIDE:SOL-	SR2SIO4	STRONTIUM-ORTHOSILICATE
SMOF:B	SAMARIUM-FLUORIDE-OXIDE:SOL-	SR2TIO4	DISTRONTIUM-TITANIUM-
SN	TIN-WHITE	SR2TIO4:1	DISTRONTIUM-TITANIUM-4-
SN(SO4)2	TIN-DISULFATE	SR2TIO4:2	DISTRONTIUM-TITANIUM-4-
SN2I4	DITIN-TETRAIODIDE-GAS	SR3(ASO4)2	STRONTIUM-ARSENATE
SN2S3	DITIN-TRISULFIDE	SR3N2	TRISTRONTIUM-DINITRIDE

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
SR4TI3O10	TETRASTRONTIUM-TRITITANIUM-	TA	TANTALUM
SR:A	STRONTIUM:SOL-A	TA2C	DITANTALUM-CARBIDE
SR:C	STRONTIUM:SOL-C	TA2N	DITANTALUM-NITRIDE
SRAL2O4	STRONTIUM-DIALUMINIUM-	TA2O5	DITANTALUM-PENTOXIDE
SRAL2O4:A	STRONTIUM-DIALUMINIUM-4-	TAB2	TANTALUM-DIBORIDE
SRAL2O4:B	STRONTIUM-DIALUMINIUM-4-	TABR5	TANTALUM-PENTABROMIDE
SRBR	STRONTIUM-MONOBROMIDE-GAS	TAC	TANTALUM-MONOCARBIDE
SRBR2	STRONTIUM-BROMIDE	TACL	TANTALUM-MONOCHLORIDE-GAS
SRBR2:A	STRONTIUM-BROMIDE:SOL-A	TACL2	TANTALUM-DICHLORIDE-GAS
SRBR2:B	STRONTIUM-BROMIDE:SOL-B	TACL2.5	TANTALUM-2.5-CHLORIDE
SRC2	STRONTIUM-DICARBIDE	TACL3	TANTALUM-TRICHLORIDE
SRCL	STRONTIUM-MONOCHLORIDE-	TACL4	TANTALUM-TETRACHLORIDE
SRCL2	STRONTIUM-CHLORIDE	TACL5	TANTALUM-PENTACHLORIDE
SRCO3	STRONTIUM-CARBONATE	TAF5	TANTALUM-PENTAFLUORIDE
SRCO3:A	STRONTIUM-CARBONATE:SOL-A	TAI5	TANTALUM-PENTAIODIDE
SRCO3:B	STRONTIUM-CARBONATE:SOL-B	TALC	MG3SI4O10(OH)2
SRF2	STRONTIUM-FLUORIDE	TAN	TANTALUM-MONONITRIDE
SRF2:1	STRONTIUM-FLUORIDE:SOL-1	TAO	TANTALUM-MONOXIDE-GAS
SRF2:2	STRONTIUM-FLUORIDE:SOL-2	TAO2	TANTALUM-DIOXIDE-GAS
SRF2:3	STRONTIUM-FLUORIDE:SOL-3	TAO2CL	TANTALUM-CHLORIDE-DIOXIDE
SRH2	STRONTIUM-HYDRIDE	TAOCL3	TANTALUM-TRICHLORIDE-OXIDE
SRI2	STRONTIUM-IODIDE	TAS	TANTALUM-MONOSULFIDE-GAS
SRMOO4	STRONTIUM-MOLYBDATE	TAS2	TANTALUM-DISULFIDE
SRO	STRONTIUM-OXIDE	TB	TERBIUM
SRO2	STRONTIUM-PEROXIDE	TB2O3	DITERBIUM-TRIOXIDE
SROH	STRONTIUM-MONOHYDROXIDE-	TB:A	TERBIUM:SOL-A
SRS	STRONTIUM-SULFIDE	TB:B	TERBIUM:SOL-B
SRSIO3	STRONTIUM-METASILICATE	TBBR3	TERBIUM-TRIBROMIDE-GAS
SRSO4	STRONTIUM-SULFATE	TBCL3	TERBIUM-TRICHLORIDE
SRSO4:1	STRONTIUM-SULFATE:SOL-1	TBCL3:A	TERBIUM-TRICHLORIDE:SOL-A
SRSO4:2	STRONTIUM-SULFATE:SOL-2	TBCL3:B	TERBIUM-TRICHLORIDE:SOL-B
SRTIO3	STRONTIUM-TITANIUM-TRIOXIDE	TBO1.72	TERBIUM-1.72-OXIDE
SRWO4	STRONTIUM-TUNGSTATE	TBO1.81	TERBIUM-1.81-OXIDE
SRZRO3	STRONTIUM-ZIRCONIUM-TRIOXIDE	TBO2	TERBIUM-DIOXIDE
SSF2	SULFINOTHIOYL-DIFLUORIDE-GAS	TBS	TERBIUM-SULFIDE-GAS

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
TBSE	TERBIUM-SELENIDE-GAS	THCL4:A	THORIUM-TETRACHLORIDE:SOL-A
TBTE	TERBIUM-TELLURIDE-GAS	THCL4:B	THORIUM-TETRACHLORIDE:SOL-B
TC	TECHNETIUM	THF2	THORIUM-DIFLUORIDE-GAS
TC2O7	DITECHNETIUM-HEPTAOXIDE	THF3	THORIUM-TRIFLUORIDE-GAS
TCO2	TECHNETIUM-DIOXIDE	THF4	THORIUM-TETRAFLUORIDE
TCO3	TECHNETIUM-TRIOXIDE	THH2	THORIUM-DIHYDRIDE
TE	TELLURIUM	THI4	THORIUM-TETRAIODIDE
TE2	TELLURIUM-DIATOMIC-GAS	THN	THORIUM-MONONITRIDE
TE2O2	DITELLURIUM-DIOXIDE-GAS	THO	THORIUM-MONOXIDE-GAS
TEBR4	TELLURIUM-TETRABROMIDE	THO2	THORIUM-DIOXIDE
TECL2	TELLURIUM-DICHLORIDE-GAS	THOBR2	THORIUM-DIBROMIDE-OXIDE
TECL4	TELLURIUM-TETRACHLORIDE	THOCL2	THORIUM-DICHLORIDE-OXIDE
TEF	TELLURIUM-MONOFLUORIDE-GAS	THOF2	THORIUM-DIFLUORIDE-OXIDE
TEF2	TELLURIUM-DIFLUORIDE-GAS	THOI2	THORIUM-DIIODIDE-OXIDE
TEF4	TELLURIUM-TETRAFLUORIDE-GAS	THP	THORIUM-MONOPHOSPHIDE
TEF5	TELLURIUM-PENTAFLUORIDE-GAS	THRE2	THORIUM-2-RHENIUM
TEF6	TELLURIUM-HEXAFLUORIDE-GAS	THS	THORIUM-MONOSULFIDE
TEO	TELLURIUM-MONOXIDE-GAS	THS2	THORIUM-DISULFIDE
TEO2	TELLURIUM-DIOXIDE	TI	TITANIUM
TH	THORIUM	TI2O3	DITITANIUM-TRIOXIDE
TH(SO4)2	THORIUM-DISULFATE	TI2O3:A	DITITANIUM-TRIOXIDE:SOL-A
TH2N2O	DITHORIUM-DINITRIDE-MONOXIDE	TI2O3:B	DITITANIUM-TRIOXIDE:SOL-B
TH2S3	DITHORIUM-TRISULFIDE	TI3(ASO4)2	TRITITANIUM-DIARSENATE
TH3N4	TRITHORIUM-TETRANITRIDE	TI3O5	TRITITANIUM-PENTOXIDE
TH3P4	TRITHORIUM-TETRAPHOSPHIDE	TI3O5:A	TRITITANIUM-PENTOXIDE:SOL-A
TH:A	THORIUM:SOL-A	TI3O5:B	TRITITANIUM-PENTOXIDE:SOL-B
TH:B	THORIUM:SOL-B	TI4O7	TETRATITANIUM-HEPTAOXIDE
THBR4	THORIUM-TETRABROMIDE	TI:A	TITANIUM:SOL-A
THBR4:A	THORIUM-TETRABROMIDE:SOL-A	TI:B	TITANIUM:SOL-B
THBR4:B	THORIUM-TETRABROMIDE:SOL-B	TIB	TITANIUM-MONOBORIDE
THC1.94	THORIUM-1.94-CARBIDE	TIB2	TITANIUM-DIBORIDE
THC1.94:A	THORIUM-1.94-CARBIDE:SOL-A	TIBR	TITANIUM-MONOBROMIDE-GAS
THC1.94:B	THORIUM-1.94-CARBIDE:SOL-B	TIBR2	TITANIUM-DIBROMIDE
THC1.94:C	THORIUM-1.94-CARBIDE:SOL-C	TIBR3	TITANIUM-TRIBROMIDE
THCL4	THORIUM-TETRACHLORIDE	TIBR4	TITANIUM-TETRABROMIDE

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
TIC	TITANIUM-MONOCARBIDE	TL2S	THALLIUM-SULFIDE
TICL	TITANIUM-MONOCHLORIDE-GAS	TL2SE	THALLIUM-SELENIDE
TICL2	TITANIUM-DICHLORIDE	TL2SO4	THALLIUM-SULFATE
TICL3	TITANIUM-TRICHLORIDE	TL2SO4:A	THALLIUM-SULFATE:SOL-A
TICL4	TITANIUM-TETRACHLORIDE	TL2SO4:B	THALLIUM-SULFATE:SOL-B
TIF	TITANIUM-MONOFLUORIDE-GAS	TL2TE	THALLIUM-TELLURIDE
TIF2	TITANIUM-DIFLUORIDE-GAS	TL:A	THALLIUM:SOL-A
TIF3	TITANIUM-TRIFLUORIDE	TL:B	THALLIUM:SOL-B
TIF4	TITANIUM-TETRAFLUORIDE	TLASO4	THALLIUM-ARSENATE
TIH2	TITANIUM-DIHYDRIDE	TLBR	THALLIUM-BROMIDE
TII	TITANIUM-MONOIODIDE-GAS	TLCL	THALLIUM-CHLORIDE
TII2	TITANIUM-DIIODIDE	TLCL3	THALLIUM-TRICHLORIDE
TII3	TITANIUM-TRIIODIDE	TLF	THALLIUM-FLUORIDE
TII4	TITANIUM-TETRAIODIDE	TLF:A	THALLIUM-FLUORIDE:SOL-A
TII4:A	TITANIUM-TETRAIODIDE:SOL-A	TLF:B	THALLIUM-FLUORIDE:SOL-B
TII4:B	TITANIUM-TETRAIODIDE:SOL-B	TLI	THALLIUM-IODIDE
TIN	TITANIUM-MONONITRIDE	TLI:A	THALLIUM-IODIDE:SOL-A
TIO	TITANIUM-MONOXIDE	TLI:B	THALLIUM-IODIDE:SOL-B
TIO2	TITANIUM-DIOXIDE-RUTILE	TLSE	THALLIUM-SELENIDE
TIO2-A	TITANIUM-DIOXIDE-ANATASE	TLSE:A	THALLIUM-SELENIDE:SOL-A
TIO:A	TITANIUM-MONOXIDE:SOL-A	TLSE:B	THALLIUM-SELENIDE:SOL-B
TIO:B	TITANIUM-MONOXIDE:SOL-B	TM	THULIUM
TIOCL	TITANIUM-CHLORIDE-OXIDE-GAS	TM2O3	DITHULIUM-TRIOXIDE
TIOCL2	TITANIUM-DICHLORIDE-OXIDE-	TM2O3:A	DITHULIUM-TRIOXIDE:SOL-A
TIOF	TITANIUM-FLUORIDE-OXIDE-GAS	TM2O3:B	DITHULIUM-TRIOXIDE:SOL-B
TIOF2	TITANIUM-DIFLUORIDE-OXIDE-GAS	TMBR3	THULIUM-TRIBROMIDE-GAS
TIS	TITANIUM-MONOSULFIDE	TMCL3	THULIUM-TRICHLORIDE
TIS2	TITANIUM-DISULFIDE	TMF3	THULIUM-TRIFLUORIDE
TIS2:A	TITANIUM-DISULFIDE:SOL-A	TMF3:A	THULIUM-TRIFLUORIDE:SOL-A
TIS2:B	TITANIUM-DISULFIDE:SOL-B	TMF3:B	THULIUM-TRIFLUORIDE:SOL-B
TL	THALLIUM	TMI3	THULIUM-TRIIODIDE-GAS
TL2CL2	DITHALLIUM-DICHLORIDE-GAS	TREMOLITE	CA2MG5SI8O23*H2O
TL2F2	DITHALLIUM-DIFLUORIDE-GAS	U	URANIUM
TL2O	THALLIUM-OXIDE	U(SO4)2	URANIUM-DISULFATE
TL2O3	DITHALLIUM-TRIOXIDE	U2C3	DIURANIUM-TRICARBIDE

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
U2S3	DIURANIUM-TRISULFIDE	UO2F2	URANIUM-DIFLUORIDE-DIOXIDE
U3O8	TRIURANIUM-OCTAOXIDE-	UO2SO4	URANIUM-SULFATE-DIOXIDE
U4O9	TETRAURANIUM-NONAOXIDE	UO3	URANIUM-TRIOXIDE-
U4O9:1	TETRAURANIUM-NONAOXIDE:SOL-	UO3*2H2O	URANIUM-TRIOXIDE-DIHYDRATE
U4O9:2	TETRAURANIUM-NONAOXIDE:SOL-	UO3*H2O	URANIUM-TRIOXIDE-
U4O9:3	TETRAURANIUM-NONAOXIDE:SOL-	UOBR2	URANIUM-DIBROMIDE-OXIDE
U:A	URANIUM:SOL-A	UOBR3	URANIUM-TRIBROMIDE-OXIDE
U:B	URANIUM:SOL-B	UOCL	URANIUM-CHLORIDE-OXIDE
U:C	URANIUM:SOL-C	UOCL2	URANIUM-DICHLORIDE-OXIDE
UB12	URANIUM-DODECABORIDE	UOCL3	URANIUM-TRICHLORIDE-OXIDE
UB2	URANIUM-DIBORIDE	US	URANIUM-SULFIDE
UB4	URANIUM-TETRABORIDE	US2	URANIUM-DISULFIDE
UBR3	URANIUM-TRIBROMIDE	USE	URANIUM-SELENIDE
UBR4	URANIUM-TETRABROMIDE	V	VANADIUM
UBR5	URANIUM-PENTABROMIDE	V2C	DIVANADIUM-CARBIDE
UC	URANIUM-MONOCARBIDE	V2O3	DIVANADIUM-TRIOXIDE
UC1.94	URANIUM-1.94-CARBIDE	V2O4	DIVANADIUM-TETRAOXIDE
UCL3	URANIUM-TRICHLORIDE	V2O4:1	DIVANADIUM-TETRAOXIDE:SOL-1
UCL4	URANIUM-TETRACHLORIDE	V2O4:2	DIVANADIUM-TETRAOXIDE:SOL-2
UCL5	URANIUM-PENTACHLORIDE	V2O5	DIVANADIUM-PENTAOXIDE
UCL6	URANIUM-HEXACHLORIDE	V3B2	TRIVANADIUM-DIBORIDE
UF3	URANIUM-TRIFLUORIDE	V3B4	TRIVANADIUM-TETRABORIDE
UF4	URANIUM-TETRAFLUORIDE	VB	VANADIUM-BORIDE
UF4.25	URANIUM-4.25-FLUORIDE	VB2	VANADIUM-DIBORIDE
UF4.5	URANIUM-4.5-FLUORIDE	VBR2	VANADIUM-DIBROMIDE
UF5	URANIUM-PENTAFLUORIDE	VBR3	VANADIUM-TRIBROMIDE
UF6	URANIUM-HEXAFLUORIDE	VBR4	VANADIUM-TETRABROMIDE-GAS
UH3-B	URANIUM-TRIHYDRIDE-BETA	VC0.88	VANADIUM-0.88-CARBIDE
UI3	URANIUM-TRIIODIDE	VCL2	VANADIUM-DICHLORIDE
UI4	URANIUM-TETRAIODIDE	VCL3	VANADIUM-TRICHLORIDE
UN	URANIUM-NITRIDE	VCL4	VANADIUM-TETRACHLORIDE
UO2	URANIUM-DIOXIDE	VF3	VANADIUM-TRIFLUORIDE
UO2(NO3)2	URANIUM-DINITRATE-DIOXIDE	VF4	VANADIUM-TETRAFLUORIDE
UO2BR2	URANIUM-DIBROMIDE-DIOXIDE	VF5	VANADIUM-PENTAFLUORIDE-GAS
UO2CL2	URANIUM-DICHLORIDE-DIOXIDE	VI2	VANADIUM-DIIODIDE

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
VI3	VANADIUM-TRIIODIDE	WO3	TUNGSTEN-TRIOXIDE
VN	VANADIUM-NITRIDE	WO3:1	TUNGSTEN-TRIOXIDE:SOL-1
VN0.465	VANADIUM-0.465-NITRIDE	WO3:2	TUNGSTEN-TRIOXIDE:SOL-2
VO	VANADIUM-OXIDE	WOCL4	TUNGSTEN-TETRACHLORIDE-
VO2	VANADIUM-DIOXIDE-GAS	WOF4	TUNGSTEN-TETRAFLUORIDE-
VOCL3	VANADIUM-TRICHLORIDE-OXIDE	WS2	TUNGSTEN-DISULFIDE
W	TUNGSTEN	XE	XENON
W(CO)6	TUNGSTEN-HEXACARBONYL	Y	YTTRIUM
W2C	DITUNGSTEN-CARBIDE	Y2O3	DIYTTRIUM-TRIOXIDE
W2CL10	DITUNGSTEN-DECACHLORIDE-	Y2O3:A	DIYTTRIUM-TRIOXIDE:SOL-A
W2O6	DITUNGSTEN-HEXAOXIDE-GAS	Y2O3:B	DIYTTRIUM-TRIOXIDE:SOL-B
W3O8	TRITUNGSTEN-OCTAOXIDE-GAS	Y2ZR2O7	DIYTTRIUM-DIZIRCONIUM-
W3O9	TRITUNGSTEN-NONAOXIDE-GAS	Y:A	YTTRIUM:SOL-A
W4O12	TETRATUNGSTEN-DODECAOXIDE-	Y:B	YTTRIUM:SOL-B
WBR	TUNGSTEN-BROMIDE-GAS	YASO4	YTTRIUM-ARSENATE
WBR5	TUNGSTEN-PENTABROMIDE	YB	YTTERBIUM
WBR6	TUNGSTEN-HEXABROMIDE	YB2O3	DIYTTERBIUM-TRIOXIDE
WC	TUNGSTEN-CARBIDE	YB2O3:A	DIYTTERBIUM-TRIOXIDE:SOL-A
WCL	TUNGSTEN-CHLORIDE-GAS	YB2O3:B	DIYTTERBIUM-TRIOXIDE:SOL-B
WCL2	TUNGSTEN-DICHLORIDE	YB:A	YTTERBIUM:SOL-A
WCL4	TUNGSTEN-TETRACHLORIDE	YB:B	YTTERBIUM:SOL-B
WCL5	TUNGSTEN-PENTACHLORIDE	YBCL2	YTTERBIUM-DICHLORIDE
WCL6	TUNGSTEN-HEXACHLORIDE	YBCL3	YTTERBIUM-TRICHLORIDE
WCL6:A1	TUNGSTEN-HEXACHLORIDE:S.-A1	YCL3	YTTRIUM-TRICHLORIDE
WCL6:A2	TUNGSTEN-HEXACHLORIDE:S.-A2	YF3	YTTRIUM-TRIFLUORIDE
WCL6:B	TUNGSTEN-HEXACHLORIDE:SOL-	YF3:A	YTTRIUM-TRIFLUORIDE:SOL-A
WF	TUNGSTEN-FLUORIDE-GAS	YF3:B	YTTRIUM-TRIFLUORIDE:SOL-B
WF6	TUNGSTEN-HEXAFLUORIDE-GAS	YI3	YTTRIUM-TRIIODIDE
WO	TUNGSTEN-OXIDE-GAS	YN	YTTRIUM-NITRIDE
WO2	TUNGSTEN-DIOXIDE	ZN	ZINC
WO2.72	TUNGSTEN-2.72-OXIDE	ZN2SIO4	ZINC-ORTHOSILICATE-WILLEMITE
WO2.90	TUNGSTEN-2.90-OXIDE	ZN2TIO4	DIZINC-TITANIUM-TETRAOXIDE
WO2.96	TUNGSTEN-2.96-OXIDE	ZN3(ASO4)2	ZINC-ARSENATE
WO2CL2	TUNGSTEN-DICHLORIDE-DIOXIDE	ZN3(PO4)2	ZINC-PHOSPHATE
WO2I2	TUNGSTEN-DIIODIDE-DIOXIDE-	ZN3AS2	ZINC-ARSENIDE

continued

Table 1.7 Components Available in the INORGANIC Databank (continued)

Alias	Component Name	Alias	Component Name
ZN3AS2:1	ZINC-ARSENIDE:SOL-1	ZR	ZIRCONIUM
ZN3AS2:2	ZINC-ARSENIDE:SOL-2	ZR:A	ZIRCONIUM:SOL-A
ZN3AS2:3	ZINC-ARSENIDE:SOL-3	ZR:B	ZIRCONIUM:SOL-B
ZN3N2	ZINC-NITRIDE	ZRB2	ZIRCONIUM-DIBORIDE
ZN3O(SO4)2	TRIZINC-DISULFATE-OXIDE	ZRBR	ZIRCONIUM-MONOBROMIDE-GAS
ZN3P2	TRIZINC-DIPHOSPHIDE	ZRBR2	ZIRCONIUM-DIBROMIDE
ZN3P2:1	TRIZINC-DIPHOSPHIDE:SOL-1	ZRBR3	ZIRCONIUM-TRIBROMIDE
ZN3P2:2	TRIZINC-DIPHOSPHIDE:SOL-2	ZRBR4	ZIRCONIUM-TETRABROMIDE
ZN3PO4-2:A	ZINC-PHOSPHATE:SOL-A	ZRC	ZIRCONIUM-CARBIDE
ZN3PO4-2:B	ZINC-PHOSPHATE:SOL-B	ZRCL	ZIRCONIUM-MONOCHLORIDE-GAS
ZNBR2	ZINC-BROMIDE	ZRCL2	ZIRCONIUM-DICHLORIDE
ZNCL2	ZINC-CHLORIDE	ZRCL3	ZIRCONIUM-TRICHLORIDE
ZNCO3	ZINC-CARBONATE	ZRCL4	ZIRCONIUM-TETRACHLORIDE
ZNF2	ZINC-FLUORIDE	ZRF	ZIRCONIUM-MONOFLUORIDE-GAS
ZNF2:A	ZINC-FLUORIDE:SOL-A	ZRF2	ZIRCONIUM-DIFLUORIDE
ZNF2:B	ZINC-FLUORIDE:SOL-B	ZRF3	ZIRCONIUM-TRIFLUORIDE
ZNI2	ZINC-IODIDE	ZRF4	ZIRCONIUM-TETRAFLUORIDE
ZNO	ZINC-OXIDE	ZRF4:A	ZIRCONIUM-TETRAFLUORIDE:SOL-
ZNP2	ZINC-DIPHOSPHIDE	ZRF4:B	ZIRCONIUM-TETRAFLUORIDE:SOL-
ZNS	ZINC-SULFIDE-WURTZITE	ZRH	ZIRCONIUM-HYDRIDE-GAS
ZNS-S	ZINC-SULFIDE-SPHALERITE	ZRI	ZIRCONIUM-MONOIODIDE-GAS
ZNSE	ZINC-SELENIDE	ZRI2	ZIRCONIUM-DIIODIDE
ZNSEO3	ZINC-SELENITE	ZRI3	ZIRCONIUM-TRIIODIDE
ZNSIO3	ZINC-METASILICATE	ZRI4	ZIRCONIUM-TETRAIODIDE
ZNSO4	ZINC-SULFATE	ZRN	ZIRCONIUM-NITRIDE
ZNSO4*2H2O	ZINC-SULFATE-DIHYDRATE	ZRO	ZIRCONIUM-MONOXIDE-GAS
ZNSO4*6H2O	ZINC-SULFATE-HEXAHYDRATE	ZRO2	ZIRCONIUM-DIOXIDE
ZNSO4*7H2O	ZINC-SULFATE-HEPTAHYDRATE	ZRO2:A	ZIRCONIUM-DIOXIDE:SOL-A
ZNSO4*H2O	ZINC-SULFATE-MONOHYDRATE	ZRO2:B	ZIRCONIUM-DIOXIDE:SOL-B
ZNSO4:1	ZINC-SULFATE:SOL-1	ZRS	ZIRCONIUM-MONOSULFIDE-GAS
ZNSO4:2	ZINC-SULFATE:SOL-2	ZRS2	ZIRCONIUM-DISULFIDE
ZNTE	ZINC-TELLURIDE	ZRSIO4	ZIRCONIUM-ORTHOSILICATE
ZNWO4	ZINC-TUNGSTATE	ZRSIO4	ZIRCONIUM-ORTHOSILICATE

Table 1.8 Parameters Available in the PURE10 Databank

Parameter Name	Description
AIT†	Auto ignition temperature
ANILPT	Aniline point
API	Standard API gravity at 60°F
ATOMNO††	Atomic number of each atom in the compound
CPDIEC	Dielectric constant
CPIGDP	DIPPR ideal gas heat capacity coefficients
CPLDIP	DIPPR liquid heat capacity coefficients
CPSDIP	DIPPR solid heat capacity coefficients
DCPLS	Difference between liquid and solid heat capacity at
DELTA	Solubility parameter at 298.2 K
DGFORM†††	Standard Gibbs free energy of formation; ideal gas at
DHFORM†††	Standard heat of formation; ideal gas at 298.2 K
DHVLB	Heat of vaporization at TB
DHVLDP	DIPPR heat of vaporization coefficients
DNLDIP	DIPPR liquid density coefficients
DNSDIP	DIPPR solid density coefficients
ENT†	Absolute entropy of formation at 298.2 K
FLML†	Lower flammability limit
FLMU†	Upper flammability limit
FP	Flash point
GMUQQ	UNIQUAC area parameter
GMUQR	UNIQUAC volume parameter
HCOM	Standard enthalpy of combustion at 298.2 K
HFUS	Enthalpy of fusion at melting point
KLDIP	DIPPR liquid thermal conductivity coefficients
KVDIP	DIPPR vapor thermal conductivity coefficients
MOCTNO	Motor octane number
MULDIP	DIPPR liquid viscosity coefficients
MUP	Dipole moment
MUVDIP	DIPPR vapor viscosity coefficients
MW	Molecular weight

† *These parameters are not used in Aspen Plus models but can be accessed by user or in-house models.*

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

††† *Contains functional group number and number of occurrences of each group.*

continued

Table 1.8 Parameters Available in the PURE10 Databank (continued)

Parameter Name	Description
NOATOM††	Number of occurrences of each atom
NTHA	Nothnagel parameters
OMEGA	Pitzer acentric factor
OMGCTD	Acentric factor for the COSTALD model
PC	Critical pressure
PLXANT	Extended Antoine vapor pressure coefficients
PRMCP	Mathias-Copeman parameters for PR equation of state
PRSRP	Schwartzentruber-Renon parameters for PR equation of
RGYR	Radius of gyration
RI	Refractive index at 298.2 K
RKSMCP	Mathias-Copeman parameters for RKS equation of state
RKSSRP	Schwartzentruber-Renon parameters for RKS equation of
RKTZRA	Rackett liquid density parameter
ROCTNO	Research octane number
SG	Standard specific gravity at 60°F
SIGDIP	DIPPR surface tension coefficients
SVRDIP†	Second virial coefficient
TB	Normal boiling point
TC	Critical temperature
TFP	Normal freezing point
TPP†	Triple point pressure
TPT	Triple point temperature
UFGRP†††	Functional group information for the UNIFAC model
UFGRPD†††	Functional group information for the Dortmund modified
UFGRPL†††	Functional group information for the Lyngby modified
VB	Liquid molar volume at TB
VC	Critical volume
VLCVT1	Scatchard-Hildebrand volume parameter
VLSTD	Standard liquid volume at 60°F
VSTCTD	Characteristic volume for the COSTALD model
WATSOL	Water solubility correlation coefficients
ZC	Critical compressibility factor

† *These parameters are not used in Aspen Plus models but can be accessed by user or in-house models.*

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

††† *Contains functional group number and number of occurrences of each group.*

Table 1.9 Components Available in the PURE10 Database

Alias	Component Name	Alias	Component Name
AIR	AIR	CCL3F	TRICHLOROFLUOROMETHANE
AG	SILVER	CCL4	CARBON-TETRACHLORIDE
AL	ALUMINUM	COF2	CARBONYL-FLUORIDE
ALCL3	ALUMINUM-CHLORIDE	CF4	CARBON-TETRAFLUORIDE
AL(OH)3	GIBBSITE	CHBR3	TRIBROMOMETHANE
ALPO4	ALUMINUM-PHOSPHATE-ORTHO	CHCLF2	CHLORODIFLUOROMETHANE
AL2O3-2	ALUMINUM-OXIDE	CHCL2F	DICHLOROMONOFLUOROMETHANE
AL2(SO4)3	ALUMINUM-SULFATE	CHCL3	CHLOROFORM
AR	ARGON	CHF3	TRIFLUOROMETHANE
AS	ARSENIC	CHN	HYDROGEN-CYANIDE
ASH3	ARSINE	NACHO2	SODIUM-FORMATE
AS2O3	ARSENIC-TRIOXIDE	NAHCO3	SODIUM-BICARBONATE
BCL3	BORON-TRICHLORIDE	CH2BRCL	BROMOCHLOROMETHANE
BF3	BORON-TRIFLUORIDE	CH2BR2	DIBROMOMETHANE
H3BO3	HYDROGEN-ORTHOBORATE	CH2CLF	CHLOROFLUOROMETHANE
NABO3	SODIUM-PERBORATE	CH2CL2	DICHLOROMETHANE
B2H6	DIBORANE	CH2F2	DIFLUOROMETHANE
B4H20NA2O17	BORAX	CH2I2	DIIODOMETHANE
BE	BERYLLIUM	CH2O	FORMALDEHYDE
BI	BISMUTH	CH2O2	FORMIC-ACID
HBR	HYDROGEN-BROMIDE	CH3BR	METHYL-BROMIDE
KBR	POTASSIUM-BROMIDE	CH3CL	METHYL-CHLORIDE
NABR	SODIUM-BROMIDE	CH3SICL3	METHYL-TRICHLOROSILANE
BR2	BROMINE	CH3F	METHYL-FLUORIDE
C	CARBON(GRAPHITE)	CH3I	METHYL-IODIDE
BACO3	BARIUM-CARBONATE	CH3NO	FORMAMIDE
CBRCLF2	BROMOCHLORODIFLUOROMETHANE	CH3NO2	NITROMETHANE
CBRCL3	BROMOTRICHLOROMETHANE	CH4	METHANE
CBRF3	TRIFLUOROBROMOMETHANE	CH4SICL2	METHYL-DICHLOROSILANE
CBR2F2	DIBROMODIFLUOROMETHANE	CH4N2O	UREA
CACO3-2	CALCIUM-CARBONATE(CALCITE)	CH4N2S	THIOUREA
CCLF3	CHLOROTRIFLUOROMETHANE	CH4O	METHANOL
CCLN	CYANOGEN-CHLORIDE	CH4O3S	METHANESULFONIC-ACID
CCL2F2	DICHLORODIFLUOROMETHANE	CH4S	METHYL-MERCAPTAN
CCL2O	PHOSGENE	CH5SICL	METHYL-CHLOROSILANE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
CH5N	METHYL-AMINE	C2HF3O2	TRIFLUOROACETIC-ACID
CH6SI	METHYL-SILANE	C2HF5	PENTAFLUOROETHANE
K2CO3	POTASSIUM-CARBONATE	C2H2	ACETYLENE
NACN	SODIUM-CYANIDE	C2H2BR4	1,1,2,2-TETRABROMOETHANE
CN4O8	TETRANITROMETHANE	C2H2CLF3	2-CHLORO-1,1,1-TRIFLUOROETHANE
NA2CO3	SODIUM-CARBONATE	C2H2CL2-D1	1,1-DICHLOROETHYLENE
CO	CARBON-MONOXIDE	C2H2CL2-D2	CIS-1,2-DICHLOROETHYLENE
COS	CARBONYL-SULFIDE	C2H2CL2-D3	TRANS-1,2-DICHLOROETHYLENE
CO2	CARBON-DIOXIDE	C2H2CL2O	CHLOROACETYL-CHLORIDE
CS2	CARBON-DISULFIDE	C2H2CL2O-D1	DICHLOROACETALDEHYDE
SIC	SILICON-CARBIDE	C2H2CL2O2	DICHLOROACETIC-ACID
C2BRF3	BROMOTRIFLUOROETHYLENE	C2H2CL3F	1,1,1-TRICHLOROFLUOROETHANE
C2BR2F4	1,2-DIBROMOTETRAFLUOROETHANE	C2H2CL4-D1	1,1,1,2-TETRACHLOROETHANE
C2CLF3	CHLOROTRIFLUOROETHYLENE	C2H2CL4-D2	1,1,2,2-TETRACHLOROETHANE
C2CLF5	CHLOROPENTAFLUOROETHANE	C2H2F2	1,1-DIFLUOROETHYLENE
C2CL2F4-1	1,1-DICHLORO-1,2,2,2-TETRAFLUORO	C2H2F4	1,1,1,2-TETRAFLUOROETHANE
C2CL2F4-2	1,2-DICHLORO-1,1,2,2-TETRAFLUORO	C2H2F4-D1	1,1,2,2-TETRAFLUOROETHANE
C2CL3F3	1,2,2-TRICHLORO-1,1,2-TRIFLUOROE	C2H2O	KETENE
C2CL4	TETRACHLOROETHYLENE	C2H2O2	GLYOXAL
C2CL4F2-D1	1,1,1,2-TETRACHLORODIFLUOROETHAN	C2H2O4	OXALIC-ACID
C2CL4F2	1,1,2,2-TETRACHLORO-1,2-DIFLUORO	C2H3BR	VINYL-BROMIDE
C2CL4O	TRICHLOROACETYL-CHLORIDE	C2H3CL	VINYL-CHLORIDE
C2CL6	HEXACHLOROETHANE	C2H3CLF2	1-CHLORO-1,1-DIFLUOROETHANE
C2F4	PERFLUOROETHENE	C2H3CLO	ACETYL-CHLORIDE
C2F6	PERFLUOROETHANE	C2H3CLO-D0	CHLOROACETALDEHYDE
C2HBRCLF3	HALOTHANE	C2H3CLO2	CHLOROACETIC-ACID
C2HCLF2	2-CHLORO-1,1-DIFLUOROETHYLENE	C2H3CLO2-D1	METHYL-CHLOROFORMATE
C2HCLF4	2-CHLORO-1,1,1,2-TETRAFLUOROETHA	C2H3CL2F	1,1-DICHLORO-1-FLUOROETHANE
C2HCL2F3-D2	1,2-DICHLORO-1,1,2-TRIFLUOROETHA	C2H3CL3-D0	1,1,1-TRICHLOROETHANE
C2HCL2F3-D1	1,1-DICHLORO-2,2,2-TRIFLUOROETHA	C2H3CL3	1,1,2-TRICHLOROETHANE
C2HCL3	TRICHLOROETHYLENE	C2H3F	VINYL-FLUORIDE
C2HCL3O	DICHLOROACETYL-CHLORIDE	C2H3F3	1,1,1-TRIFLUOROETHANE
C2HCL3O-D1	TRICHLOROACETALDEHYDE	KC2H3O2	POTASSIUM-ACETATE
C2HCL3O2	TRICHLOROACETIC-ACID	C2H3N	ACETONITRILE
C2HCL5	PENTACHLOROETHANE	C2H3NO-E1	HYDROXYACETONITRILE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C2H3NO	METHYL-ISOCYANATE	C2H6O-1	DIMETHYL-ETHER
C2H3NAO2	SODIUM-ACETATE	C2H6O-2	ETHANOL
C2H4	ETHYLENE	C2H6OS	DIMETHYL-SULFOXIDE
C2H4BR2-D1	1,1-DIBROMOETHANE	C2H6OS-D1	2-MERCAPTOETHANOL
C2H4BR2	1,2-DIBROMOETHANE	C2H6O2	ETHYLENE-GLYCOL
C2H4CL2-1	1,1-DICHLOROETHANE	C2H6O4S	DIMETHYL-SULFATE
C2H4CL2-2	1,2-DICHLOROETHANE	C2H6S-2	DIMETHYL-SULFIDE
C2H4CL2O	BIS-CHLOROMETHYL-ETHER	C2H6S-1	ETHYL-MERCAPTAN
C2H4F2	1,1-DIFLUOROETHANE	C2H6S2	DIMETHYL-DISULFIDE
C2H4F2-D1	1,2-DIFLUOROETHANE	C2H6S2-D1	1,2-ETHANEDITHIOL
C2H4N2	AMINOACETONITRILE	C2H7SICL	DIMETHYLCHLOROSILANE
C2H4N2O6	ETHYLENE-GLYCOL-DINITRATE	C2H7N-2	DIMETHYLAMINE
C2H4N4	DICYANDIAMIDE	C2H7N-1	ETHYL-AMINE
C2H4O-1	ACETALDEHYDE	C2H7NO	MONOETHANOLAMINE
C2H4O-2	ETHYLENE-OXIDE	C2H7NO2	AMMONIUM-ACETATE
C2H4O2-1	ACETIC-ACID	C2H8N2	ETHYLENEDIAMINE
C2H4O2-2	METHYL-FORMATE	C2H8N2O4	AMMONIUM-OXALATE
C2H4O2S	THIOGLYCOLIC-ACID	C2H8P2O6	1,2-ETHANE-DIPHOSPHONIC-ACID
C2H4O3-D1	GLYCOLIC-ACID	C2H8SI	DIMETHYL-SILANE
C2H4O3-D2	PERACETIC-ACID	C2N2	CYANOGEN
C2H4S	THIACYCLOPROPANE	C3CL2F6	1,3-DICHLOROHEXAFLUOROPROPANE
C2H5BR	ETHYL-BROMIDE	C3F6	HEXAFLUOROPROPYLENE
C2H5CL	ETHYL-CHLORIDE	C3F6O	HEXAFLUOROACETONE
C2H5CLO	2-CHLOROETHANOL	C3F8	OCTAFLUOROPROPANE
C2H5CLO-D1	CHLOROMETHYL-METHYL-ETHER	C3H2N2	MALONONITRILE
C2H5F	ETHYL-FLUORIDE	C3H3CL	PROPARGYL-CHLORIDE
C2H5I	ETHYL-IODIDE	C3H3F5	1,1,1,2,2-PENTAFLUOROPROPANE
C2H5N	ETHYLENE-IMINE	C3H3N	ACRYLONITRILE
C2H5NO-D1	ACETAMIDE	C3H3NO	OXAZOLE
C2H5NO-D2	N-METHYLFORMAMIDE	C3H4-2	METHYL-ACETYLENE
C2H5NO2-D1	GLYCINE	C3H4-1	PROPADIENE
C2H5NO2	NITROETHANE	C3H4CL2	2,3-DICHLOROPROPENE
C2H6	ETHANE	C3H4N2	PYRAZOLE
C2H6ALCL	DIMETHYLALUMINUM-CHLORIDE	C3H4O	ACROLEIN
C2H6SICL2	DIMETHYLDICHLOROSILANE	C3H4O-D0	PROPARGYL-ALCOHOL

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C3H4O2-1	ACRYLIC-ACID	C3H6O3-D3	DIMETHYL-CARBONATE
C3H4O2-D0	BETA-PROPIOLACTONE	C3H6O3-D1	LACTIC-ACID
C3H4O2-2	VINYL-FORMATE	C3H6O3	METHOXYACETIC-ACID
C3H4O3	ETHYLENE-CARBONATE	C3H6O3-D2	TRIOXANE
C3H4O3-D1	PYRUVIC-ACID	C3H6S	TRIMETHYLENE-SULFIDE
C3H4O4	MALONIC-ACID	C3H7BR-D1	1-BROMOPROPANE
C3H5CL-D0	2-CHLOROPROPENE	C3H7BR-D2	2-BROMOPROPANE
C3H5CL	ALLYL-CHLORIDE	C3H7CL-2	ISOPROPYL-CHLORIDE
C3H5CLO	ALPHA-EPICHLOROHYDRIN	C3H7CL-1	PROPYL-CHLORIDE
C3H5CLO2-D1	ETHYL-CHLOROFORMATE	C3H7I-D1	ISOPROPYL-IODIDE
C3H5CLO2	METHYL-CHLOROACETATE	C3H7I-D2	N-PROPYL-IODIDE
C3H5CL3	1,2,3-TRICHLOROPROPANE	C3H7N	ALLYLAMINE
C3H5N	PROPIONITRILE	C3H7N-D1	PROPYLENEIMINE
C3H5NO-D1	ACRYLAMIDE	C3H7NO	N,N-DIMETHYLFORMAMIDE
C3H5NO-D2	HYDRACRYLONITRILE	C3H7NO-D1	N-METHYLACETAMIDE
C3H5NO	LACTONITRILE	C3H7NO2-D1	1-NITROPROPANE
C3H5N3O9	NITROGLYCERINE	C3H7NO2-D2	2-NITROPROPANE
C3H6-1	CYCLOPROPANE	C3H8	PROPANE
C3H6-2	PROPYLENE	C3H8O-2	ISOPROPYL-ALCOHOL
C3H6CL2-D1	1,1-DICHLOROPROPANE	C3H8O-3	METHYL-ETHYL-ETHER
C3H6CL2	1,2-DICHLOROPROPANE	C3H8O-1	1-PROPANOL
C3H6CL2-D2	1,3-DICHLOROPROPANE	C3H8O2	2-METHOXYETHANOL
C3H6N6	MELAMINE	C3H8O2-1	METHYLAL
C3H6O-1	ACETONE	C3H8O2-2	PROPANEDIOL-1,2
C3H6O-2	ALLYL-ALCOHOL	C3H8O2-3	1,3-PROPANEDIOL
C3H6O-5	VINYL-METHYL-ETHER	C3H8O3	GLYCEROL
C3H6O-3	N-PROPIONALDEHYDE	C3H8S-D1	ISOPROPYL-MERCAPTAN
C3H6O-4	PROPYLENE-OXIDE	C3H8S-E2	METHYL-ETHYL-SULFIDE
C3H6O-D0	1,3-PROPYLENE-OXIDE	C3H8S-E1	N-PROPYLMERCAPTAN
C3H6O2-D1	ACETOL	C3H9AL	TRIMETHYLALUMINUM
C3H6O2-D2	2,3-EPOXY-1-PROPANOL	C3H9SICL	TRIMETHYLCHLOROSILANE
C3H6O2-2	ETHYL-FORMATE	C3H9GA	TRIMETHYLGALLIUM
C3H6O2-3	METHYL-ACETATE	C3H9N-2	ISOPROPYL-AMINE
C3H6O2-1	PROPIONIC-ACID	C3H9N-1	N-PROPYL-AMINE
C3H6O2S	3-MERCAPTOPROPIONIC-ACID	C3H9N-3	TRIMETHYL-AMINE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C3H9NO-D1	1-AMINO-2-PROPANOL	C4H6-3	1,2-BUTADIENE
C3H9NO-D2	3-AMINO-1-PROPANOL	C4H6-4	1,3-BUTADIENE
C3H9NO	METHYL-ETHANOLAMINE	C4H6-2	2-BUTYNE
C3H9O4P	TRIMETHYL-PHOSPHATE	C4H6-1	1-BUTYNE
C3H10N2	1,2-PROPANEDIAMINE	C4H6CL2-E1	1,3-DICHLORO-TRANS-2-BUTENE
C3H10SI	TRIMETHYL-SILANE	C4H6CL2-E3	1,4-DICHLORO-CIS-2-BUTENE
C4CL2F6	1,2-DICHLOROHEXAFLUOROCYCLOBUTAN	C4H6CL2	1,4-DICHLORO-TRANS-2-BUTENE
C4CL4S	TETRACHLOROTHIOPHENE	C4H6CL2-E2	3,4-DICHLORO-1-BUTENE
C4CL6	HEXACHLORO-1,3-BUTADIENE	C4H6O-D1	TRANS-CROTONALDEHYDE
C4F8-D1	OCTAFLUORO-2-BUTENE	C4H6O-D4	2,3-DIHYDROFURAN
C4F8-D2	OCTAFLUOROCYCLOBUTANE	C4H6O	2,5-DIHYDROFURAN
C4F10	DECAFLUOROBUTANE	C4H6O-D2	DIVINYL-ETHER
C4H2N2-D1	FUMARONITRILE	C4H6O-D3	METHACROLEIN
C4H2O3	MALEIC-ANHYDRIDE	C4H6O2-D1	2-BUTYNE-1,4-DIOL
C4H4	VINYLACETYLENE	C4H6O2-D2	GAMMA-BUTYROLACTONE
C4H2N2-D2	MALEONITRILE	C4H6O2-D3	CIS-CROTONIC-ACID
C4H4N2-D1	PYRAZINE	C4H6O2-D4	TRANS-CROTONIC-ACID
C4H4N2-D2	PYRIDAZINE	C4H6O2-D5	METHACRYLIC-ACID
C4H4N2-D3	PYRIMIDINE	C4H6O2-2	METHYL-ACRYLATE
C4H4N2	SUCCINONITRILE	C4H6O2-1	VINYL-ACETATE
C4H4O	FURAN	C4H6O2S	SULFOLENE
C4H4O2	DIKETENE	C4H6O3	ACETIC-ANHYDRIDE
C4H4O3	SUCCINIC-ANHYDRIDE	C4H6O3-D1	PROPYLENE-CARBONATE
C4H4O4-D1	FUMARIC-ACID	C4H6O4-2	SUCCINIC-ACID
C4H4O4-D2	MALEIC-ACID	C4H6O5	DIGLYCOLIC-ACID
C4H4S	THIOPHENE	C4H6O5-D1	MALIC-ACID
C4H5CL	CHLOROPRENE	C4H6O6	TARTARIC-ACID
C4H5N-E3	CIS-CROTONITRILE	C4H7CLO2	ETHYLCHLOROACETATE
C4H5N-E1	TRANS-CROTONITRILE	C4H7N	BUTYRONITRILE
C4H5N	METHACRYLONITRILE	C4H7N-D0	ISOBUTYRONITRILE
C4H5N-2	PYRROLE	C4H7NO-D1	ACETONE-CYANOHYDRIN
C4H5N-1	ALLYL-CYANIDE	C4H7NO-E1	2-METHACRYLAMIDE
C4H5NO	ACROLEIN-CYANOHYDRIN	C4H7NO-E2	3-METHOXYPROPIONITRILE
C4H5NO2	METHYL-CYANOACETATE	C4H7NO-D2	2-PYRROLIDONE
C4H5N3	2,2-IMINOBIS-ACETONITRILE	C4H8-1	1-BUTENE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C4H8-2	CIS-2-BUTENE	C4H9N	PYRROLIDINE
C4H8-3	TRANS-2-BUTENE	C4H9NO-D0	N,N-DIMETHYLACETAMIDE
C4H8-4	CYCLOBUTANE	C4H9NO	MORPHOLINE
C4H8-5	ISOBUTYLENE	C4H10-1	N-BUTANE
C4H8CL2-D1	1,2-DICHLOROBUTANE	C4H10-2	ISOBUTANE
C4H8CL2	1,4-DICHLOROBUTANE	C4H10N2	PIPERAZINE
C4H8CL2-D2	2,3-DICHLOROBUTANE	C4H10O-1	N-BUTANOL
C4H8O-1	N-BUTYRALDEHYDE	C4H10O-2	2-BUTANOL
C4H8O	1,2-EPOXYBUTANE	C4H10O-5	DIETHYL-ETHER
C4H8O-D1	1,2-EPOXY-2-METHYLPROPANE	C4H10O-D1	METHYL-ISOPROPYL-ETHER
C4H8O-5	VINYL-ETHYL-ETHER	C4H10O-3	ISOBUTANOL
C4H8O-3	METHYL-ETHYL-KETONE	C4H10O-4	TERT-BUTYL-ALCOHOL
C4H8O-2	ISOBUTYRALDEHYDE	C4H10O-D2	METHYL-N-PROPYL-ETHER
C4H8O-4	TETRAHYDROFURAN	C4H10OS	ETHYLTHIOETHANOL
C4H8O2-D1	ACETALDOL	C4H10OS2	DIMERCAPTOETHYL-ETHER
C4H8O2-D2	CIS-2-BUTENE-1,4-DIOL	C4H10O2-D6	1,2-BUTANEDIOL
C4H8O2-D3	TRANS-2-BUTENE-1,4-DIOL	C4H10O2-D1	1,3-BUTANEDIOL
C4H8O2-1	N-BUTYRIC-ACID	C4H10O2-D2	1,4-BUTANEDIOL
C4H8O2-D4	1,3-DIOXANE	C4H10O2-D5	2,3-BUTANEDIOL
C4H8O2-2	1,4-DIOXANE	C4H10O2-D3	T-BUTYL-HYDROPEROXIDE
C4H8O2-3	ETHYL-ACETATE	C4H10O2	1,2-DIMETHOXYETHANE
C4H8O2-D6	4-HYDROXYBUTYRALDEHYDE	C4H10O2-D4	2-ETHOXYETHANOL
C4H8O2-D5	3-HYDROXY-2-METHYL-PROPIONALDEHY	C4H10O2-D9	2-METHOXY-PROPANOL-1
C4H8O2-4	ISOBUTYRIC-ACID	C4H10O2-D8	2-METHYL-1,3-PROPANEDIOL
C4H8O2-5	METHYL-PROPIONATE	C4H10O2-D7	PG-MONOMETHYL-ETHER
C4H8O2-6	N-PROPYL-FORMATE	C4H10O2S	THIODIGLYCOL
C4H8O2S	SULFOLANE	C4H10O3	DIETHYLENE-GLYCOL
C4H8O3	METHYL-LACTATE	C4H10SO3	DIETHYLSULFITE
C4H8S	TETRAHYDROTHIOPHENE	C4H10O4S	DIETHYL-SULFATE
C4H9BR-D1	1-BROMOBUTANE	C4H10S-D1	N-BUTYL-MERCAPTAN
C4H9BR-D2	2-BROMOBUTANE	C4H10S-E1	SEC-BUTYL-MERCAPTAN
C4H9CL-1	1-CHLOROBUTANE	C4H10S-D2	TERT-BUTYL-MERCAPTAN
C4H9CL-2	2-CHLOROBUTANE	C4H10S	DIETHYL-SULFIDE
C4H9CL-3	TERT-BUTYL-CHLORIDE	C4H10S-E2	ISOBUTYL-MERCAPTAN
C4H9CL-D1	ISOBUTYL-CHLORIDE	C4H10S-D3	METHYL-N-PROPYL-SULFIDE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C4H10S2	DIETHYL-DISULFIDE	C5H8	CIS-1,3-PENTADIENE
C4H11N-1	N-BUTYL-AMINE	C5H8-3	1-TRANS-3-PENTADIENE
C4H11N-D1	SEC-BUTYLAMINE	C5H8-4	1,4-PENTADIENE
C4H11N-D2	TERT-BUTYLAMINE	C5H8-E4	2,3-PENTADIENE
C4H11N-3	DIETHYL-AMINE	C5H8-5	1-PENTYNE
C4H11N-2	ISOBUTYL-AMINE	C5H8-E5	2-PENTYNE
C4H11NO	DIMETHYLETHANOLAMINE	NAC5H8NO4	MONOSODIUM-GLUTAMATE
C4H11NO2-2	DIGLYCOLAMINE	C5H8N4O12	PENTAERYTHRITOL-TETRANITRATE
C4H11NO2-1	DIETHANOLAMINE	C5H8O	CYCLOPENTANONE
C4H12N2O	N-AMINOETHYL-ETHANOLAMINE	C5H8O-D1	METHYL-ISOPROPENYL-KETONE
C4H12SIO2	DIMETHYLDIMETHOXYSILANE	C5H8O2-D1	ACETYLACETONE
C4H12SI	TETRAMETHYLSILANE	C5H8O2-D2	ALLYL-ACETATE
C4H13N3	DIETHYLENE-TRIAMINE	C5H8O2	ETHYL-ACRYLATE
C5CL6	HEXACHLOROCYCLOPENTADIENE	C5H8O2-D6	GLUTARALDEHYDE
C5H4O2	FURFURAL	C5H8O2-D3	METHYL-METHACRYLATE
C5H4O3	METHYL-MALEIC-ANHYDRIDE	C5H8O2-D4	GAMMA-VALEROLACTONE
C5H5N	PYRIDINE	C5H8O2-D5	VINYL-PROPIONATE
C5H6	CYCLOPENTADIENE	C5H8O3	2-HYDROXYETHYL-ACRYLATE
C5H6-E1	2-METHYL-1-BUTENE-3-YNE	C5H8O3-D1	LEVULINIC-ACID
C5H6-E2	1-PENTENE-3-YNE	C5H8O3-D2	METHYL-ACETOACETATE
C5H6-E3	1-PENTENE-4-YNE	C5H8O4	GLUTARIC-ACID
C5H6N2	GLUTARONITRILE	C5H9N	VALERONITRILE
C5H6O2	FURFURYL-ALCOHOL	C5H9NO-D1	N-BUTYL-ISOCYANATE
C5H6O3	GLUTARIC-ANHYDRIDE	C5H9NO-D2	N-METHYL-2-PYRROLIDONE
C5H6O4-E1	CITRACONIC-ACID	C5H9NO4	L-GLUTAMIC-ACID
C5H6O4-E2	ITACONIC-ACID	C5H9NS	N-METHYLTHIOPYRROLIDONE
C5H6S-E1	2-METHYLTHIOPHENE	C5H10-1	CYCLOPENTANE
C5H6S-E2	3-METHYLTHIOPHENE	C5H10-5	2-METHYL-1-BUTENE
C5H7N	N-METHYLPYRROLE	C5H10-6	2-METHYL-2-BUTENE
C5H7NO2	ETHYL-CYANOACETATE	C5H10-7	3-METHYL-1-BUTENE
C5H8-1	CYCLOPENTENE	C5H10-2	1-PENTENE
C5H8-6	2-METHYL-1,3-BUTADIENE	C5H10-3	CIS-2-PENTENE
C5H8-7	3-METHYL-1,2-BUTADIENE	C5H10-4	TRANS-2-PENTENE
C5H8-E2	3-METHYL-1-BUTYNE	C5H10CL2	1,5-DICHLOROPENTANE
C5H8-2	1,2-PENTADIENE	C5H10NNAS2	SODIUM-DIETHYLDITHIOCARBAMATE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C5H10O-3	METHYL-ISOPROPYL-KETONE	C5H12O-E2	METHYL-N-BUTYL-ETHER
C5H10O-1	VALERALDEHYDE	C5H12O	METHYL-SEC-BUTYL-ETHER
C5H10O-2	METHYL-N-PROPYL-KETONE	C5H12O-D2	METHYL-TERT-BUTYL-ETHER
C5H10O-4	DIETHYL-KETONE	C5H12O-E1	METHYL-ISOBUTYL-ETHER
C5H10O2-D1	N-BUTYL-FORMATE	C5H12O-1	1-PENTANOL
C5H10O2-D6	SEC-BUTYL-FORMATE	C5H12O-D3	2-PENTANOL
C5H10O2-D7	TERT-BUTYL-FORMATE	C5H12O-D4	3-PENTANOL
C5H10O2-4	ETHYL-PROPIONATE	C5H12O2-D4	ETHYLAL
C5H10O2-2	ISOBUTYL-FORMATE	C5H12O2-D3	ETHYLENE-GLYCOL-MONOPROPYL-ETHER
C5H10O2-D2	ISOPROPYL-ACETATE	C5H12O2-D1	NEOPENTYL-GLYCOL
C5H10O2-D3	ISOVALERIC-ACID	C5H12O2-D2	1,5-PENTANEDIOL
C5H10O2-5	METHYL-BUTYRATE	C5H12O2-D5	2,4-PENTANEDIOL
C5H10O2-D4	2-METHYLBUTYRIC-ACID	C5H12O3	2-2-METHOXYETHOXY-ETHANOL
C5H10O2-6	METHYL-ISOBUTYRATE	C5H12O4	PENTAERYTHRITOL
C5H10O2	NEOPENTANOIC-ACID	C5H12S-D2	METHYL-N-BUTYL-SULFIDE
C5H10O2-1	N-VALERIC-ACID	C5H12S-D1	METHYL-T-BUTYL-SULFIDE
C5H10O2-3	N-PROPYL-ACETATE	C5H12S	1-PENTANETHIOL
C5H10O2-D5	TETRAHYDROFURFURYL-ALCOHOL	C5H13N	N-PENTYLAMINE
C5H10O2S	3-METHYL-SULFOLANE	C5H13NO2	METHYL-DIETHANOLAMINE
C5H10O3-D1	DIETHYL-CARBONATE	C6CL6	HEXACHLOROBENZENE
C5H10O3-D2	ETHYL-LACTATE	C6F6	PERFLUOROBENZENE
C5H11CL	1-CHLOROPENTANE	C6H3CLN2O4	1-CHLORO-2,4-DINITROBENZENE
C5H11N-D0	N-METHYLPYRROLIDINE	C6H3CL2NO2	1,2-DICHLORO-4-NITROBENZENE
C5H11N	PIPERIDINE	C6H3CL3	1,2,4-TRICHLOROBENZENE
C5H11NO	TERT-BUTYLFORMAMIDE	C6H3CL3-D1	1,3,5-TRICHLOROBENZENE
C5H12-2	2-METHYL-BUTANE	C6H3N3O6	1,3,5-TRINITROBENZENE
C5H12-3	2,2-DIMETHYL-PROPANE	C6H4BR2	M-DIBROMOBENZENE
C5H12-1	N-PENTANE	C6H4CLNO2-D1	M-CHLORONITROBENZENE
C5H12O-5	2,2-DIMETHYL-1-PROPANOL	C6H4CLNO2-D2	O-CHLORONITROBENZENE
C5H12O-D5	ETHYL-ISOPROPYL-ETHER	C6H4CLNO2-D3	P-CHLORONITROBENZENE
C5H12O-6	ETHYL-PROPYL-ETHER	C6H4CL2-2	M-DICHLOROBENZENE
C5H12O-2	2-METHYL-1-BUTANOL	C6H4CL2-1	O-DICHLOROBENZENE
C5H12O-4	2-METHYL-2-BUTANOL	C6H4CL2-3	P-DICHLOROBENZENE
C5H12O-3	3-METHYL-1-BUTANOL	C6H4N2	NICOTINONITRILE
C5H12O-D1	3-METHYL-2-BUTANOL	C6H4N2O4-E1	M-DINITROBENZENE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C6H4N2O4-E2	O-DINITROBENZENE	C6H7N-2	4-METHYLPYRIDINE
C6H4N2O4-E3	P-DINITROBENZENE	C6H7NO3S	SULFANILIC-ACID
C6H4O2	QUINONE	C6H8-E1	1,3-CYCLOHEXADIENE
C6H5BR	BROMOBENZENE	C6H8-E3	1,4-CYCLOHEXADIENE
C6H5CL	CHLOROBENZENE	C6H8-E2	METHYLCYCLOPENTADIENE
C6H5CLO-E1	M-CHLOROPHENOL	C6H8N2-D1	ADIPONITRILE
C6H5CLO-E2	O-CHLOROPHENOL	C6H8N2	METHYLGLUTARONITRILE
C6H5CLO-E3	P-CHLOROPHENOL	C6H8N2-D2	M-PHENYLENEDIAMINE
C6H5CL2N	3,4-DICHLOROANILINE	C6H8N2-D3	O-PHENYLENEDIAMINE
C6H5SICL3	PHENYLTRICHLOROSILANE	C6H8N2-D4	P-PHENYLENEDIAMINE
C6H5F	FLUOROBENZENE	C6H8N2-D5	PHENYLHYDRAZINE
C6H5I	IODOBENZENE	C6H8N2O	BIS-CYANOETHYL-ETHER
C6H5NO2-D1	NIACIN	C6H8O4	DIMETHYL-MALEATE
C6H5NO2	NITROBENZENE	C6H8O6	ASCORBIC-ACID
C6H6	BENZENE	C6H8O7	CITRIC-ACID
C6H6CLN-D1	M-CHLOROANILINE	C6H10-2	CYCLOHEXENE
C6H6CLN-D2	O-CHLOROANILINE	C6H10-E3	2,3-DIMETHYL-1,3-BUTADIENE
C6H6CLN-D3	P-CHLOROANILINE	C6H10-D4	1,2-HEXADIENE
C6H6N2-E1	CIS-DICYANO-1-BUTENE	C6H10-E8	1,4-HEXADIENE
C6H6N2-E2	TRANS-DICYANO-1-BUTENE	C6H10-1	1,5-HEXADIENE
C6H6N2-E3	1,4-DICYANO-2-BUTENE	C6H10-E4	CIS,TRANS-2,4-HEXADIENE
C6H6N2O2-D1	M-NITROANILINE	C6H10-E5	TRANS,TRANS-2,4-HEXADIENE
C6H6N2O2-D2	O-NITROANILINE	C6H10-E2	1-HEXYNE
C6H6N2O2-D3	P-NITROANILINE	C6H10-E6	2-HEXYNE
C6H6N4	2,2,2-NITRILOTRIS-ACETONITRILE	C6H10-E7	3-HEXYNE
C6H6O	PHENOL	C6H10-D1	1-METHYLCYCLOPENTENE
C6H6O2-E1	1,2-BENZENEDIOL	C6H10-D2	3-METHYLCYCLOPENTENE
C6H6O2-E2	1,3-BENZENEDIOL	C6H10-D3	4-METHYLCYCLOPENTENE
C6H6O2	P-HYDROQUINONE	C6H10O	CYCLOHEXANONE
C6H6O3	1,2,3-BENZENETRIOL	C6H10O-D0	MESITYL-OXIDE
C6H6O3S	BENZENESULFONIC-ACID	C6H10O2-D1	CAPROLACTONE
C6H6S	PHENYL-MERCAPTAN	C6H10O2-D2	ETHYL-METHACRYLATE
C6H7N-1	ANILINE	C6H10O2-D5	ISOPROPYL-ACRYLATE
C6H7N-D1	2-METHYLPYRIDINE	C6H10O2-D4	METHOXYDIHYDROPYRAN
C6H7N-D2	3-METHYLPYRIDINE	C6H10O2-D3	N-PROPYL-ACRYLATE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C6H10O3-D1	ETHYLACETOACETATE	C6H12O-D1	BUTYL-VINYL-ETHER
C6H10O3	2-HYDROXYETHYL-METHACRYLATE	C6H12O-1	CYCLOHEXANOL
C6H10O3-D2	PROPIONIC-ANHYDRIDE	C6H12O-E3	3,3-DIMETHYL-2-BUTANONE
C6H10O4-D1	ADIPIC-ACID	C6H12O-E1	ETHYL-ISOPROPYL-KETONE
C6H10O4-D2	DIETHYL-OXALATE	C6H12O-D2	1-HEXANAL
C6H10O4-D3	ETHYLENE-GLYCOL-DIACETATE	C6H12O-D3	2-HEXANONE
C6H10O4	ETHYLIDENE-DIACETATE	C6H12O	3-HEXANONE
C6H10O5	DILACTIC-ACID	C6H12O-2	METHYL-ISOBUTYL-KETONE
C6H11N-D1	DIALLYLAMINE	C6H12O-E2	3-METHYL-2-PENTANONE
C6H11N	HEXANENITRILE	C6H12O2-1	N-BUTYL-ACETATE
C6H11NO	EPSILON-CAPROLACTAM	C6H12O2-D1	SEC-BUTYL-ACETATE
C6H11NO-D1	CYCLOHEXANONE-OXIME	C6H12O2	TERT-BUTYL-ACETATE
C6H12-1	CYCLOHEXANE	C6H12O2-D2	CYCLOHEXYL-PEROXIDE
C6H12-13	2,3-DIMETHYL-1-BUTENE	C6H12O2-D3	DIACETONE-ALCOHOL
C6H12-14	2,3-DIMETHYL-2-BUTENE	C6H12O2-3	ETHYL-BUTYRATE
C6H12-15	3,3-DIMETHYL-1-BUTENE	C6H12O2-D4	2-ETHYL-BUTYRIC-ACID
C6H12-D1	2-ETHYL-1-BUTENE	C6H12O2-4	ETHYL-ISOBUTYRATE
C6H12-3	1-HEXENE	C6H12O2-D5	N-HEXANOIC-ACID
C6H12-4	CIS-2-HEXENE	C6H12O2-2	ISOBUTYL-ACETATE
C6H12-5	TRANS-2-HEXENE	C6H12O2-D6	NEOHEXANOIC-ACID
C6H12-6	CIS-3-HEXENE	C6H12O2-E1	N-PENTYL-FORMATE
C6H12-7	TRANS-3-HEXENE	C6H12O2-5	N-PROPYL-PROPIONATE
C6H12-2	METHYLCYCLOPENTANE	C6H12O3-D1	2-ETHOXYETHYL-ACETATE
C6H12-D2	2-METHYL-1-PENTENE	C6H12O3-E1	HYDROXYCAPROIC-ACID
C6H12-8	2-METHYL-2-PENTENE	C6H12O3	6-HYDROXYHEXANOIC-ACID
C6H12-E3	3-METHYL-1-PENTENE	C6H12O3-D2	PARALDEHYDE
C6H12-9	3-METHYL-CIS-2-PENTENE	C6H12O3-E2	PG-MONOMETHYL-ETHER-ACETATE
C6H12-10	3-METHYL-TRANS-2-PENTENE	C6H12O6	DEXTROSE
C6H12-D3	4-METHYL-1-PENTENE	C6H12O6-D1	INOSITOL
C6H12-11	4-METHYL-CIS-2-PENTENE	C6H12S	CYCLOHEXYL-MERCAPTAN
C6H12-12	4-METHYL-TRANS-2-PENTENE	C6H13N-D1	CYCLOHEXYLAMINE
C6H12CL3PO3	BIS-2-CHLOROETHYL-2-CHLOROETHYL	C6H13N-D2	HEXAMETHYLENEIMINE
C6H12N2-E1	AMINOCAPRONITRILE	C6H14-4	2,2-DIMETHYL-BUTANE
C6H12N2-E2	TRIETHYLENEDIAMINE	C6H14-5	2,3-DIMETHYL-BUTANE
C6H12N4	HEXAMETHYLENETETRAMINE	C6H14-1	N-HEXANE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C6H14-2	2-METHYL-PENTANE	C6H15N-1	DIPROPYLAMINE
C6H14-3	3-METHYL-PENTANE	C6H15N-D2	N-HEXYLAMINE
C6H14N2O	N-2-HYDROXYETHYL-PIPERAZINE	C6H15N-2	TRIETHYLAMINE
C6H14N2O2	LYSINE	C6H15NO	6-AMINOHEXANOL
C6H14O-2	ETHYL-BUTYL-ETHER	C6H15NO-D1	DIETHYLETHANOLAMINE
C6H14O-E3	TERT-BUTYL-ETHYL-ETHER	C6H15NO2	DIISOPROPANOLAMINE
C6H14O-3	DIISOPROPYL-ETHER	C6H15NO3	TRIETHANOLAMINE
C6H14O-D1	DI-N-PROPYL-ETHER	C6H15N3	N-AMINOETHYL-PIPERAZINE
C6H14O-D2	2-ETHYL-1-BUTANOL	C6H15O4P	TRIETHYL-PHOSPHATE
C6H14O-1	1-HEXANOL	C6H16N2	HEXAMETHYLENEDIAMINE
C6H14O-E1	2-HEXANOL	C6H16N2-D1	TETRAMETHYLETHYLENEDIAMINE
C6H14O-D3	2-METHYL-1-PENTANOL	C6H18N3OP	HEXAMETHYL-PHOSPHORAMIDE
C6H14O-D4	4-METHYL-2-PENTANOL	C6H18N4	TRIETHYLENE-TETRAMINE
C6H14O-E4	METHYL-N-PENTYL-ETHER	C6H18OSI2	HEXAMETHYLDISILOXANE
C6H14O-E2	METHYL-TERT-PENTYL-ETHER	C6H18O3SI3	HEXAMETHYLCYCLOTRISILOXANE
C6H14O2-D1	ACETAL	C6H19NSI2	HEXAMETHYLDISILAZANE
C6H14O2-D2	2-BUTOXYETHANOL	C7H3CLF3NO2	4-CHLORO-3-NITROBENZOTRIFLUORIDE
C6H14O2-D5	1,2-DIETHOXYETHANE	C7H3CL2F3	2,4-DICHLOROBENZOTRIFLUORIDE
C6H14O2-D3	1,6-HEXANEDIOL	C7H3CL2NO	3,4-DICHLOROPHENYL-ISOCYANATE
C6H14O2-D4	HEXYLENE-GLYCOL	C7H4CLF3	P-CHLOROBENZOTRIFLUORIDE
C6H14O2S	DI-N-PROPYL-SULFONE	C7H4CL2O	M-CHLOROBENZOYL-CHLORIDE
C6H14O3-D1	DIETHYLENE-GLYCOL-DIMETHYL-ETHER	C7H4F3NO2	3-NITROBENZOTRIFLUORIDE
C6H14O3-D2	DIPROPYLENE-GLYCOL	C7H5CLO	BENZOYL-CHLORIDE
C6H14O3-D3	2-2-ETHOXYETHOXY-ETHANOL	C7H5CLO2	O-CHLOROBENZOIC-ACID
C6H14O3-D4	TRIMETHYLOLPROPANE	C7H5CL3	BENZOTRICHLORIDE
C6H14O4	TRIETHYLENE-GLYCOL	C7H5F3	BENZOTRIFLUORIDE
C6H14O6	SORBITOL	C7H5N	BENZONITRILE
C6H14S-D1	DI-N-PROPYL-SULFIDE	C7H5NO	PHENYL-ISOCYANATE
C6H14S-D3	ETHYL-T-BUTYL-SULFIDE	C7H5NS2	2-MERCAPTOBENZOTHIAZOLE
C6H14S	N-HEXYLMERCAPTAN	C7H5N3O6	2,4,6-TRINITROTOLUENE
C6H14S-D2	METHYL-T-PENTYL-SULFIDE	C7H5N5O8	TETRYL
C6H14S2	DI-N-PROPYLDISULFIDE	C7H5NAO2	SODIUM-BENZOATE
C6H15AL	TRIETHYL-ALUMINUM	C7H6CL2-D1	BENZYL-DICHLORIDE
C6H15AL2CL3	ETHYL-ALUMINUM-SESQUICHLORIDE	C7H6CL2	2,4-DICHLOROTOLUENE
C6H15N-D1	DIISOPROPYLAMINE	C7H6N2O4-E1	2,4-DINITROTOLUENE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C7H6N2O4-E2	2,5-DINITROTOLUENE	C7H9N-8	P-TOLUIDINE
C7H6N2O4-E3	2,6-DINITROTOLUENE	C7H10	2-NORBORNENE
C7H6N2O4-E4	3,4-DINITROTOLUENE	C7H10N2	TOLUENEDIAMINE
C7H6N2O4-E5	3,5-DINITROTOLUENE	C7H10O2	ALLYL-METHACRYLATE
C7H6O	BENZALDEHYDE	C7H11NO	CYCLOHEXYL-ISOCYANATE
C7H6O2	BENZOIC-ACID	C7H12	CYCLOHEPTENE
C7H6O2-E1	P-HYDROXY-BENZALDEHYDE	C7H12-D1	1-HEPTYNE
C7H6O2-D0	SALICYLALDEHYDE	C7H12O2-D1	N-BUTYL-ACRYLATE
C7H6O3	SALICYLIC-ACID	C7H12O2-D4	CYCLOHEXYL-FORMATE
C7H7BR	P-BROMOTOLUENE	C7H12O2	CYCLOPENTYLACETIC-ACID
C7H7CL-D1	BENZYL-CHLORIDE	C7H12O2-D2	ISOBUTYL-ACRYLATE
C7H7CL-D2	O-CHLOROTOLUENE	C7H12O2-D3	N-PROPYL-METHACRYLATE
C7H7CL-D3	P-CHLOROTOLUENE	C7H12O4	DIETHYL-MALONATE
C7H7NO	FORMANILIDE	C7H12O4-D1	PIMELIC-ACID
C7H7NO2-D1	M-NITROTOLUENE	C7H14-1	CYCLOHEPTANE
C7H7NO2-D2	O-NITROTOLUENE	C7H14-2	1,1-DIMETHYLCYCLOPENTANE
C7H7NO2-D3	P-NITROTOLUENE	C7H14-3	CIS-1,2-DIMETHYLCYCLOPENTANE
C7H7NO3	O-NITROANISOLE	C7H14-4	TRANS-1,2-DIMETHYLCYCLOPENTANE
C7H8	TOLUENE	C7H14-E2	CIS-1,3-DIMETHYLCYCLOPENTANE
C7H8SICL2	PHENYLMETHYLDICHLOROSILANE	C7H14-E3	TRANS-1,3-DIMETHYLCYCLOPENTANE
C7H8O-1	METHYL-PHENYL-ETHER	C7H14-5	ETHYLCYCLOPENTANE
C7H8O-2	BENZYL-ALCOHOL	C7H14-E7	2-ETHYL-1-PENTENE
C7H8O-4	M-CRESOL	C7H14-E8	3-ETHYL-1-PENTENE
C7H8O-3	O-CRESOL	C7H14-7	1-HEPTENE
C7H8O-5	P-CRESOL	C7H14-D1	CIS-2-HEPTENE
C7H8O2-E1	GUAIACOL	C7H14-E4	TRANS-2-HEPTENE
C7H8O2	P-METHOXYPHENOL	C7H14-D2	CIS-3-HEPTENE
C7H8O3S-D1	O-TOLUENESULFONIC-ACID	C7H14-E5	TRANS-3-HEPTENE
C7H8O3S	P-TOLUENESULFONIC-ACID	C7H14-6	METHYLCYCLOHEXANE
C7H8S	BENZYL-MERCAPTAN	C7H14-E9	2-METHYL-1-HEXENE
C7H9N-D1	BENZYLAMINE	C7H14-E10	3-METHYL-1-HEXENE
C7H9N-D2	2,6-DIMETHYLPYRIDINE	C7H14-E6	4-METHYL-1-HEXENE
C7H9N-5	METHYLPHENYLAMINE	C7H14-8	2,3,3-TRIMETHYL-1-BUTENE
C7H9N-7	M-TOLUIDINE	C7H14O	DIISOPROPYL-KETONE
C7H9N-6	O-TOLUIDINE	C7H14O-D1	1-HEPTANAL

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C7H14O-D2	2-HEPTANONE	C7H16O	1-HEPTANOL
C7H14O-E1	3-HEPTANONE	C7H16O-D0	2-HEPTANOL
C7H14O-E2	4-HEPTANONE	C7H16O-D1	ISOPROPYL-BUTYL-ETHER
C7H14O-D3	1-METHYLCYCLOHEXANOL	C7H16O-D2	ISOPROPYL-ISOBUTYL-ETHER
C7H14O-D4	CIS-2-METHYLCYCLOHEXANOL	C7H16O-E1	ISOHEPTANOL
C7H14O-D5	TRANS-2-METHYLCYCLOHEXANOL	C7H16O2	PG-1-TERT-BUTYL-ETHER
C7H14O-D6	CIS-3-METHYLCYCLOHEXANOL	C7H16O2-D1	PG-2-TERT-BUTYL-ETHER
C7H14O-D7	TRANS-3-METHYLCYCLOHEXANOL	C7H16O3-D1	DIETHYLENE-GLYCOL-PROPYL-ETHER
C7H14O-D8	CIS-4-METHYLCYCLOHEXANOL	C7H16O3	DPG-MONOMETHYL-ETHER
C7H14O-D9	TRANS-4-METHYLCYCLOHEXANOL	C7H16S	N-HEPTYL-MERCAPTAN
C7H14O-E3	2-METHYLHEXANAL	C7H17N	1-AMINOHEPTANE
C7H14O-E4	3-METHYLHEXANAL	C8H4CL2O2	ISOPHTHALOYL-CHLORIDE
C7H14O-D10	5-METHYL-2-HEXANONE	C8H4O3	PHTHALIC-ANHYDRIDE
C7H14O2-D1	N-BUTYL-PROPIONATE	C8H6	ETHYNYLBENZENE
C7H14O2-D2	ETHYL-ISOVALERATE	C8H6O2	TEREPHTHALDEHYDE
C7H14O2-D3	N-HEPTANOIC-ACID	C8H6O3	4-CARBOXYBENZALDEHYDE
C7H14O2-D8	N-HEXYL-FORMATE	C8H6O3-D1	2-FORMYL-BENZOIC-ACID
C7H14O2-D4	ISOPENTYL-ACETATE	C8H6O4-D1	ISOPHTHALIC-ACID
C7H14O2-D9	NEOHEPTANOIC-ACID	C8H6O4-D2	PHTHALIC-ACID
C7H14O2-D5	N-PENTYL-ACETATE	C8H6O4-D3	TEREPHTHALIC-ACID
C7H14O2-D6	N-PROPYL-N-BUTYRATE	C8H6S	BENZOTHIOPHENE
C7H14O2-D7	N-PROPYL-ISOBUTYRATE	C8H7N	INDOLE
C7H14O3	ETHYL-3-ETHOXYPROPIONATE	C8H7N-D1	PHENYLACETONITRILE
C7H15BR	1-BROMOHEPTANE	C8H8	STYRENE
C7H15N	N-METHYLCYCLOHEXYLAMINE	C8H8O	METHYL-PHENYL-KETONE
C7H16-4	2,2-DIMETHYLPENTANE	C8H8O-D1	4-HYDROXYSTYRENE
C7H16-5	2,3-DIMETHYLPENTANE	C8H8O-D2	O-TOLUALDEHYDE
C7H16-6	2,4-DIMETHYLPENTANE	C8H8O-D0	P-TOLUALDEHYDE
C7H16-7	3,3-DIMETHYLPENTANE	C8H8O2-D3	BENZYL-FORMATE
C7H16-8	3-ETHYLPENTANE	C8H8O2-D4	2-HYDROXYACETOPHENONE
C7H16-1	N-HEPTANE	C8H8O2-D5	4-HYDROXYACETOPHENONE
C7H16-2	2-METHYLHEXANE	C8H8O2	METHYL-BENZOATE
C7H16-3	3-METHYLHEXANE	C8H8O2-D1	O-TOLUIC-ACID
C7H16-9	2,2,3-TRIMETHYLBUTANE	C8H8O2-D2	P-TOLUIC-ACID
C7H16O-E2	ETHYL-TERT-PENTYL-ETHER	C8H8O3	METHYL-SALICYLATE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C8H8O3-D1	VANILLIN	C8H14O2	N-BUTYL-METHACRYLATE
C8H9NO	ACETANILIDE	C8H14O2-D2	CYCLOHEXYL-ACETATE
C8H9NO2	ACETAMINOPHEN	C8H14O2-D1	ISOBUTYL-METHACRYLATE
C8H10-4	ETHYLBENZENE	C8H14O3	BUTYRIC-ANHYDRIDE
C8H10-2	M-XYLENE	C8H14O4	DIETHYL-SUCCINATE
C8H10-1	O-XYLENE	C5H8O3-D3	DIETHYLENE-GLYCOL-MONOACRYLATE
C8H10-3	P-XYLENE	C8H14O4-D1	SUBERIC-ACID
C8H10N4O2	CAFFEINE	C8H16-D6	CYCLOOCTANE
C8H10O-3	P-ETHYLPHENOL	C8H16-1	1,1-DIMETHYLCYCLOHEXANE
C8H10O-D1	ALPHA-METHYLBENZYL-ALCOHOL	C8H16-2	CIS-1,2-DIMETHYLCYCLOHEXANE
C8H10O-4	PHENETOLE	C8H16-3	TRANS-1,2-DIMETHYLCYCLOHEXANE
C8H10O	2-PHENYLETHANOL	C8H16-4	CIS-1,3-DIMETHYLCYCLOHEXANE
C8H10O-D2	P-TOLUALCOHOL	C8H16-5	TRANS-1,3-DIMETHYLCYCLOHEXANE
C8H10O-5	2,3-XYLENOL	C8H16-6	CIS-1,4-DIMETHYLCYCLOHEXANE
C8H10O-6	2,4-XYLENOL	C8H16-7	TRANS-1,4-DIMETHYLCYCLOHEXANE
C8H10O-7	2,5-XYLENOL	C8H16-E1	2,3-DIMETHYL-1-HEXENE
C8H10O-8	2,6-XYLENOL	C8H16-8	ETHYLCYCLOHEXANE
C8H10O-9	3,4-XYLENOL	C8H16-D1	2-ETHYL-1-HEXENE
C8H10O-10	3,5-XYLENOL	C8H16-15	ISOPROPYLCYCLOPENTANE
C8H10O2	ETHYLBENZENE-HYDROPEROXIDE	C8H16-13	1-METHYL-1-ETHYLCYCLOPENTANE
C8H10O4	ETHYLENE-GLYCOL-DIACRYLATE	C8H16-E2	2-METHYL-1-HEPTENE
C8H11N	N,N-DIMETHYLANILINE	C8H16-16	1-OCTENE
C8H11N-D2	N-ETHYLANILINE	C8H16-D7	CIS-2-OCTENE
C8H11N-D0	O-ETHYLANILINE	C8H16-17	TRANS-2-OCTENE
C8H11N-D1	2,4,6-TRIMETHYLPYRIDINE	C8H16-D9	CIS-3-OCTENE
C8H11NO	P-PHENETIDINE	C8H16-D2	TRANS-3-OCTENE
C8H12-D1	1,5-CYCLOOCTADIENE	C8H16-D8	CIS-4-OCTENE
C8H12-D2	METHYLNORBORNENE	C8H16-D3	TRANS-4-OCTENE
C8H12	VINYLCYCLOHEXENE	C8H16-14	N-PROPYLCYCLOPENTANE
C8H12O4-E1	1,4-CYCLOHEXANEDICARBOXYLIC-ACID	C8H16-D4	2,4,4-TRIMETHYL-1-PENTENE
C8H12O4-E2	DIETHYL-MALEATE	C8H16-D5	2,4,4-TRIMETHYL-2-PENTENE
C8H14	CYCLOOCTENE	C8H16O	2-ETHYLHEXANAL
C8H14-D2	2,5-DIMETHYL-1,5-HEXADIENE	C8H16O-E1	1-OCTANAL
C8H14-D3	2,5-DIMETHYL-2,4-HEXADIENE	C8H16O-E2	2-OCTANONE
C8H14-D1	1-OCTYNE	C8H16O2-D1	N-BUTYL-N-BUTYRATE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C8H16O2	1,4-CYCLOHEXANEDIMETHANOL	C8H18O2-D1	2-HEXOXYETHANOL
C8H16O2-D6	2-ETHYL-HEXANOIC-ACID	C8H18O2-E2	2,2,4-TRIMETHYL-1,3-PENTANEDIOL
C8H16O2-D5	N-HEPTYL-FORMATE	C8H18O2S	DI-N-BUTYL-SULFONE
C8H16O2-D4	N-HEXYL-ACETATE	C8H18O3-D1	DIETHYLENE-GLYCOL-DIETHYL-ETHER
C8H16O2-D2	ISOBUTYL-ISOBUTYRATE	C8H18O3	DIETHYLENE-GLYCOL-MONOBUTYL-ETHE
C8H16O2-D3	N-OCTANOIC-ACID	C8H18O4-D1	TRIETHYLENE-GLYCOL-ETHYL-ETHER
C8H16O3	EG-MONOBUTYL-ETHER-ACETATE	C8H18O4	TRIETHYLENE-GLYCOL-DIMETHYL-ETHE
C8H16O4	2-2-ETHOXYETHOXY-ETHYL-ACETATE	C8H18SO4	DI-N-BUTYL-SULFATE
C8H18-5	2,2-DIMETHYLHEXANE	C8H18O5	TETRAETHYLENE-GLYCOL
C8H18-6	2,3-DIMETHYLHEXANE	C8H18S-D1	N-OCTYL-MERCAPTAN
C8H18-7	2,4-DIMETHYLHEXANE	C8H18S	TERT-OCTYLMERCAPTAN
C8H18-8	2,5-DIMETHYLHEXANE	C8H19N	DIBUTYLAMINE
C8H18-9	3,3-DIMETHYLHEXANE	C8H19N-D1	DIISOBUTYLAMINE
C8H18-10	3,4-DIMETHYLHEXANE	C8H19N-D0	N-OCTYLAMINE
C8H18-11	3-ETHYLHEXANE	C8H20PB	TETRAETHYL-LEAD
C8H18-16	2-METHYL-3-ETHYLPENTANE	C8H20SI	TETRAETHYL-SILANE
C8H18-17	3-METHYL-3-ETHYLPENTANE	C8H23N5	TETRAETHYLENEPENTAMINE
C8H18-2	2-METHYLHEPTANE	C8H24O4SI4	OCTAMETHYLCYCLOTETRASILOXANE
C8H18-3	3-METHYLHEPTANE	C9H4O5	TRIMELLITIC-ANHYDRIDE
C8H18-4	4-METHYLHEPTANE	C9H6N2O2	TOLUENE-DIISOCYANATE
C8H18-1	N-OCTANE	C9H6O6	TRIMELLITIC-ACID
C8H18	2,2,3,3-TETRAMETHYLBUTANE	C9H7N-D1	ISOQUINOLINE
C8H18-12	2,2,3-TRIMETHYLPENTANE	C9H7N-D2	QUINOLINE
C8H18-13	2,2,4-TRIMETHYLPENTANE	C9H7NO	8-HYDROXYQUINOLINE
C8H18-14	2,3,3-TRIMETHYLPENTANE	C9H8	INDENE
C8H18-15	2,3,4-TRIMETHYLPENTANE	C9H8O	2-METHYLBENZOFURAN
C8H18O-4	BUTYL-ETHER	C9H8O2	CINNAMIC-ACID
C8H18O-D1	DI-SEC-BUTYL-ETHER	C9H8O4	ACETYLSALICYLIC-ACID
C8H18O	DI-TERT-BUTYL-ETHER	C9H10-E1	INDANE
C8H18O-D2	DIISOBUTYL-ETHER	C9H10	ALPHA-METHYL-STYRENE
C8H18O-3	2-ETHYLHEXANOL	C9H10-E2	M-METHYL-STYRENE
C8H18O-D3	ETHYL-N-HEXYL-ETHER	C9H10-E3	O-METHYL-STYRENE
C8H18O-1	1-OCTANOL	C9H10-E4	P-METHYL-STYRENE
C8H18O-2	2-OCTANOL	C9H10-E5	CIS-1-PROPENYLBENZENE
C8H18O2	DI-T-BUTYL-PEROXIDE	C9H10-E6	TRANS-1-PROPENYLBENZENE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C9H10O2-D0	BENZYL-ACETATE	C9H18O-E1	2-NONANONE
C9H10O2	ETHYL-BENZOATE	C9H18O-E2	5-NONANONE
C9H10O3-D1	ACETOVANILLONE	C9H18O2-D1	N-BUTYL-VALERATE
C9H10O3	ETHYL-VANILLIN	C9H18O2-D3	N-HEPTYL-ACETATE
C9H11NO	P-DIMETHYLAMINOBENZALDEHYDE	C9H18O2	N-NONANOIC-ACID
C9H11NO2	L-PHENYLALANINE	C9H18O2-D2	N-OCTYL-FORMATE
C9H12-2	ISOPROPYLBENZENE	C9H18O3	TRIACETONE-ALCOHOL
C9H12	5-ETHYLIDENE-2-NORBORNENE	C9H18O4	DPG-MONOMETHYL-ETHER-ACETATE
C9H12-4	1-METHYL-3-ETHYLBENZENE	C9H20-5	3,3-DIETHYLPENTANE
C9H12-3	1-METHYL-2-ETHYLBENZENE	C9H20-E3	2,2-DIMETHYL-3-ETHYLPENTANE
C9H12-5	1-METHYL-4-ETHYLBENZENE	C9H20-E4	2,4-DIMETHYL-3-ETHYLPENTANE
C9H12-8	1,3,5-TRIMETHYLBENZENE	C9H20-E1	2,2-DIMETHYLHEPTANE
C9H12-1	N-PROPYLBENZENE	C9H20-E2	2,6-DIMETHYLHEPTANE
C9H12-6	1,2,3-TRIMETHYLBENZENE	C9H20-E5	3-ETHYLHEPTANE
C9H12-7	1,2,4-TRIMETHYLBENZENE	C9H20-D1	2-METHYLOCTANE
C9H12-D1	VINYLNORBORNENE	C9H20-D2	3-METHYLOCTANE
C9H12O	BENZYL-ETHYL-ETHER	C9H20-D3	4-METHYLOCTANE
C9H12O-D1	1-PHENYL-1-PROPANOL	C9H20-1	N-NONANE
C9H12O-D3	2-PHENYL-1-PROPANOL	C9H20-6	2,2,3,3-TETRAMETHYLPENTANE
C9H12O-D2	1-PHENYL-2-PROPANOL	C9H20-7	2,2,3,4-TETRAMETHYLPENTANE
C9H12O-E1	DIMETHYL-PHENYL-CARBINOL	C9H20-8	2,2,4,4-TETRAMETHYLPENTANE
C9H12O2	CUMENE-HYDROPEROXIDE	C9H20-9	2,3,3,4-TETRAMETHYLPENTANE
C9H14-D1	ETHYLNORBORNENE	C9H20-4	2,2,5-TRIMETHYLHEXANE
C9H14-D2	1-METHYL-4-VINYLCYCLOHEXENE	C9H20-D4	2,4,4-TRIMETHYLHEXANE
C9H14O	ISOPHORONE	C9H20O-D1	2,6-DIMETHYL-4-HEPTANOL
C9H14O6	GLYCERYL-TRIACETATE	C9H20O-D2	1-NONANOL
C9H15N	TRIALLYLAMINE	C9H20O-E1	2-NONANOL
C9H16O4	AZELAIC-ACID	C9H20O4	TRIPROPYLENE-GLYCOL
C9H18-D1	N-BUTYLCYCLOPENTANE	C9H20S	N-NONYL-MERCAPTAN
C9H18-2	ISOPROPYLCYCLOHEXANE	C9H20S-D1	TERT-NONYL-MERCAPTAN
C9H18-3	1-NONENE	C9H21N-D1	N-NONYLAMINE
C9H18-1	N-PROPYLCYCLOHEXANE	C9H21N-D2	TRIPROPYLAMINE
C9H18	1-TRANS-3,5-TRIMETHYLCYCLOHEXANE	C10H6O8	PYROMELLITIC-ACID
C9H18O-D1	DIISOBUTYL-KETONE	C10H7BR	1-BROMONAPHTHALENE
C9H18O	1-NONANAL	C10H7CL	1-CHLORONAPHTHALENE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C10H8	NAPHTHALENE	C10H14-E10	1-METHYL-4-N-PROPYLBENZENE
C10H9N	QUINALDINE	C10H14-E7	1,2,3,4-TETRAMETHYL-BENZENE
C10H10-D1	M-DIVINYLBENZENE	C10H14-E6	1,2,3,5-TETRAMETHYL-BENZENE
C10H10-D2	1-METHYLINDENE	C10H14-9	1,2,4,5-TETRAMETHYLBENZENE
C10H10-D3	2-METHYLINDENE	C10H14O	P-TERT-BUTYLPHENOL
C10H10O4-D3	DIMETHYL-ISOPHTHALATE	C10H14O2	P-TERT-BUTYLCATECHOL
C10H10O4-D1	O-DIMETHYL-PHTHALATE	C10H14O5	2-ACETOACETOXY-ETHYL-METHACRYLAT
C10H10O4-D2	DIMETHYL-TEREPHTHALATE	C10H15N-E1	N,N-DIETHYLANILINE
C10H11NO2	ACETOACETANILIDE	C10H15N-E2	2,6-DIETHYLANILINE
C10H12-D0	DICYCLOPENTADIENE	C10H16-D5	ADAMANTANE
C10H12-E1	2-PHENYLBUTENE-1	C10H16-E1	CAMPHENE
C10H12-E2	CIS-2-PHENYLBUTENE-2	C10H16-D1	D-LIMONENE
C10H12-E3	TRANS-2-PHENYLBUTENE-2	C10H16-E2	ALPHA-PHELLANDRENE
C10H12	1,2,3,4-TETRAHYDRONAPHTHALENE	C10H16-E3	BETA-PHELLANDRENE
C10H12O	ANETHOLE	C10H16-D2	ALPHA-PINENE
C10H12O2	N-PROPYL-BENZOATE	C10H16-D3	BETA-PINENE
C10H12O4	DIALLYL-MALEATE	C10H16-E4	ALPHA-TERPINENE
C10H14-1	N-BUTYLBENZENE	C10H16-E5	GAMMA-TERPINENE
C10H14-3	SEC-BUTYLBENZENE	C10H16-D4	TERPINOLENE
C10H14-4	TERT-BUTYLBENZENE	C10H16N2O8	ETHYLENEDIAMINETETRAACETIC-ACID
C10H14-6	1-METHYL-3-ISOPROPYLBENZENE	C10H16O	CAMPHOR
C10H14-5	1-METHYL-2-ISOPROPYLBENZENE	C10H16O4-D1	DIMETHYL-1,4-CYCLOHEXANEDICARBOX
C10H14-7	1-METHYL-4-ISOPROPYLBENZENE	C10H16O4	DIPROPYL-MALEATE
C10H14-D1	M-DIETHYLBENZENE	C10H18-1	CIS-DECALIN
C10H14-D2	O-DIETHYLBENZENE	C10H18-2	TRANS-DECALIN
C10H14-8	1,4-DIETHYLBENZENE	C10H18O4	SEBACIC-ACID
C10H14-E1	2-ETHYL-M-XYLENE	C10H19O6PS2	MALATHION
C10H14-E2	2-ETHYL-P-XYLENE	C10H20-1	N-BUTYLCYCLOHEXANE
C10H14-D3	1,2-DIMETHYL-3-ETHYLBENZENE	C10H20-5	1-DECENE
C10H14-E3	4-ETHYL-M-XYLENE	C10H20-D1	CIS-2-DECENE
C10H14-E4	4-ETHYL-O-XYLENE	C10H20-D2	TRANS-2-DECENE
C10H14-E5	5-ETHYL-M-XYLENE	C10H20-D3	1,1-DIETHYLCYCLOHEXANE
C10H14-2	ISOBUTYLBENZENE	C10H20-D4	1,2,3,4-TETRAMETHYLCYCLOHEXANE
C10H14-E8	1-METHYL-2-N-PROPYLBENZENE	C10H20O	1-DECANAL
C10H14-E9	1-METHYL-3-N-PROPYLBENZENE	C10H20O-D1	L-MENTHOL

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C10H20O2-D1	N-DECANOIC-ACID	C10H30SI5O5	DECAMETHYLCYCLOPENTASILOXANE
C10H20O2-D2	2-ETHYLHEXYL-ACETATE	C11H10-1	1-METHYLNAPHTHALENE
C10H20O2-D3	ISOPENTYL-ISOVALERATE	C11H10-2	2-METHYLNAPHTHALENE
C10H20O2	P-MENTHANE-HYDROPEROXIDE	C11H12	P-ISOPROPENYLSTYRENE
C10H20O2-D5	N-NONYL-FORMATE	C11H14O2	BUTYL-BENZOATE
C10H20O2-D4	N-OCTYL-ACETATE	C11H16-D1	1-ETHYL-2-ISOPROPYLBENZENE
C10H20O4	DIGLYCOL-MONOBUTYL-ETHER-ACETATE	C11H16-D2	PENTAMETHYLBENZENE
C10H22-1	N-DECANE	C11H16	N-PENTYLBENZENE
C10H22-E1	2,2-DIMETHYL-OCTANE	C11H16O	P-TERT-AMYLPHENOL
C10H22-D1	2,3-DIMETHYLOCTANE	C11H20O2	2-ETHYLHEXYL-ACRYLATE
C10H22-D2	2,4-DIMETHYLOCTANE	C11H22-2	1-UNDECENE
C10H22-D3	2,5-DIMETHYLOCTANE	C11H22O	1-UNDECANAL
C10H22-D4	2,6-DIMETHYLOCTANE	C11H22O2-D1	N-DECYL-FORMATE
C10H22-D5	2,7-DIMETHYLOCTANE	C11H22O2-D2	METHYL-DECANOATE
C10H22-E2	2-METHYLNONANE	C11H22O2	N-NONYL-ACETATE
C10H22-E3	3-METHYLNONANE	C11H22O2-D3	N-UNDECANOIC-ACID
C10H22-E4	4-METHYLNONANE	C11H24	N-UNDECANE
C10H22-E5	5-METHYLNONANE	C11H24O	1-UNDECANOL
C10H22-3	2,2,3,3-TETRAMETHYLHEXANE	C11H24S	UNDECYL-MERCAPTAN
C10H22-4	2,2,5,5-TETRAMETHYLHEXANE	C11H25N	UNDECYLAMINE
C10H22-2	3,3,5-TRIMETHYLHEPTANE	C12H6N2O2	1,5-NAPHTHALENE-DIISOCYANATE
C10H22O	1-DECANOL	C12H8	ACENAPHTHALENE
C10H22O-D1	DI-N-PENTYL-ETHER	C12H8O	DIBENZOFURAN
C10H22O-D0	ISODECANOL	C12H8S	DIBENZOTHIOPHENE
C10H22O2	ETHYLENE-GLYCOL-2-ETHYLHEXYL-ETH	C12H9N	DIBENZOPYRROLE
C10H22O3-E1	DIPROPYLENE-GLYCOL-T-BUTYL-ETHER	C12H9N3O4	4,4-DINITRODIPHENYLAMINE
C10H22O3-D1	2-2-HEXOXYETHOXY-ETHANOL	C12H10-D0	ACENAPHTHENE
C10H22O4-D1	TRIETHYLENE-GLYCOL-BUTYL-ETHER	C12H10	DIPHENYL
C10H22O4	TRIPROPYLENE-GLYCOL-MONOMETHYL-E	C12H10N2O2-A	O-NITRODIPHENYLAMINE
C10H22O5	TETRAETHYLENE-GLYCOL-DIMETHYL-ET	C12H10N2O2-B	P-NITRODIPHENYLAMINE
C10H22S	N-DECYL-MERCAPTAN	C12H10O	DIPHENYL-ETHER
C10H23N	N-DECYLAMINE	C12H11N-D1	P-AMINODIPHENYL
C10H23N-D1	DIAMYLAMINE	C12H11N	DIPHENYLAMINE
C10H24N2	N,N-DI-TERT-BUTYLETHYLENEDIAMINE	C12H11N3-E1	P-AMINOAZOBENZENE
C10H30SI4O3	DECAMETHYLTETRASILOXANE	C12H11N3-E2	1,3-DIPHENYLTRIAZENE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C12H12-E1	2,6-DIMETHYLNAPHTHALENE	C12H26O3	DIETHYLENE-GLYCOL-DI-N-BUTYL-ETH
C12H12-E2	2,7-DIMETHYLNAPHTHALENE	C12H26S	N-DODECYL-MERCAPTAN
C12H12-E3	1-ETHYLNAPHTHALENE	C12H26S-E1	TERT-DODECYL-MERCAPTAN
C12H12-E4	2-ETHYLNAPHTHALENE	C12H27BO3	TRI-N-BUTYL-BORATE
C12H12N2-D1	P-AMINODIPHENYLAMINE	C12H27N-D0	DODECYLAMINE
C12H12N2-D3	BENZIDINE	C12H27N	TRIBUTYLAMINE
C12H12N2-D2	HYDRAZOBENZENE	C12H36SI6O6	DODECAMETHYLCYCLOHEXASILOXANE
C12H14	1,2,3-TRIMETHYLINDENE	C13H9N	ACRIDINE
C12H14O4	DIETHYL-PHTHALATE	C13H10	FLUORENE
C12H14O6	BIS-2-HYDROXYETHYL-TEREPHTHALATE	C13H10O	BENZOPHENONE
C12H16-D1	P-TERT-BUTYLSTYRENE	C13H12	DIPHENYLMETHANE
C12H16	CYCLOHEXYLBENZENE	C13H14	1-N-PROPYLNAPHTHALENE
C12H16-D2	4-ISOBUTYLSTYRENE	C13H18O2	IBUPROFEN
C12H18-D4	P-TERT-BUTYL-ETHYLBENZENE	C13H20	N-HEPTYLBENZENE
C12H18-D5	1,5,9-CYCLODODECATRIENE	C13H26-2	1-TRIDECENE
C12H18-D1	M-DIISOPROPYLBENZENE	C13H26O	1-TRIDECANAL
C12H18-D2	P-DIISOPROPYLBENZENE	C13H26O2-D1	N-BUTYL-NONANOATE
C12H18-D7	HEXAMETHYLBENZENE	C13H26O2	METHYL-DODECANOATE
C12H18-D3	N-HEXYLBENZENE	C13H26O2-D2	N-TRIDECANOIC-ACID
C12H18-D8	1,2,3-TRIETHYLBENZENE	C13H28	N-TRIDECANE
C12H18-D6	1,2,4-TRIETHYLBENZENE	C13H28O	1-TRIDECANOL
C12H18O2	M-DIISOPROPYL-BENZENE-HYDROPEROX	C14H8O2	ANTHRAQUINONE
C12H18O2-D1	P-DIISOPROPYLBENZ-HYDROPEROXIDE	C14H10-1	ANTHRACENE
C12H20O	2-CYCLOHEXYL-CYCLOHEXANONE	C14H10	DIPHENYLACETYLENE
C12H20O4	DIBUTYL-MALEATE	C14H10-2	PHENANTHRENE
C12H22	BICYCLOHEXYL	C14H10O4	BENZOYL-PEROXIDE
C12H22O11	SUCROSE	C14H12-D1	CIS-STILBENE
C12H23N	DICYCLOHEXYLAMINE	C14H12-D2	TRANS-STILBENE
C12H24-2	1-DODECENE	C14H12O2	BENZYL-BENZOATE
C12H24O	1-DODECANAL	C14H14-D1	1,1-DIPHENYLETHANE
C12H24O2-E1	N-DECYL-ACETATE	C14H14-D2	1,2-DIPHENYLETHANE
C12H24O2	N-DODECANOIC-ACID	C14H14O	DIBENZYL-ETHER
C12H26	N-DODECANE	C14H16	1-N-BUTYLNAPHTHALENE
C12H26O-1	DIHEXYLETHER	C14H16-D1	2,6-DIETHYLNAPHTHALENE
C12H26O-2	DODECANOL	C14H18O4	DIPROPYL-PHTHALATE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C14H20	DIAMANTANE	C16H34-D1	2,2,4,4,6,8,8-HEPTAMETHYLNONANE
C14H22	N-OCTYLBENZENE	C16H34	N-HEXADECANE
C14H22-D1	1,2,3,5-TETRAETHYLBENZENE	C16H34O-D1	DI-N-OCTYL-ETHER
C14H22O	P-TERT-OCTYLPHENOL	C16H34O	1-HEXADECANOL
C14H28-2	1-TETRADECENE	C17H28	N-UNDECYLBENZENE
C14H28O2	N-TETRADECANOIC-ACID	C17H34-D1	1-HEPTADECENE
C14H30	N-TETRADECANE	C17H34O2	N-HEPTADECANOIC-ACID
C14H30O	1-TETRADECANOL	C17H34O2-D1	ISOPROPYL-MYRISTATE
C14H31N	TETRADECYLAMINE	C17H36	N-HEPTADECANE
C14H42SI6O5	TETRADECAMETHYLHEXASILOXANE	C17H36O	HEPTADECANOL
C15H10N2O2	DIPHENYLMETHANE-4,4-DIISOCYANATE	C18H12	CHRYSENE
C15H12	1-PHENYLINDENE	C18H13N3O4	4,4-DINITROTRIPHENYLAMINE
C15H16O	P-CUMYLPHENOL	C18H14-2	M-TERPHENYL
C15H16O2	BISPHENOL-A	C18H14-1	O-TERPHENYL
C15H18	1-N-PENTYLNAPHTHALENE	C18H14-3	P-TERPHENYL
C15H24	N-NONYLBENZENE	C18H15PO	TRIPHENYLPHOSPHINE-OXIDE
C15H24O-D1	2,6-DI-TERT-BUTYL-P-CRESOL	C18H15O4P	TRIPHENYL-PHOSPHATE
C15H24O-D2	NONYLPHENOL	C18H15P	TRIPHENYLPHOSPHINE
C15H30-2	1-PENTADECENE	C18H16N2	N-N-DIPHENYL-P-PHENYLENEDIAMINE
C15H30O2	PENTADECANOIC-ACID	C18H20	2,4-DIPHENYL-4-METHYLPENTENE-1
C15H32	N-PENTADECANE	C18H22	2,3-DIMETHYL-2,3-DIPHENYLBUTANE
C15H32O	1-PENTADECANOL	C18H22O2	DICUMYLPEROXIDE
C15H33N	TRIAMYLAMINE	C18H30	N-DODECYLBENZENE
C16H10-D1	FLUORANTHENE	C18H30O2	LINOLENIC-ACID
C16H10-D2	PYRENE	C18H32O2	LINOLEIC-ACID
C16H12	1-PHENYLNAPHTHALENE	C18H34O2	OLEIC-ACID
C16H18	1-4-ETHYLPHENYL-2-PHENYLETHANE	C18H34O4-D1	DIBUTYL-SEBACATE
C16H20	1-N-HEXYLNAPHTHALENE	C18H34O4-D2	DIHEXYL-ADIPATE
C16H22O4	DIBUTYL-O-PHTHALATE	C18H36-1	1-OCTADECENE
C16H22O4-D1	DIISOBUTYL-PHTHALATE	C18H36O2	STEARIC-ACID
C16H24	1-N-HEXYL-1,2,3,4-TETRAHYDRONAPH	C18H38	N-OCTADECANE
C16H26	N-DECYLBENZENE	C18H38O-D0	DINONYL-ETHER
C16H32-1	N-DECYLCYCLOHEXANE	C18H38O	1-OCTADECANOL
C16H32-2	1-HEXADECENE	C19H16	TRIPHENYLMETHANE
C16H32O2	N-HEXADECANOIC-ACID	C19H26	1-N-NONYLNAPHTHALENE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C19H32	N-TRIDECYLBENZENE	C25H52	N-PENTACOSANE
C19H36O2	METHYL-OLEATE	C26H20	TETRAPHENYLETHYLENE
C19H38-D1	1-NONADECENE	C26H22	1,1,2,2-TETRAPHENYLETHANE
C19H38O2	NONADECANOIC-ACID	C26H42O4	DI-N-NONYL-PHTHALATE
C19H40	N-NONADECANE	C26H54	N-HEXACOSANE
C19H40O	1-NONADECANOL	C27H46O	BETA-CHOLESTEROL
C20H16	TRIPHENYLETHYLENE	C27H56	N-HEPTACOSANE
C20H18	1,1,2-TRIPHENYLETHANE	C28H46O4	DIISODECYL-PHTHALATE
C20H28	1-N-DECYLNAPHTHALENE	C28H58	N-OCTACOSANE
C20H30O2	ABIETIC-ACID	C29H60	N-NONACOSANE
C20H31N	DEHYDROABIETYLAMINE	C30H62-D1	SQUALANE
C20H34	N-TETRADECYLBENZENE	C30H62	N-TRIACONTANE
C20H37NAO7S	DIOCTYLSODIUM-SULFOSUCCINATE	C32H66	N-DOTRIACONTANE
C20H38O2	CETYL-METHACRYLATE	C36H74	N-HEXATRIACONTANE
C20H40-D1	1-EICOSENE	CA	CALCIUM
C20H40O2	N-EICOSANIC-ACID	CACL2	CALCIUM-CHLORIDE
C20H42	N-EICOSANE	CACL2O2	CALCIUM-HYPOCHLORITE
C20H42O	1-EICOSANOL	CAF2	CALCIUM-FLUORIDE
C21H21O4P	TRI-O-CRESYL-PHOSPHATE	CA(OH)2	CALCIUM-HYDROXIDE
C21H36	N-PENTADECYLBENZENE	CAO	CALCIUM-OXIDE
C21H44	N-HENEICOSANE	CASO4	CALCIUM-SULFATE
C22H34O4	DIHEPTYL-PHTHALATE	CUCL	CUPROUS-CHLORIDE
C22H38	N-HEXADECYLBENZENE	CLO3F	PERCHLORYL-FLUORIDE
C22H42O4	DI-2-ETHYLHEXYL-ADIPATE	HCL	HYDROGEN-CHLORIDE
C22H44O2	N-BUTYL-STEARATE	HCLO	HYPOCHLOROUS-ACID
C22H46	N-DOCOSANE	CLHO3S	CHLOROSULFONIC-ACID
C23H40	N-HEPTADECYLBENZENE	HCLO4	PERCHLORIC-ACID
C23H48	N-TRICOSANE	NH4CL	AMMONIUM-CHLORIDE
C24H38O4-D1	DIISOOCTYL-PHTHALATE	CLH4NO	HYDROXYLAMINE-HYDROCHLORIDE
C24H38O4	DIOCTYL-PHTHALATE	NH4CLO4	AMMONIUM-PERCHLORATE
C24H38O4-D2	DIOCTYL-TEREPHTHALATE	KCL	POTASSIUM-CHLORIDE
C24H42	N-OCTADECYLBENZENE	NOCL	NITROSYL-CHLORIDE
C24H42O	DINONYLPHENOL	NACL	SODIUM-CHLORIDE
C24H50	N-TETRACOSANE	NACLO	SODIUM-HYPOCHLORITE
C25H20	TETRAPHENYLMETHANE	NACLO3	SODIUM-CHLORATE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
CLO2	CHLORINE-DIOXIDE	FECL2	FERROUS-CHLORIDE
KCLO3	POTASSIUM-CHLORATE	FECL3	FERRIC-CHLORIDE
CL2	CHLORINE	FEO	FERROUS-OXIDE
CUCL2	CUPRIC-CHLORIDE	FESO4	FERROUS-SULFATE
SIH2CL2	DICHLOROSILANE	FE2O3	FERRIC-OXIDE
SOCL2	THIONYL-CHLORIDE	GE	GERMANIUM
SO2CL2	SULFURYL-CHLORIDE	GEH4	GERMANIUM-TETRAHYDRIDE
SCL2	SULFUR-DICHLORIDE	HI	HYDROGEN-IODIDE
GACL3	GALLIUM-TRICHLORIDE	KOH	POTASSIUM-HYDROXIDE
SIHCL3	TRICHLOROSILANE	K2HPO4	DIPOTASSIUM-PHOSPHATE
NCL3	NITROGEN-TRICHLORIDE	HNO2	NITROUS-ACID
POCL3	PHOSPHORUS-OXYCHLORIDE	HNO3	NITRIC-ACID
VCL3O	VANADIUM-OXYTRICHLORIDE	HNO5S	NITROSYLSULFURIC-ACID
PCL3	PHOSPHORUS-TRICHLORIDE	NAOH	SODIUM-HYDROXIDE
PSCL3	PHOSPHORUS-THIOCHLORIDE	NAHSO3	SODIUM-BISULFITE
SBCL3	ANTIMONY-TRICHLORIDE	NAHSO4	SODIUM-BISULFATE
TICL3	TITANIUM-TRICHLORIDE	NA2HPO4	DISODIUM-PHOSPHATE
SICL4	SILICON-TETRACHLORIDE	H2	HYDROGEN
TICL4	TITANIUM-TETRACHLORIDE	H2-PARA	HYDROGEN-PARA
VCL4	VANADIUM-TETRACHLORIDE	NANH2	SODIUM-AMIDE
PCL5	PHOSPHORUS-PENTACHLORIDE	NAH2PO4	MONOSODIUM-PHOSPHATE
CRO3	CHROMIUM-TRIOXIDE	H2O	WATER
NA2CR2O7	SODIUM-DICHROMATE	H2O2	HYDROGEN-PEROXIDE
CUSO4	CUPRIC-SULFATE	H2SO4	SULFURIC-ACID
D2	DEUTERIUM	H2S	HYDROGEN-SULFIDE
D2O	DEUTERIUM-OXIDE	H2SE	HYDROGEN-SELENIDE
HF	HYDROGEN-FLUORIDE	H3N	AMMONIA
FHO3S	FLUOROSULFONIC-ACID	H3NO	HYDROXYLAMINE
NAF	SODIUM-FLUORIDE	H3NO3S	SULFAMIC-ACID
F2	FLUORINE	H3PO2	HYPOPHOSPHOROUS-ACID
NF3	NITROGEN-TRIFLUORIDE	H3PO3	PHOSPHOROUS-ACID
N2F4	TETRAFLUOROHYDRAZINE	H3PO4	ORTHOPHOSPHORIC-ACID
SIF4	SILICON-TETRAFLUORIDE	PH3	PHOSPHINE
SF6	SULFUR-HEXAFLUORIDE	H4N2	HYDRAZINE
FE	IRON	NH4NO3	AMMONIUM-NITRATE

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
SIH4	SILANE	NA2S2O4	SODIUM-HYDROSULFITE
NH4OH	AMMONIUM-HYDROXIDE	NA2S	SODIUM-SULFIDE
NH5SO3	AMMONIUM-BISULFITE	NA3PO4	TRISODIUM-PHOSPHATE
NH4HSO4	AMMONIUM-BISULFATE	NA4P2O7	TETRASODIUM-PYROPHOSPHATE
NH6PO4	AMMONIUM-PHOSPHATE	NA5P3O10	SODIUM-TRIPOLYPHOSPHATE
SI2H6	DISILANE	NA6P6O18	SODIUM-HEXAMETAPHOSPHATE
N2H8SO3	AMMONIUM-SULFITE	NE	NEON
(NH4)2SO4	AMMONIUM-SULFATE	ZNO	ZINC-OXIDE
(NH4)2HPO4	DIAMMONIUM-PHOSPHATE	O2	OXYGEN
HE-3	HELIUM-3	O2S	SULFUR-DIOXIDE
HE-4	HELIUM-4	SIO2	SILICON-DIOXIDE
HG	MERCURY	TIO2	TITANIUM-OXIDE(RUTILE)
KI	POTASSIUM-IODIDE	O3	OZONE
NAI	SODIUM-IODIDE	O3S	SULFUR-TRIOXIDE
I2	IODINE	ZNSO4	ZINC-SULFATE
K	POTASSIUM	(P2O5)2	PHOSPHORUS-PENTOXIDE(DIMERIC)
KR	KRYPTON	P	PHOSPHORUS-WHITE
LI	LITHIUM	P4S10	PHOSPHORUS-PENTASULFIDE
MG(NO3)2	MAGNESIUM-NITRATE	S	SULFUR
MGO	PERICLASE	SI	SILICON
MGSO4	MAGNESIUM-SULFATE	V	VANADIUM
NANO2	SODIUM-NITRITE	XE	XENON
NANO3	SODIUM-NITRATE	ZN	ZINC
NO	NITRIC-OXIDE	CH6N2	METHYL-HYDRAZINE
NO2	NITROGEN-DIOXIDE	C4H6O4-1	DIMETHYL-OXALATE
N2	NITROGEN	C6F12	PERFLUOROCYCLOHEXANE
N2O	NITROUS-OXIDE	C6F14	PERFLUORO-N-HEXANE
N2O3	NITROGEN-TRIOXIDE	C7F14	PERFLUOROMETHYLCYCLOHEXANE
N2O4	NITROGEN-TETROXIDE	C7F16	PERFLUORO-N-HEPTANE
N2O5	NITROGEN-PENTOXIDE	C7H9N-1	2,3-DIMETHYLPYRIDINE
NA	SODIUM	C7H9N-2	2,5-DIMETHYLPYRIDINE
NA2O2	SODIUM-PEROXIDE	C7H9N-3	3,4-DIMETHYLPYRIDINE
NA2S2O3	SODIUM-THIOSULFATE	C7H9N-4	3,5-DIMETHYLPYRIDINE
NA2SIO3	SODIUM-SILICATE	C8H10O-1	O-ETHYLPHENOL
NA2SO4	SODIUM-SULFATE	C8H10O-2	M-ETHYLPHENOL

continued

Table 1.9 Components Available in the PURE10 Database (continued)

Alias	Component Name	Alias	Component Name
C8H16-9	1,1,2-TRIMETHYLCYCLOPENTANE	C11H22-1	N-HEXYLCYCLOPENTANE
C8H16-10	1,1,3-TRIMETHYLCYCLOPENTANE	C12H24-1	N-HEPTYLCYCLOPENTANE
C8H16-11	CIS,CIS,TRANS-1,2,4-TRIMETHYLCYC	C13H26-1	N-OCTYLCYCLOPENTANE
C8H16-12	CIS,TRANS,CIS-1,2,4-TRIMETHYLCYC	C14H28-1	N-NONYLCYCLOPENTANE
C9H20-2	2,2,3-TRIMETHYLHEXANE	C15H30-1	N-DECYLCYCLOPENTANE
C9H20-3	2,2,4-TRIMETHYLHEXANE	C17H34	N-DODECYLCYCLOPENTANE
C10H15N	N-BUTYLANILINE	C18H36-2	N-TRIDECYLCYCLOPENTANE
C10H19N	CAPRINITRILE	C19H38	N-TETRADECYLCYCLOPENTANE
C10H20-2	ISOBUTYLCYCLOHEXANE	C20H40	N-PENTADECYLCYCLOPENTANE
C10H20-3	SEC-BUTYLCYCLOHEXANE	C21H42	N-HEXADECYLCYCLOPENTANE
C10H20-4	TERT-BUTYLCYCLOHEXANE	C21H42	N-HEXADECYLCYCLOPENTANE

Table 1.9 Components Available in the PURE10 Database for Heating Fluids

Alias	Component Name	Alias	Component Name
CALFLO-AF	CALFLO-AF	R502	REFRIGERANT-502
CALFLO-HTF	CALFLO-HTF	SHELL15	SHELL15
CACL2-15	CALCIUM-CHLORIDE-15-WT-%	SHELL33	SHELL33
CACL2-25	CALCIUM-CHLORIDE-25-WT%	SYL800	SYLTHERM-800
CHEM550	CHEMTHERM-550	SYL-XLT	SYLTHERM-XLT
DEGLY-20	DIETHLENE-GLYCOL-20-WT-%	SYN350	SYNTREL-350
DEGLY-40	DIETHYLENE-GLYCOL-40-WT-%	THERMVP1	THERMINOL-VP-1
DEGLY-80	DIETHLENE-GLYCOL-80-WT-%	TEGLY-L	TEGLY-L
DEGLY-60	DIETHYLENE-GLYCOL-60-WT-%	TEGLY-40	TRIETHYLENE-GLYCOL-40-WT-%
DOWA	DOWTHERM-A	TEGLY-80	TRIETHYLENE-GLYCOL-80-WT-%
DOWG	DOWTHERM-G	THERMFG1	THERMFG1
DOWJ	DOWTHERM-J	THERM550	THERMALANE-550-(FG-1)
EGLY-20	ETHYLENE-GLYCOL-20-WT-%	THERM800	THERMALANE-800
EGLY-40	ETHYLENE-GLYCOL-40-WT-%	THERM600	THERMALANE-600
EGLY-60	ETHYLENE-GLYCOL-60-WT-%	THERMFR1	THERMINOL-FR-1
MARLO-S	MARLOTHERM-S	THERMFR2	THERMINOL-FR-2
MBL605	MOBILTHERM-605	THERMFR3	THERMINOL-FR-3
MBLLIGHT	MOBILTHERM-LIGHT	THERM55	THERMINOL-55

Continued

Table 1.9 Components Available in the PURE10 Database for Heating Fluids (continued)

Alias	Component Name	Alias	Component Name
MBL603	MOBILTHERM-603	THERM66	THERMINOL-66
PGLY-20	PROPYLENE-GLYCOL-20-WT-%	THERM77	THERMINOL-77
PGLY-60	PROPYLENE-GLYCOL-60-WT-%	THERM44	THERMINOL-44
R503	REFRIGERANT-503	THERM60	THERMINOL-60
R123	REFRIGERANT-123	THERMFR0	THERMINOL-FR-0

Table 1.9A Parameters Available in the PURE93 Databank

Parameter Name	Description
AIT †	Auto ignition temperature
ANILPT	Aniline point
API	Standard API gravity at 60°F
ATOMNO ††	Atomic number of each atom in the compound
CPDIEC	Dielectric constant
CPIGDP	DIPPR ideal gas heat capacity coefficients
CPLDIP	DIPPR liquid heat capacity coefficients
CPSDIP	DIPPR solid heat capacity coefficients
DCPLS	Difference between liquid and solid heat capacity at
DELTA	Solubility parameter at 298.2 K
DGFORM	Standard Gibbs free energy of formation; ideal gas at
DHFORM	Standard heat of formation; ideal gas at 298.2 K
DHVLB	Heat of vaporization at TB
DHVLDP	DIPPR heat of vaporization coefficients
DNLDIP	DIPPR liquid density coefficients
DNSDIP	DIPPR solid density coefficients
ENT †	Absolute entropy of formation at 298.2 K
FLML †	Lower flammability limit
FLMU †	Upper flammability limit
FP	Flash point
GMUQQ	UNIQUAC area parameter
GMUQR	UNIQUAC volume parameter
HCOM	Standard enthalpy of combustion at 298.2 K
HFUS	Enthalpy of fusion at melting point
KLDIP	DIPPR liquid thermal conductivity coefficients
KVDIP	DIPPR vapor thermal conductivity coefficients
MOCTNO	Motor octane number
MULDIP	DIPPR liquid viscosity coefficients
MUP	Dipole moment
MUVDIP	DIPPR vapor viscosity coefficients
MW	Molecular weight

† *These parameters are not used in Aspen Plus models but can be accessed by user or in-house models.*

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

continued

Table 1.9A Parameters Available in the PURE93 Databank (continued)

Parameter Name	Description
NOATOM††	Number of occurrences of each atom
NTHA	Nothnagel parameters
OMEGA	Pitzer acentric factor
OMGCTD	Acentric factor for the COSTALD model
PC	Critical pressure
PLXANT	Extended Antoine vapor pressure coefficients
PRMCP	Mathias-Copeman parameters for PR equation of state
PRSRP	Schwartzentruber-Renon parameters for PR equation of
RGYR	Radius of gyration
RI	Refractive index at 298.2 K
RKSMCP	Mathias-Copeman parameters for RKS equation of state
RKSSRP	Schwartzentruber-Renon parameters for RKS equation of
RKTZRA	Rackett liquid density parameter
ROCTNO	Research octane number
SG	Standard specific gravity at 60°F
SIGDIP	DIPPR surface tension coefficients
SVRDIP†	Second virial coefficient
TB	Normal boiling point
TC	Critical temperature
TFP	Normal freezing point
TPP†	Triple point pressure
TPT	Triple point temperature
UFGRP†††	Functional group information for the UNIFAC model
UFGRPD†††	Functional group information for the Dortmund modified
UFGRPL†††	Functional group information for the Lyngby modified
VB	Liquid molar volume at TB
VC	Critical volume
VLCVT1	Scatchard-Hildebrand volume parameter
VLSTD	Standard liquid volume at 60°F
VSTCTD	Characteristic volume for the COSTALD model
WATSOL	Water solubility correlation coefficients
ZC	Critical compressibility factor

† *These parameters are not used in Aspen Plus models but can be accessed by user or in-house models.*

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

††† *Contains functional group number and number of occurrences of each group.*

Table 1.9B Components Available in the PURE93 Databank

Alias	Component Name	Alias	Component Name
AIR	AIR	CF4	CARBON-TETRAFLUORIDE
AG	SILVER	CHBR3	TRIBROMOMETHANE
AL	ALUMINUM	CHCLF2	CHLORODIFLUOROMETHANE
ALCL3	ALUMINUM-CHLORIDE	CHCL2F	DICHLOROMONOFLUOROMETHANE
AL(OH)3	GIBBSITE	CHCL3	CHLOROFORM
ALPO4	ALUMINUM-PHOSPHATE-ORTHO	CHF3	TRIFLUOROMETHANE
AL2O3-2	ALUMINUM-OXIDE	CHN	HYDROGEN-CYANIDE
AL2(SO4)3	ALUMINUM-SULFATE	NACHO2	SODIUM-FORMATE
AR	ARGON	NAHCO3	SODIUM-BICARBONATE
AS	ARSENIC	CH2BRCL	BROMOCHLOROMETHANE
ASH3	ARSINE	CH2BR2	DIBROMOMETHANE
AS2O3	ARSENIC-TRIOXIDE	CH2CL2	DICHLOROMETHANE
BCL3	BORON-TRICHLORIDE	CH2F2	DIFLUOROMETHANE
BF3	BORON-TRIFLUORIDE	CH2I2	DIIODOMETHANE
H3BO3	HYDROGEN-ORTHOBORATE	CH2O	FORMALDEHYDE
NABO3	SODIUM-PERBORATE	CH2O2	FORMIC-ACID
B2H6	DIBORANE	CH3BR	METHYL-BROMIDE
B4H20NA2O17	BORAX	CH3CL	METHYL-CHLORIDE
BE	BERYLLIUM	CH3SICL3	METHYL-TRICHLOROSILANE
BI	BISMUTH	CH3F	METHYL-FLUORIDE
KBR	POTASSIUM-BROMIDE	CH3I	METHYL-IODIDE
NABR	SODIUM-BROMIDE	CH3NO	FORMAMIDE
BR2	BROMINE	CH3NO2	NITROMETHANE
C	CARBON(GRAPHITE)	CH4	METHANE
BACO3	BARIUM-CARBONATE	CH4SICL2	METHYL-DICHLOROSILANE
CBRCLF2	BROMOCHLORODIFLUOROMETHANE	CH4N2O	UREA
CBRCL3	BROMOTRICHLOROMETHANE	CH4N2S	THIOUREA
CBRF3	TRIFLUOROBROMOMETHANE	CH4O	METHANOL
CBR2F2	DIBROMODIFLUOROMETHANE	CH4O3S	METHANESULFONIC-ACID
CACO3-2	CALCIUM-CARBONATE(CALCITE)	CH4S	METHYL-MERCAPTAN
CCLF3	CHLOROTRIFLUOROMETHANE	CH5SICL	METHYL-CHLOROSILANE
CCLN	CYANOGEN-CHLORIDE	CH5N	METHYL-AMINE
CCL2F2	DICHLORODIFLUOROMETHANE	CH6N2	METHYL-HYDRAZINE
CCL2O	PHOSGENE	CH6SI	METHYL-SILANE
CCL3F	TRICHLOROFLUOROMETHANE	K2CO3	POTASSIUM-CARBONATE
CCL4	CARBON-TETRACHLORIDE	NACN	SODIUM-CYANIDE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
CN4O8	TETRANITROMETHANE	C2H2CL2-D1	1,1-DICHLOROETHYLENE
NA2CO3	SODIUM-CARBONATE	C2H2CL2-D2	CIS-1,2-DICHLOROETHYLENE
CO	CARBON-MONOXIDE	C2H2CL2-D3	TRANS-1,2-DICHLOROETHYLENE
COF2	CARBONYL-FLUORIDE	C2H2CL2O	CHLOROACETYL-CHLORIDE
COS	CARBONYL-SULFIDE	C2H2CL2O-D1	DICHLOROACETALDEHYDE
CO2	CARBON-DIOXIDE	C2H2CL2O2	DICHLOROACETIC-ACID
CS2	CARBON-DISULFIDE	C2H2CL3F	1,1,1-TRICHLOROFLUOROETHANE
SIC	SILICON-CARBIDE	C2H2CL4-D1	1,1,1,2-TETRACHLOROETHANE
C2BRF3	BROMOTRIFLUOROETHYLENE	C2H2CL4-D2	1,1,2,2-TETRACHLOROETHANE
C2BR2F4	1,2-DIBROMOTETRAFLUOROETHANE	C2H2F2	1,1-DIFLUOROETHYLENE
C2CLF3	CHLOROTRIFLUOROETHYLENE	C2H2F4	1,1,1,2-TETRAFLUOROETHANE
C2CLF5	CHLOROPENTAFLUOROETHANE	C2H2F4-D1	1,1,2,2-TETRAFLUOROETHANE
C2CL2F4-1	1,1-DICHLORO-1,2,2,2-TETRAFLUORO	C2H2O	KETENE
C2CL2F4-2	1,2-DICHLORO-1,1,2,2-TETRAFLUORO	C2H2O2	GLYOXAL
C2CL3F3	1,2,2-TRICHLORO-1,1,2-TRIFLUOROE	C2H2O4	OXALIC-ACID
C2CL4	TETRACHLOROETHYLENE	C2H3BR	VINYL-BROMIDE
C2CL4F2	1,1,2,2-TETRACHLORO-1,2-DIFLUORO	C2H3CL	VINYL-CHLORIDE
C2CL4F2-D1	1,1,1,2-TETRACHLORODIFLUOROETHAN	C2H3CLF2	1-CHLORO-1,1-DIFLUOROETHANE
C2CL4O	TRICHLOROACETYL-CHLORIDE	C2H3CLO	ACETYL-CHLORIDE
C2CL6	HEXACHLOROETHANE	C2H3CLO-D0	CHLOROACETALDEHYDE
C2F4	PERFLUOROETHENE	C2H3CLO2	CHLOROACETIC-ACID
C2F6	PERFLUOROETHANE	C2H3CLO2-D1	METHYL-CHLOROFORMATE
C2HBRCLF3	HALOTHANE	C2H3CL2F	1,1-DICHLORO-1-FLUOROETHANE
C2HCLF2	2-CHLORO-1,1-DIFLUOROETHYLENE	C2H3CL3	1,1,2-TRICHLOROETHANE
C2HCLF4	2-CHLORO-1,1,1,2-TETRAFLUOROETHA	C2H3CL3-D0	1,1,1-TRICHLOROETHANE
C2HCL2F3-D1	1,1-DICHLORO-2,2,2-TRIFLUOROETHA	C2H3F	VINYL-FLUORIDE
C2HCL2F3-D2	1,2-DICHLORO-1,1,2-TRIFLUOROETHA	C2H3F3	1,1,1-TRIFLUOROETHANE
C2HCL3	TRICHLOROETHYLENE	KC2H3O2	POTASSIUM-ACETATE
C2HCL3O	DICHLOROACETYL-CHLORIDE	C2H3N	ACETONITRILE
C2HCL3O-D1	TRICHLOROACETALDEHYDE	C2H3NO	METHYL-ISOCYANATE
C2HCL3O2	TRICHLOROACETIC-ACID	C2H3NO-E1	HYDROXYACETONITRILE
C2HCL5	PENTACHLOROETHANE	C2H3NAO2	SODIUM-ACETATE
C2HF3O2	TRIFLUOROACETIC-ACID	C2H4	ETHYLENE
C2HF5	PENTAFLUOROETHANE	C2H4BR2	1,2-DIBROMOETHANE
C2H2	ACETYLENE	C2H4BR2-D1	1,1-DIBROMOETHANE
C2H2BR4	1,1,2,2-TETRABROMOETHANE	C2H4CL2-1	1,1-DICHLOROETHANE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C2H4CL2-2	1,2-DICHLOROETHANE	C2H6S2	DIMETHYL-DISULFIDE
C2H4CL2O	BIS-CHLOROMETHYL-ETHER	C2H6S2-D1	1,2-ETHANEDITHIOL
C2H4F2	1,1-DIFLUOROETHANE	C2H7SICL	DIMETHYLCHLOROSILANE
C2H4F2-D1	1,2-DIFLUOROETHANE	C2H7N-1	ETHYL-AMINE
C2H4N2	AMINOACETONITRILE	C2H7N-2	DIMETHYLAMINE
C2H4N2O6	ETHYLENE-GLYCOL-DINITRATE	C2H7NO	MONOETHANOLAMINE
C2H4N4	DICYANDIAMIDE	C2H7NO2	AMMONIUM-ACETATE
C2H4O-1	ACETALDEHYDE	C2H8N2	ETHYLENEDIAMINE
C2H4O-2	ETHYLENE-OXIDE	C2H8N2O4	AMMONIUM-OXALATE
C2H4O2-1	ACETIC-ACID	C2H8P2O6	1,2-ETHANE-DIPHOSPHONIC-ACID
C2H4O2-2	METHYL-FORMATE	C2H8SI	DIMETHYL-SILANE
C2H4O2S	THIOGLYCOLIC-ACID	C2N2	CYANOGEN
C2H4O3-D1	GLYCOLIC-ACID	C3F6	HEXAFLUOROPROPYLENE
C2H4O3-D2	PERACETIC-ACID	C3F6O	HEXAFLUOROACETONE
C2H5BR	ETHYL-BROMIDE	C3F8	OCTAFLUOROPROPANE
C2H5CL	ETHYL-CHLORIDE	C3H2N2	MALONONITRILE
C2H5CLO	2-CHLOROETHANOL	C3H3CL	PROPARGYL-CHLORIDE
C2H5CLO-D1	CHLOROMETHYL-METHYL-ETHER	C3H3N	ACRYLONITRILE
C2H5F	ETHYL-FLUORIDE	C3H3NO	OXAZOLE
C2H5I	ETHYL-IODIDE	C3H4-1	PROPADIENE
C2H5N	ETHYLENE-IMINE	C3H4-2	METHYL-ACETYLENE
C2H5NO-D1	ACETAMIDE	C3H4CL2	2,3-DICHLOROPROPENE
C2H5NO-D2	N-METHYLFORMAMIDE	C3H4O	ACROLEIN
C2H5NO2	NITROETHANE	C3H4O-D0	PROPARGYL-ALCOHOL
C2H5NO2-D1	GLYCINE	C3H4O2-1	ACRYLIC-ACID
C2H6	ETHANE	C3H4O2-2	VINYL-FORMATE
C2H6ALCL	DIMETHYLALUMINUM-CHLORIDE	C3H4O2-D0	BETA-PROPIOLACTONE
C2H6SICL2	DIMETHYLDICHLOROSILANE	C3H4O3	ETHYLENE-CARBONATE
C2H6O-1	DIMETHYL-ETHER	C3H4O3-D1	PYRUVIC-ACID
C2H6O-2	ETHANOL	C3H4O4	MALONIC-ACID
C2H6OS	DIMETHYL-SULFOXIDE	C3H5CL	ALLYL-CHLORIDE
C2H6OS-D1	2-MERCAPTOETHANOL	C3H5CL-D0	2-CHLOROPROPENE
C2H6O2	ETHYLENE-GLYCOL	C3H5CLO	ALPHA-EPICHLOROHYDRIN
C2H6O4S	DIMETHYL-SULFATE	C3H5CLO2	METHYL-CHLOROACETATE
C2H6S-1	ETHYL-MERCAPTAN	C3H5CLO2-D1	ETHYL-CHLOROFORMATE
C2H6S-2	DIMETHYL-SULFIDE	C3H5CL3	1,2,3-TRICHLOROPROPANE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C3H5N	PROPIONITRILE	C3H7NO-D1	N-METHYLACETAMIDE
C3H5NO	LACTONITRILE	C3H7NO2-D1	1-NITROPROPANE
C3H5NO-D1	ACRYLAMIDE	C3H7NO2-D2	2-NITROPROPANE
C3H5NO-D2	HYDRACRYLONITRILE	C3H8	PROPANE
C3H5N3O9	NITROGLYCERINE	C3H8O-1	1-PROPANOL
C3H6-1	CYCLOPROPANE	C3H8O-2	ISOPROPYL-ALCOHOL
C3H6-2	PROPYLENE	C3H8O-3	METHYL-ETHYL-ETHER
C3H6CL2	1,2-DICHLOROPROPANE	C3H8O2	2-METHOXYETHANOL
C3H6CL2-D1	1,1-DICHLOROPROPANE	C3H8O2-1	METHYLAL
C3H6CL2-D2	1,3-DICHLOROPROPANE	C3H8O2-2	PROPANEDIOL-1,2
C3H6N6	MELAMINE	C3H8O2-3	1,3-PROPANEDIOL
C3H6O-1	ACETONE	C3H8O3	GLYCEROL
C3H6O-2	ALLYL-ALCOHOL	C3H8S-D1	ISOPROPYL-MERCAPTAN
C3H6O-3	N-PROPIONALDEHYDE	C3H8S-E1	N-PROPYLMERCAPTAN
C3H6O-4	PROPYLENE-OXIDE	C3H8S-E2	METHYL-ETHYL-SULFIDE
C3H6O-5	VINYL-METHYL-ETHER	C3H9AL	TRIMETHYLALUMINUM
C3H6O-D0	1,3-PROPYLENE-OXIDE	C3H9SICL	TRIMETHYLCHLOROSILANE
C3H6O2-1	PROPIONIC-ACID	C3H9GA	TRIMETHYLGALLIUM
C3H6O2-2	ETHYL-FORMATE	C3H9N-1	N-PROPYL-AMINE
C3H6O2-3	METHYL-ACETATE	C3H9N-2	ISOPROPYL-AMINE
C3H6O2-D1	ACETOL	C3H9N-3	TRIMETHYL-AMINE
C3H6O2-D2	2,3-EPOXY-1-PROPANOL	C3H9NO	METHYL-ETHANOLAMINE
C3H6O2S	3-MERCAPTOPROPIONIC-ACID	C3H9NO-D1	1-AMINO-2-PROPANOL
C3H6O3	METHOXYACETIC-ACID	C3H9NO-D2	3-AMINO-1-PROPANOL
C3H6O3-D1	LACTIC-ACID	C3H9O4P	TRIMETHYL-PHOSPHATE
C3H6O3-D2	TRIOXANE	C3H10N2	1,2-PROPANEDIAMINE
C3H6O3-D3	DIMETHYL-CARBONATE	C3H10SI	TRIMETHYL-SILANE
C3H7BR-D1	1-BROMOPROPANE	C4CL4S	TETRACHLOROTHIOPHENE
C3H7BR-D2	2-BROMOPROPANE	C4CL6	HEXACHLORO-1,3-BUTADIENE
C3H7CL-1	PROPYL-CHLORIDE	C4F8-D1	OCTAFLUORO-2-BUTENE
C3H7CL-2	ISOPROPYL-CHLORIDE	C4F8-D2	OCTAFLUOROCYCLOBUTANE
C3H7I-D1	ISOPROPYL-IODIDE	C4F10	DECAFLUOROBUTANE
C3H7I-D2	N-PROPYL-IODIDE	C4H2O3	MALEIC-ANHYDRIDE
C3H7N	ALLYLAMINE	C4H4	VINYLACETYLENE
C3H7N-D1	PROPYLENEIMINE	C4H4N2	SUCCINONITRILE
C3H7NO	N,N-DIMETHYLFORMAMIDE	C4H4O	FURAN

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C4H4O2	DIKETENE	C4H6O4-2	SUCCINIC-ACID
C4H4O3	SUCCINIC-ANHYDRIDE	C4H6O5	DIGLYCOLIC-ACID
C4H4O4-D1	FUMARIC-ACID	C4H6O5-D1	MALIC-ACID
C4H4O4-D2	MALEIC-ACID	C4H6O6	TARTARIC-ACID
C4H4S	THIOPHENE	C4H7CLO2	ETHYLCHLOROACETATE
C4H5CL	CHLOROPRENE	C4H7N	BUTYRONITRILE
C4H5N	METHACRYLONITRILE	C4H7N-D0	ISOBUTYRONITRILE
C4H5N-1	ALLYL-CYANIDE	C4H7NO-D1	ACETONE-CYANOHYDRIN
C4H5N-2	PYRROLE	C4H7NO-D2	2-PYRROLIDONE
C4H5N-E1	TRANS-CROTONITRILE	C4H7NO-E1	2-METHACRYLAMIDE
C4H5N-E3	CIS-CROTONITRILE	C4H7NO-E2	3-METHOXYPROPIONITRILE
C4H5NO2	METHYL-CYANOACETATE	C4H8-1	1-BUTENE
C4H5N3	2,2-IMINOBIS-ACETONITRILE	C4H8-2	CIS-2-BUTENE
C4H6-1	1-BUTYNE	C4H8-3	TRANS-2-BUTENE
C4H6-2	2-BUTYNE	C4H8-4	CYCLOBUTANE
C4H6-3	1,2-BUTADIENE	C4H8-5	ISOBUTYLENE
C4H6-4	1,3-BUTADIENE	C4H8CL2	1,4-DICHLOROBUTANE
C4H6CL2	1,4-DICHLORO-TRANS-2-BUTENE	C4H8Cl2-D1	1,2-DICHLOROBUTANE
C4H6CL2-E1	1,3-DICHLORO-TRANS-2-BUTENE	C4H8Cl2-D2	2,3-DICHLOROBUTANE
C4H6CL2-E2	3,4-DICHLORO-1-BUTENE	C4H8O	1,2-EPOXYBUTANE
C4H6CL2-E3	1,4-DICHLORO-CIS-2-BUTENE	C4H8O-1	N-BUTYRALDEHYDE
C4H6O	2,5-DIHYDROFURAN	C4H8O-2	ISOBUTYRALDEHYDE
C4H6O-D1	TRANS-CROTONALDEHYDE	C4H8O-3	METHYL-ETHYL-KETONE
C4H6O-D2	DIVINYL-ETHER	C4H8O-4	TETRAHYDROFURAN
C4H6O-D3	METHACROLEIN	C4H8O-5	VINYL-ETHYL-ETHER
C4H6O2-1	VINYL-ACETATE	C4H8O-D1	1,2-EPOXY-2-METHYLPROPANE
C4H6O2-2	METHYL-ACRYLATE	C4H8O2-1	N-BUTYRIC-ACID
C4H6O2-D1	2-BUTYNE-1,4-DIOL	C4H8O2-2	1,4-DIOXANE
C4H6O2-D2	GAMMA-BUTYROLACTONE	C4H8O2-3	ETHYL-ACETATE
C4H6O2-D3	CIS-CROTONIC-ACID	C4H8O2-4	ISOBUTYRIC-ACID
C4H6O2-D4	TRANS-CROTONIC-ACID	C4H8O2-5	METHYL-PROPIONATE
C4H6O2-D5	METHACRYLIC-ACID	C4H8O2-6	N-PROPYL-FORMATE
C4H6O2S	SULFOLENE	C4H8O2-D1	ACETALDOL
C4H6O3	ACETIC-ANHYDRIDE	C4H8O2-D2	CIS-2-BUTENE-1,4-DIOL
C4H6O3-D1	PROPYLENE-CARBONATE	C4H8O2-D3	TRANS-2-BUTENE-1,4-DIOL
C4H6O4-1	DIMETHYL-OXALATE	C4H8O2-D4	1,3-DIOXANE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C4H8O2-D5	3-HYDROXY-2-METHYL-PROPIONALDEHY	C4H10SO3	DIETHYLSULFITE
C4H8O2-D6	4-HYDROXYBUTYRALDEHYDE	C4H10O4S	DIETHYL-SULFATE
C4H8O2S	SULFOLANE	C4H10S	DIETHYL-SULFIDE
C4H8S	TETRAHYDROTHIOPHENE	C4H10S-D1	N-BUTYL-MERCAPTAN
C4H9BR-D1	1-BROMOBUTANE	C4H10S-D2	TERT-BUTYL-MERCAPTAN
C4H9BR-D2	2-BROMOBUTANE	C4H10S-D3	METHYL-N-PROPYL-SULFIDE
C4H9CL-1	1-CHLOROBUTANE	C4H10S-E1	SEC-BUTYL-MERCAPTAN
C4H9CL-2	2-CHLOROBUTANE	C4H10S-E2	ISOBUTYL-MERCAPTAN
C4H9CL-3	TERT-BUTYL-CHLORIDE	C4H10S2	DIETHYL-DISULFIDE
C4H9CL-D1	ISOBUTYL-CHLORIDE	C4H11N-1	N-BUTYL-AMINE
C4H9N	PYRROLIDINE	C4H11N-2	ISOBUTYL-AMINE
C4H9NO	MORPHOLINE	C4H11N-3	DIETHYL-AMINE
C4H9NO-D0	N,N-DIMETHYLACETAMIDE	C4H11N-D1	SEC-BUTYLAMINE
C4H10-1	N-BUTANE	C4H11N-D2	TERT-BUTYLAMINE
C4H10-2	ISOBUTANE	C4H11NO	DIMETHYLETHANOLAMINE
C4H10N2	PIPERAZINE	C4H11NO2-1	DIETHANOLAMINE
C4H10O-1	N-BUTANOL	C4H11NO2-2	DIGLYCOLAMINE
C4H10O-2	2-BUTANOL	C4H12N2O	N-AMINOETHYL-ETHANOLAMINE
C4H10O-3	ISOBUTANOL	C4H12SI	TETRAMETHYLSILANE
C4H10O-4	TERT-BUTYL-ALCOHOL	C4H13N3	DIETHYLENE-TRIAMINE
C4H10O-5	DIETHYL-ETHER	C5CL6	HEXACHLOROCYCLOPENTADIENE
C4H10O-D1	METHYL-ISOPROPYL-ETHER	C5H4O2	FURFURAL
C4H10O-D2	METHYL-N-PROPYL-ETHER	C5H5N	PYRIDINE
C4H10OS	ETHYLTHIOETHANOL	C5H6	CYCLOPENTADIENE
C4H10OS2	DIMERCAPTOETHYL-ETHER	C5H6-E1	2-METHYL-1-BUTENE-3-YNE
C4H10O2	1,2-DIMETHOXYETHANE	C5H6-E2	1-PENTENE-3-YNE
C4H10O2-D1	1,3-BUTANEDIOL	C5H6-E3	1-PENTENE-4-YNE
C4H10O2-D2	1,4-BUTANEDIOL	C5H6N2	GLUTARONITRILE
C4H10O2-D3	T-BUTYL-HYDROPEROXIDE	C5H6O2	FURFURYL-ALCOHOL
C4H10O2-D4	2-ETHOXYETHANOL	C5H6O3	GLUTARIC-ANHYDRIDE
C4H10O2-D5	2,3-BUTANEDIOL	C5H6O4-E1	CITRACONIC-ACID
C4H10O2-D6	1,2-BUTANEDIOL	C5H6O4-E2	ITACONIC-ACID
C4H10O2-D7	PG-MONOMETHYL-ETHER	C5H6S-E1	2-METHYLTHIOPHENE
C4H10O2-D8	2-METHYL-1,3-PROPANEDIOL	C5H6S-E2	3-METHYLTHIOPHENE
C4H10O2S	THIODIGLYCOL	C5H7N	N-METHYLPYRROLE
C4H10O3	DIETHYLENE-GLYCOL	C5H7NO2	ETHYL-CYANOACETATE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C5H8	CIS-1,3-PENTADIENE	C5H10-6	2-METHYL-2-BUTENE
C5H8-1	CYCLOPENTENE	C5H10-7	3-METHYL-1-BUTENE
C5H8-2	1,2-PENTADIENE	C5H10CL2	1,5-DICHLOROPENTANE
C5H8-3	1-TRANS-3-PENTADIENE	C5H10NNAS2	SODIUM-DIETHYLDITHIOCARBAMATE
C5H8-4	1,4-PENTADIENE	C5H10O-1	VALERALDEHYDE
C5H8-5	1-PENTYNE	C5H10O-2	METHYL-N-PROPYL-KETONE
C5H8-6	2-METHYL-1,3-BUTADIENE	C5H10O-3	METHYL-ISOPROPYL-KETONE
C5H8-7	3-METHYL-1,2-BUTADIENE	C5H10O-4	DIETHYL-KETONE
C5H8-E2	3-METHYL-1-BUTYNE	C5H10O2	NEOPENTANOIC-ACID
C5H8-E4	2,3-PENTADIENE	C5H10O2-1	N-VALERIC-ACID
C5H8-E5	2-PENTYNE	C5H10O2-2	ISOBUTYL-FORMATE
NAC5H8NO4	MONOSODIUM-GLUTAMATE	C5H10O2-3	N-PROPYL-ACETATE
C5H8N4O12	PENTAERYTHRITOL-TETRANITRATE	C5H10O2-4	ETHYL-PROPIONATE
C5H8O	CYCLOPENTANONE	C5H10O2-5	METHYL-BUTYRATE
C5H8O-D1	METHYL-ISOPROPENYL-KETONE	C5H10O2-6	METHYL-ISOBUTYRATE
C5H8O2	ETHYL-ACRYLATE	C5H10O2-D1	N-BUTYL-FORMATE
C5H8O2-D1	ACETYLACETONE	C5H10O2-D2	ISOPROPYL-ACETATE
C5H8O2-D2	ALLYL-ACETATE	C5H10O2-D3	ISOVALERIC-ACID
C5H8O2-D3	METHYL-METHACRYLATE	C5H10O2-D4	2-METHYLBUTYRIC-ACID
C5H8O2-D4	GAMMA-VALEROLACTONE	C5H10O2-D5	TETRAHYDROFURFURYL-ALCOHOL
C5H8O2-D5	VINYL-PROPIONATE	C5H10O2-D6	SEC-BUTYL-FORMATE
C5H8O2-D6	GLUTARALDEHYDE	C5H10O2-D7	TERT-BUTYL-FORMATE
C5H8O3	2-HYDROXYETHYL-ACRYLATE	C5H10O2S	3-METHYL-SULFOLANE
C5H8O3-D1	LEVULINIC-ACID	C5H10O3-D1	DIETHYL-CARBONATE
C5H8O3-D2	METHYL-ACETOACETATE	C5H10O3-D2	ETHYL-LACTATE
C5H8O4	GLUTARIC-ACID	C5H11CL	1-CHLOROPENTANE
C5H9N	VALERONITRILE	C5H11N	PIPERIDINE
C5H9NO-D1	N-BUTYL-ISOCYANATE	C5H11N-D0	N-METHYLPYRROLIDINE
C5H9NO-D2	N-METHYL-2-PYRROLIDONE	C5H11NO	TERT-BUTYLFORMAMIDE
C5H9NO4	L-GLUTAMIC-ACID	C5H12-1	N-PENTANE
C5H9NS	N-METHYLTHIOPYRROLIDONE	C5H12-2	2-METHYL-BUTANE
C5H10-1	CYCLOPENTANE	C5H12-3	2,2-DIMETHYL-PROPANE
C5H10-2	1-PENTENE	C5H12O	METHYL-SEC-BUTYL-ETHER
C5H10-3	CIS-2-PENTENE	C5H12O-1	1-PENTANOL
C5H10-4	TRANS-2-PENTENE	C5H12O-2	2-METHYL-1-BUTANOL
C5H10-5	2-METHYL-1-BUTENE	C5H12O-3	3-METHYL-1-BUTANOL

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C5H12O-4	2-METHYL-2-BUTANOL	C6H4CL2-2	M-DICHLOROBENZENE
C5H12O-5	2,2-DIMETHYL-1-PROPANOL	C6H4CL2-3	P-DICHLOROBENZENE
C5H12O-6	ETHYL-PROPYL-ETHER	C6H4N2O4-E1	M-DINITROBENZENE
C5H12O-D1	3-METHYL-2-BUTANOL	C6H4N2O4-E2	O-DINITROBENZENE
C5H12O-D2	METHYL-TERT-BUTYL-ETHER	C6H4N2O4-E3	P-DINITROBENZENE
C5H12O-D3	2-PENTANOL	C6H4O2	QUINONE
C5H12O-D4	3-PENTANOL	C6H5BR	BROMOBENZENE
C5H12O-D5	ETHYL-ISOPROPYL-ETHER	C6H5CL	CHLOROBENZENE
C5H12O-E1	METHYL-ISOBUTYL-ETHER	C6H5CLO-E1	M-CHLOROPHENOL
C5H12O-E2	METHYL-N-BUTYL-ETHER	C6H5CLO-E2	O-CHLOROPHENOL
C5H12O2-D1	NEOPENTYL-GLYCOL	C6H5CLO-E3	P-CHLOROPHENOL
C5H12O2-D2	1,5-PENTANEDIOL	C6H5CL2N	3,4-DICHLOROANILINE
C5H12O2-D3	ETHYLENE-GLYCOL-MONOPROPYL-ETHER	C6H5F	FLUOROBENZENE
C5H12O2-D4	ETHYLAL	C6H5I	IODOBENZENE
C5H12O2-D5	2,4-PENTANEDIOL	C6H5NO2	NITROBENZENE
C5H12O3	2-2-METHOXYETHOXY-ETHANOL	C6H5NO2-D1	NIACIN
C5H12O4	PENTAERYTHRITOL	C6H6	BENZENE
C5H12S	1-PENTANETHIOL	C6H6CLN-D1	M-CHLOROANILINE
C5H12S-D1	METHYL-T-BUTYL-SULFIDE	C6H6CLN-D2	O-CHLOROANILINE
C5H12S-D2	METHYL-N-BUTYL-SULFIDE	C6H6CLN-D3	P-CHLOROANILINE
C5H13N	N-PENTYLAMINE	C6H6N2-E1	CIS-DICYANO-1-BUTENE
C5H13NO2	METHYL-DIETHANOLAMINE	C6H6N2-E2	TRANS-DICYANO-1-BUTENE
C6CL6	HEXACHLOROBENZENE	C6H6N2-E3	1,4-DICYANO-2-BUTENE
C6F6	PERFLUOROBENZENE	C6H6N2O2-D1	M-NITROANILINE
C6F12	PERFLUOROCYCLOHEXANE	C6H6N2O2-D2	O-NITROANILINE
C6F14	PERFLUORO-N-HEXANE	C6H6N2O2-D3	P-NITROANILINE
C6H3CLN2O4	1-CHLORO-2,4-DINITROBENZENE	C6H6N4	\2,2,2-NITRILOTRIS-ACETONITRILE
C6H3CL2NO2	1,2-DICHLORO-4-NITROBENZENE	C6H6O	PHENOL
C6H3CL3	1,2,4-TRICHLOROBENZENE	C6H6O2	P-HYDROQUINONE
C6H3CL3-D1	1,3,5-TRICHLOROBENZENE	C6H6O2-E1	1,2-BENZENEDIOL
C6H3N3O6	1,3,5-TRINITROBENZENE	C6H6O2-E2	1,3-BENZENEDIOL
C6H4BR2	M-DIBROMOBENZENE	C6H6O3	1,2,3-BENZENETRIOL
C6H4CLNO2-D1	M-CHLORONITROBENZENE	C6H6O3S	BENZENESULFONIC-ACID
C6H4CLNO2-D2	O-CHLORONITROBENZENE	C6H6S	PHENYL-MERCAPTAN
C6H4CLNO2-D3	P-CHLORONITROBENZENE	C6H7N-1	ANILINE
C6H4CL2-1	O-DICHLOROBENZENE	C6H7N-2	4-METHYLPYRIDINE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C6H7N-D1	2-METHYLPYRIDINE	C6H10O4	ETHYLIDENE-DIACETATE
C6H7N-D2	3-METHYLPYRIDINE	C6H10O4-D1	ADIPIC-ACID
C6H7NO3S	SULFANILIC-ACID	C6H10O4-D2	DIETHYL-OXALATE
C6H8-E1	1,3-CYCLOHEXADIENE	C6H10O4-D3	ETHYLENE-GLYCOL-DIACETATE
C6H8-E2	METHYLCYCLOPENTADIENE	C6H11N	HEXANENITRILE
C6H8-E3	1,4-CYCLOHEXADIENE	C6H11N-D1	DIALLYLAMINE
C6H8N2	METHYLGLUTARONITRILE	C6H11NO	EPSILON-CAPROLACTAM
C6H8N2-D1	ADIPONITRILE	C6H11NO-D1	CYCLOHEXANONE-OXIME
C6H8N2-D2	M-PHENYLENEDIAMINE	C6H12-1	CYCLOHEXANE
C6H8N2-D3	O-PHENYLENEDIAMINE	C6H12-10	3-METHYL-TRANS-2-PENTENE
C6H8N2-D4	P-PHENYLENEDIAMINE	C6H12-11	4-METHYL-CIS-2-PENTENE
C6H8N2-D5	PHENYLHYDRAZINE	C6H12-12	4-METHYL-TRANS-2-PENTENE
C6H8N2O	BIS-CYANOETHYL-ETHER	C6H12-13	2,3-DIMETHYL-1-BUTENE
C6H8O4	DIMETHYL-MALEATE	C6H12-14	2,3-DIMETHYL-2-BUTENE
C6H8O6	ASCORBIC-ACID	C6H12-15	3,3-DIMETHYL-1-BUTENE
C6H8O7	CITRIC-ACID	C6H12-2	METHYLCYCLOPENTANE
C6H10-1	1,5-HEXADIENE	C6H12-3	1-HEXENE
C6H10-2	CYCLOHEXENE	C6H12-4	CIS-2-HEXENE
C6H10-D1	1-METHYLCYCLOPENTENE	C6H12-5	TRANS-2-HEXENE
C6H10-D2	3-METHYLCYCLOPENTENE	C6H12-6	CIS-3-HEXENE
C6H10-D3	4-METHYLCYCLOPENTENE	C6H12-7	TRANS-3-HEXENE
C6H10-D4	1,2-HEXADIENE	C6H12-8	2-METHYL-2-PENTENE
C6H10-E2	1-HEXYNE	C6H12-9	3-METHYL-CIS-2-PENTENE
C6H10-E3	2,3-DIMETHYL-1,3-BUTADIENE	C6H12-D1	2-ETHYL-1-BUTENE
C6H10-E4	CIS,TRANS-2,4-HEXADIENE	C6H12-D2	2-METHYL-1-PENTENE
C6H10-E5	TRANS,TRANS-2,4-HEXADIENE	C6H12-D3	4-METHYL-1-PENTENE
C6H10-E6	2-HEXYNE	C6H12-E3	3-METHYL-1-PENTENE
C6H10-E7	3-HEXYNE	C6H12CL3PO3	BIS-2-CHLOROETHYL-2-CHLOROETHYL
C6H10-E8	1,4-HEXADIENE	C6H12N2-E1	AMINOCAPRONITRILE
C6H10O	CYCLOHEXANONE	C6H12N2-E2	TRIETHYLENEDIAMINE
C6H10O-D0	MESITYL-OXIDE	C6H12N4	HEXAMETHYLENETETRAMINE
C6H10O2-D1	CAPROLACTONE	C6H12O	3-HEXANONE
C6H10O2-D2	ETHYL-METHACRYLATE	C6H12O-1	CYCLOHEXANOL
C6H10O2-D3	N-PROPYL-ACRYLATE	C6H12O-2	METHYL-ISOBUTYL-KETONE
C6H10O3-D1	ETHYLACETOACETATE	C6H12O-D1	BUTYL-VINYL-ETHER
C6H10O3-D2	PROPIONIC-ANHYDRIDE	C6H12O-D2	1-HEXANAL

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C6H12O-D3	2-HEXANONE	C6H14O-D2	2-ETHYL-1-BUTANOL
C6H12O-E1	ETHYL-ISOPROPYL-KETONE	C6H14O-D3	2-METHYL-1-PENTANOL
C6H12O-E2	3-METHYL-2-PENTANONE	C6H14O-D4	4-METHYL-2-PENTANOL
C6H12O-E3	3,3-DIMETHYL-2-BUTANONE	C6H14O-E1	2-HEXANOL
C6H12O2	TERT-BUTYL-ACETATE	C6H14O-E2	METHYL-TERT-PENTYL-ETHER
C6H12O2-1	N-BUTYL-ACETATE	C6H14O-E3	TERT-BUTYL-ETHYL-ETHER
C6H12O2-2	ISOBUTYL-ACETATE	C6H14O-E4	METHYL-N-PENTYL-ETHER
C6H12O2-3	ETHYL-BUTYRATE	C6H14O2-D1	ACETAL
C6H12O2-4	ETHYL-ISOBUTYRATE	C6H14O2-D2	2-BUTOXYETHANOL
C6H12O2-5	N-PROPYL-PROPIONATE	C6H14O2-D3	1,6-HEXANEDIOL
C6H12O2-D1	SEC-BUTYL-ACETATE	C6H14O2-D4	HEXYLENE-GLYCOL
C6H12O2-D2	CYCLOHEXYL-PEROXIDE	C6H14O2-D5	1,2-DIETHOXYETHANE
C6H12O2-D3	DIACETONE-ALCOHOL	C6H14O2S	DI-N-PROPYL-SULFONE
C6H12O2-D4	2-ETHYL-BUTYRIC-ACID	C6H14O3-D1	DIETHYLENE-GLYCOL-DIMETHYL-ETHER
C6H12O2-D5	N-HEXANOIC-ACID	C6H14O3-D2	DIPROPYLENE-GLYCOL
C6H12O2-D6	NEOHEXANOIC-ACID	C6H14O3-D3	2-2-ETHOXYETHOXY-ETHANOL
C6H12O2-E1	N-PENTYL-FORMATE	C6H14O3-D4	TRIMETHYLOLPROPANE
C6H12O3-D1	2-ETHOXYETHYL-ACETATE	C6H14O4	TRIETHYLENE-GLYCOL
C6H12O3-D2	PARALDEHYDE	C6H14O6	SORBITOL
C6H12O3-E1	HYDROXYCAPROIC-ACID	C6H14S	N-HEXYLMERCAPTAN
C6H12O3-E2	PG-MONOMETHYL-ETHER-ACETATE	C6H14S-D1	DI-N-PROPYL-SULFIDE
C6H12O6	DEXTROSE	C6H14S-D2	METHYL-T-PENTYL-SULFIDE
C6H12O6-D1	INOSITOL	C6H14S-D3	ETHYL-T-BUTYL-SULFIDE
C6H12S	CYCLOHEXYL-MERCAPTAN	C6H14S2	DI-N-PROPYLDISULFIDE
C6H13N-D1	CYCLOHEXYLAMINE	C6H15AL	TRIETHYL-ALUMINUM
C6H13N-D2	HEXAMETHYLENEIMINE	C6H15AL2CL3	ETHYL-ALUMINUM-SESQUICHLORIDE
C6H14-1	N-HEXANE	C6H15N-1	DIPROPYLAMINE
C6H14-2	2-METHYL-PENTANE	C6H15N-2	TRIETHYLAMINE
C6H14-3	3-METHYL-PENTANE	C6H15N-D1	DIISOPROPYLAMINE
C6H14-4	2,2-DIMETHYL-BUTANE	C6H15N-D2	N-HEXYLAMINE
C6H14-5	2,3-DIMETHYL-BUTANE	C6H15NO	6-AMINOHEXANOL
C6H14N2O2	LYSINE	C6H15NO2	DIISOPROPANOLAMINE
C6H14O-1	1-HEXANOL	C6H15NO3	TRIETHANOLAMINE
C6H14O-2	ETHYL-BUTYL-ETHER	C6H15N3	N-AMINOETHYL-PIPERAZINE
C6H14O-3	DIISOPROPYL-ETHER	C6H15O4P	TRIETHYLPHOSPHATE
C6H14O-D1	DI-N-PROPYL-ETHER	C6H16N2	HEXAMETHYLENEDIAMINE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C6H18N3OP	HEXAMETHYL-PHOSPHORAMIDE	C7H7CL-D1	BENZYLCHLORIDE
C6H18N4	TRIETHYLENE-TETRAMINE	C7H7CL-D2	O-CHLOROTOLUENE
C6H18OSI2	HEXAMETHYLDISILOXANE	C7H7CL-D3	P-CHLOROTOLUENE
C6H18O3SI3	HEXAMETHYLCYCLOTRISILOXANE	C7H7NO	FORMANILIDE
C6H19NSI2	HEXAMETHYLDISILAZANE	C7H7NO2-D1	M-NITROTOLUENE
C7F14	PERFLUOROMETHYLCYCLOHEXANE	C7H7NO2-D2	O-NITROTOLUENE
C7F16	PERFLUORO-N-HEPTANE	C7H7NO2-D3	P-NITROTOLUENE
C7H3CLF3NO2	4-CHLORO-3-NITROBENZOTRIFLUORIDE	C7H7NO3	O-NITROANISOLE
C7H3CL2F3	2,4-DICHLOROBENZOTRIFLUORIDE	C7H8	TOLUENE
C7H3CL2NO	3,4-DICHLOROPHENYL-ISOCYANATE	C7H8O-1	METHYLPHENYL-ETHER
C7H4CLF3	P-CHLOROBENZOTRIFLUORIDE	C7H8O-2	BENZYLALCOHOL
C7H4CL2O	M-CHLOROBENZOYL-CHLORIDE	C7H8O-3	O-CRESOL
C7H4F3NO2	3-NITROBENZOTRIFLUORIDE	C7H8O-4	M-CRESOL
C7H5CLO	BENZOYL-CHLORIDE	C7H8O-5	P-CRESOL
C7H5CLO2	O-CHLOROBENZOIC-ACID	C7H8O2	P-METHOXYPHENOL
C7H5CL3	BENZOTRICHLORIDE	C7H8O2-E1	GUAIACOL
C7H5F3	BENZOTRIFLUORIDE	C7H8O3S	P-TOLUENESULFONIC-ACID
C7H5N	BENZONITRILE	C7H8O3S-D1	O-TOLUENESULFONIC-ACID
C7H5NO	PHENYL-ISOCYANATE	C7H8S	BENZYL-MERCAPTAN
C7H5NS2	2-MERCAPTOBENZOTHIAZOLE	C7H9N-1	2,3-DIMETHYLPYRIDINE
C7H5N3O6	2,4,6-TRINITROTOLUENE	C7H9N-2	2,5-DIMETHYLPYRIDINE
C7H5N5O8	TETRYL	C7H9N-3	3,4-DIMETHYLPYRIDINE
C7H5NAO2	SODIUM-BENZOATE	C7H9N-4	3,5-DIMETHYLPYRIDINE
C7H6CL2	2,4-DICHLOROTOLUENE	C7H9N-5	METHYLPHENYLAMINE
C7H6CL2-D1	BENZYL-DICHLORIDE	C7H9N-6	O-TOLUIDINE
C7H6N2O4-E1	2,4-DINITROTOLUENE	C7H9N-7	M-TOLUIDINE
C7H6N2O4-E2	2,5-DINITROTOLUENE	C7H9N-8	P-TOLUIDINE
C7H6N2O4-E3	2,6-DINITROTOLUENE	C7H9N-D1	BENZYLAMINE
C7H6N2O4-E4	3,4-DINITROTOLUENE	C7H9N-D2	2,6-DIMETHYLPYRIDINE
C7H6N2O4-E5	3,5-DINITROTOLUENE	C7H10	2-NORBORNENE
C7H6O	BENZALDEHYDE	C7H10N2	TOLUENEDIAMINE
C7H6O2	BENZOIC-ACID	C7H10O2	ALLYL-METHACRYLATE
C7H6O2-D0	SALICYLALDEHYDE	C7H11NO	CYCLOHEXYL-ISOCYANATE
C7H6O2-E1	P-HYDROXY-BENZALDEHYDE	C7H12	CYCLOHEPTENE
C7H6O3	SALICYLIC-ACID	C7H12-D1	1-HEPTYNE
C7H7BR	P-BROMOTOLUENE	C7H12O2-D1	N-BUTYL-ACRYLATE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C7H12O2-D2	ISOBUTYL-ACRYLATE	C7H14O-E2	4-HEPTANONE
C7H12O2-D3	N-PROPYL-METHACRYLATE	C7H14O-E3	2-METHYLHEXANAL
C7H12O2-D4	CYCLOHEXYL-FORMATE	C7H14O-E4	3-METHYLHEXANAL
C7H12O4	DIETHYL-MALONATE	C7H14O2-D1	N-BUTYL-PROPIONATE
C7H12O4-D1	PIMELIC-ACID	C7H14O2-D2	ETHYL-ISOVALERATE
C7H14-1	CYCLOHEPTANE	C7H14O2-D3	N-HEPTANOIC-ACID
C7H14-2	1,1-DIMETHYLCYCLOPENTANE	C7H14O2-D4	ISOPENTYL-ACETATE
C7H14-3	CIS-1,2-DIMETHYLCYCLOPENTANE	C7H14O2-D5	N-PENTYL-ACETATE
C7H14-4	TRANS-1,2-DIMETHYLCYCLOPENTANE	C7H14O2-D6	N-PROPYL-N-BUTYRATE
C7H14-5	ETHYLCYCLOPENTANE	C7H14O2-D7	N-PROPYL-ISOBUTYRATE
C7H14-6	METHYLCYCLOHEXANE	C7H14O2-D8	N-HEXYL-FORMATE
C7H14-7	1-HEPTENE	C7H14O2-D9	NEOHEPTANOIC-ACID
C7H14-8	2,3,3-TRIMETHYL-1-BUTENE	C7H14O3	ETHYL-3-ETHOXYPROPIONATE
C7H14-D1	CIS-2-HEPTENE	C7H15BR	1-BROMOHEPTANE
C7H14-D2	CIS-3-HEPTENE	C7H15N	N-METHYLCYCLOHEXYLAMINE
C7H14-E10	3-METHYL-1-HEXENE	C7H16-1	N-HEPTANE
C7H14-E2	CIS-1,3-DIMETHYLCYCLOPENTANE	C7H16-2	2-METHYLHEXANE
C7H14-E3	TRANS-1,3-DIMETHYLCYCLOPENTANE	C7H16-3	3-METHYLHEXANE
C7H14-E4	TRANS-2-HEPTENE	C7H16-4	2,2-DIMETHYLPENTANE
C7H14-E5	TRANS-3-HEPTENE	C7H16-5	2,3-DIMETHYLPENTANE
C7H14-E6	4-METHYL-1-HEXENE	C7H16-6	2,4-DIMETHYLPENTANE
C7H14-E7	2-ETHYL-1-PENTENE	C7H16-7	3,3-DIMETHYLPENTANE
C7H14-E8	3-ETHYL-1-PENTENE	C7H16-8	3-ETHYLPENTANE
C7H14-E9	2-METHYL-1-HEXENE	C7H16-9	2,2,3-TRIMETHYLBUTANE
C7H14O	DIISOPROPYL-KETONE	C7H16O	1-HEPTANOL
C7H14O-D1	1-HEPTANAL	C7H16O-D0	2-HEPTANOL
C7H14O-D10	5-METHYL-2-HEXANONE	C7H16O-D1	ISOPROPYL-BUTYL-ETHER
C7H14O-D2	2-HEPTANONE	C7H16O-D2	ISOPROPYL-ISOBUTYL-ETHER
C7H14O-D3	1-METHYLCYCLOHEXANOL	C7H16O-E1	ISOHEPTANOL
C7H14O-D4	CIS-2-METHYLCYCLOHEXANOL	C7H16O-E2	ETHYL-TERT-PENTYL-ETHER
C7H14O-D5	TRANS-2-METHYLCYCLOHEXANOL	C7H16O2	PG-1-TERT-BUTYL-ETHER
C7H14O-D6	CIS-3-METHYLCYCLOHEXANOL	C7H16O2-D1	PG-2-TERT-BUTYL-ETHER
C7H14O-D7	TRANS-3-METHYLCYCLOHEXANOL	C7H16O3	DPG-MONOMETHYL-ETHER
C7H14O-D8	CIS-4-METHYLCYCLOHEXANOL	C7H16O3-D1	DIETHYLENE-GLYCOL-PROPYL-ETHER
C7H14O-D9	TRANS-4-METHYLCYCLOHEXANOL	C7H16S	N-HEPTYL-MERCAPTAN
C7H14O-E1	3-HEPTANONE	C7H17N	1-AMINOHEPTANE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C8H4CL2O2	ISOPHTHALOYL-CHLORIDE	C8H10O-5	2,3-XYLENOL
C8H4O3	PHTHALIC-ANHYDRIDE	C8H10O-6	2,4-XYLENOL
C8H6	ETHYNYLBENZENE	C8H10O-7	2,5-XYLENOL
C8H6O2	TEREPHTHALDEHYDE	C8H10O-8	2,6-XYLENOL
C8H6O3	4-CARBOXYBENZALDEHYDE	C8H10O-9	3,4-XYLENOL
C8H6O4-D1	ISOPHTHALIC-ACID	C8H10O-D1	ALPHA-METHYLBENZYL-ALCOHOL
C8H6O4-D2	PHTHALIC-ACID	C8H10O2	ETHYLBENZENE-HYDROPEROXIDE
C8H6O4-D3	TEREPHTHALIC-ACID	C8H10O4	ETHYLENE-GLYCOL-DIACRYLATE
C8H6S	BENZOTHIOPHENE	C8H11N	N,N-DIMETHYLANILINE
C8H7N	INDOLE	C8H11N-D0	O-ETHYLANILINE
C8H7N-D1	PHENYLACETONITRILE	C8H11N-D1	2,4,6-TRIMETHYLPYRIDINE
C8H8	STYRENE	C8H11N-D2	N-ETHYLANILINE
C8H8O	METHYL-PHENYL-KETONE	C8H11NO	P-PHENETIDINE
C8H8O-D0	P-TOLUALDEHYDE	C8H12	VINYLCYCLOHEXENE
C8H8O-D1	4-HYDROXYSTYRENE	C8H12-D1	1,5-CYCLOOCTADIENE
C8H8O2	METHYL-BENZOATE	C8H12O4-E1	1,4-CYCLOHEXANEDICARBOXYLIC-ACID
C8H8O2-D1	O-TOLUIC-ACID	C8H12O4-E2	DIETHYL-MALEATE
C8H8O2-D2	P-TOLUIC-ACID	C8H14	CYCLOOCTENE
C8H8O2-D3	BENZYL-FORMATE	C8H14-D1	1-OCTYNE
C8H8O2-D4	2-HYDROXYACETOPHENONE	C8H14-D2	2,5-DIMETHYL-1,5-HEXADIENE
C8H8O2-D5	4-HYDROXYACETOPHENONE	C8H14-D3	2,5-DIMETHYL-2,4-HEXADIENE
C8H8O3	METHYL-SALICYLATE	C8H14O2	N-BUTYL-METHACRYLATE
C8H8O3-D1	VANILLIN	C8H14O2-D1	ISOBUTYL-METHACRYLATE
C8H9NO	ACETANILIDE	C8H14O2-D2	CYCLOHEXYL-ACETATE
C8H9NO2	ACETAMINOPHEN	C8H14O3	BUTYRIC-ANHYDRIDE
C8H10-1	O-XYLENE	C8H14O4	DIETHYL-SUCCINATE
C8H10-2	M-XYLENE	C8H14O4-D1	SUBERIC-ACID
C8H10-3	P-XYLENE	C8H16-1	1,1-DIMETHYLCYCLOHEXANE
C8H10-4	ETHYLBENZENE	C8H16-10	1,1,3-TRIMETHYLCYCLOPENTANE
C8H10N4O2	CAFFEINE	C8H16-11	CIS,CIS,TRANS-1,2,4-TRIMETHYLCYC
C8H10O	2-PHENYLETHANOL	C8H16-12	CIS,TRANS,CIS-1,2,4-TRIMETHYLCYC
C8H10O-1	O-ETHYLPHENOL	C8H16-13	1-METHYL-1-ETHYLCYCLOPENTANE
C8H10O-10	3,5-XYLENOL	C8H16-14	N-PROPYLCYCLOPENTANE
C8H10O-2	M-ETHYLPHENOL	C8H16-15	ISOPROPYLCYCLOPENTANE
C8H10O-3	P-ETHYLPHENOL	C8H16-16	1-OCTENE
C8H10O-4	PHENETOLE	C8H16-17	TRANS-2-OCTENE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C8H16-2	CIS-1,2-DIMETHYLCYCLOHEXANE	C8H18-15	2,3,4-TRIMETHYLPENTANE
C8H16-3	TRANS-1,2-DIMETHYLCYCLOHEXANE	C8H18-16	2-METHYL-3-ETHYLPENTANE
C8H16-4	CIS-1,3-DIMETHYLCYCLOHEXANE	C8H18-17	3-METHYL-3-ETHYLPENTANE
C8H16-5	TRANS-1,3-DIMETHYLCYCLOHEXANE	C8H18-2	2-METHYLHEPTANE
C8H16-6	CIS-1,4-DIMETHYLCYCLOHEXANE	C8H18-3	3-METHYLHEPTANE
C8H16-7	TRANS-1,4-DIMETHYLCYCLOHEXANE	C8H18-4	4-METHYLHEPTANE
C8H16-8	ETHYLCYCLOHEXANE	C8H18-5	2,2-DIMETHYLHEXANE
C8H16-9	1,1,2-TRIMETHYLCYCLOPENTANE	C8H18-6	2,3-DIMETHYLHEXANE
C8H16-D1	2-ETHYL-1-HEXENE	C8H18-7	2,4-DIMETHYLHEXANE
C8H16-D2	TRANS-3-OCTENE	C8H18-8	2,5-DIMETHYLHEXANE
C8H16-D3	TRANS-4-OCTENE	C8H18-9	3,3-DIMETHYLHEXANE
C8H16-D4	2,4,4-TRIMETHYL-1-PENTENE	C8H18O	DI-TERT-BUTYL-ETHER
C8H16-D5	2,4,4-TRIMETHYL-2-PENTENE	C8H18O-1	1-OCTANOL
C8H16-D6	CYCLOOCTANE	C8H18O-2	2-OCTANOL
C8H16-D7	CIS-2-OCTENE	C8H18O-3	2-ETHYLHEXANOL
C8H16-D8	CIS-4-OCTENE	C8H18O-4	BUTYL-ETHER
C8H16-D9	CIS-3-OCTENE	C8H18O-D1	DI-SEC-BUTYL-ETHER
C8H16-E1	2,3-DIMETHYL-1-HEXENE	C8H18O-D2	DIISOBUTYL-ETHER
C8H16-E2	2-METHYL-1-HEPTENE	C8H18O-D3	ETHYL-N-HEXYL-ETHER
C8H16O	2-ETHYLHEXANAL	C8H18O2	DI-T-BUTYL-PEROXIDE
C8H16O-E1	1-OCTANAL	C8H18O2S	DI-N-BUTYL-SULFONE
C8H16O-E2	2-OCTANONE	C8H18O3	DIETHYLENE-GLYCOL-MONOBUTYL-ETHE
C8H16O2-D1	N-BUTYL-N-BUTYRATE	C8H18O3-D1	DIETHYLENE-GLYCOL-DIETHYL-ETHER
C8H16O2-D2	ISOBUTYL-ISOBUTYRATE	C8H18O4	TRIETHYLENE-GLYCOL-DIMETHYL-ETHE
C8H16O2-D3	N-OCTANOIC-ACID	C8H18SO4	DI-N-BUTYL-SULFATE
C8H16O2-D4	N-HEXYL-ACETATE	C8H18O5	TETRAETHYLENE-GLYCOL
C8H16O2-D5	N-HEPTYL-FORMATE	C8H18S	TERT-OCTYLMERCAPTAN
C8H16O2-D6	2-ETHYL-HEXANOIC-ACID	C8H18S-D1	N-OCTYL-MERCAPTAN
C8H16O4	2-2-ETHOXYETHOXY-ETHYL-ACETATE	C8H19N	DIBUTYLAMINE
C8H18	2,2,3,3-TETRAMETHYLBUTANE	C8H19N-D0	N-OCTYLAMINE
C8H18-1	N-OCTANE	C8H19N-D1	DIISOBUTYLAMINE
C8H18-10	3,4-DIMETHYLHEXANE	C8H20PB	TETRAETHYL-LEAD
C8H18-11	3-ETHYLHEXANE	C8H20SI	TETRAETHYL-SILANE
C8H18-12	2,2,3-TRIMETHYLPENTANE	C8H23N5	TETRAETHYLENEPENTAMINE
C8H18-13	2,2,4-TRIMETHYLPENTANE	C8H24O4SI4	OCTAMETHYLCYCLOTETRASILOXANE
C8H18-14	2,3,3-TRIMETHYLPENTANE	C9H4O5	TRIMELLITIC-ANHYDRIDE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C9H6N2O2	TOLUENE-DIISOCYANATE	C9H14O6	GLYCERYL-TRIACETATE
C9H7N-D1	ISOQUINOLINE	C9H16O4	AZELAIC-ACID
C9H7N-D2	QUINOLINE	C9H18-1	N-PROPYLCYCLOHEXANE
C9H7NO	8-HYDROXYQUINOLINE	C9H18-2	ISOPROPYLCYCLOHEXANE
C9H8	INDENE	C9H18-3	1-NONENE
C9H8O	2-METHYLBENZOFURAN	C9H18-D1	N-BUTYLCYCLOPENTANE
C9H8O2	CINNAMIC-ACID	C9H18O	1-NONANAL
C9H8O4	ACETYLSALICYLIC-ACID	C9H18O-D1	DIISOBUTYL-KETONE
C9H10	ALPHA-METHYL-STYRENE	C9H18O-E1	2-NONANONE
C9H10-E1	INDANE	C9H18O-E2	5-NONANONE
C9H10-E2	M-METHYL-STYRENE	C9H18O2	N-NONANOIC-ACID
C9H10-E3	O-METHYL-STYRENE	C9H18O2-D1	N-BUTYL-VALERATE
C9H10-E4	P-METHYL-STYRENE	C9H18O2-D2	N-OCTYL-FORMATE
C9H10-E5	CIS-1-PROPENYLBENZENE	C9H18O2-D3	N-HEPTYL-ACETATE
C9H10-E6	TRANS-1-PROPENYLBENZENE	C9H18O4	DPG-MONOMETHYL-ETHER-ACETATE
C9H10O2	ETHYL-BENZOATE	C9H20-1	N-NONANE
C9H10O2-D0	BENZYL-ACETATE	C9H20-2	2,2,3-TRIMETHYLHEXANE
C9H10O3	ETHYL-VANILLIN	C9H20-3	2,2,4-TRIMETHYLHEXANE
C9H10O3-D1	ACETOVANILLONE	C9H20-4	2,2,5-TRIMETHYLHEXANE
C9H11NO	P-DIMETHYLAMINOBENZALDEHYDE	C9H20-5	3,3-DIETHYLPENTANE
C9H11NO2	L-PHENYLALANINE	C9H20-6	2,2,3,3-TETRAMETHYLPENTANE
C9H12-1	N-PROPYLBENZENE	C9H20-7	2,2,3,4-TETRAMETHYLPENTANE
C9H12-2	ISOPROPYLBENZENE	C9H20-8	2,2,4,4-TETRAMETHYLPENTANE
C9H12-3	1-METHYL-2-ETHYLBENZENE	C9H20-9	2,3,3,4-TETRAMETHYLPENTANE
C9H12-4	1-METHYL-3-ETHYLBENZENE	C9H20-D1	2-METHYLOCTANE
C9H12-5	1-METHYL-4-ETHYLBENZENE	C9H20-D2	3-METHYLOCTANE
C9H12-6	1,2,3-TRIMETHYLBENZENE	C9H20-D3	4-METHYLOCTANE
C9H12-7	1,2,4-TRIMETHYLBENZENE	C9H20-E1	2,2-DIMETHYLHEPTANE
C9H12-8	1,3,5-TRIMETHYLBENZENE	C9H20-E2	2,6-DIMETHYLHEPTANE
C9H12-D1	VINYLNORBORNENE	C9H20-E3	2,2-DIMETHYL-3-ETHYLPENTANE
C9H12O	BENZYL-ETHYL-ETHER	C9H20-E4	2,4-DIMETHYL-3-ETHYLPENTANE
C9H12O-D1	1-PHENYL-1-PROPANOL	C9H20-E5	3-ETHYLHEPTANE
C9H12O-D2	1-PHENYL-2-PROPANOL	C9H20-E6	2,4,4-TRIMETHYLHEXANE
C9H12O-E1	DIMETHYL-PHENYL-CARBINOL	C9H20O-D1	2,6-DIMETHYL-4-HEPTANOL
C9H12O2	CUMENE-HYDROPEROXIDE	C9H20O-D2	1-NONANOL
C9H14O	ISOPHORONE	C9H20O-E1	2-NONANOL

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C9H20O4	TRIPROPYLENE-GLYCOL	C10H14-E1	2-ETHYL-M-XYLENE
C9H20S	N-NONYL-MERCAPTAN	C10H14-E10	1-METHYL-4-N-PROPYLBENZENE
C9H21N-D1	N-NONYLAMINE	C10H14-E2	2-ETHYL-P-XYLENE
C9H21N-D2	TRIPROPYLAMINE	C10H14-E3	4-ETHYL-M-XYLENE
C10H6O8	PYROMELLITIC-ACID	C10H14-E4	4-ETHYL-O-XYLENE
C10H7BR	1-BROMONAPHTHALENE	C10H14-E5	5-ETHYL-M-XYLENE
C10H7CL	1-CHLORONAPHTHALENE	C10H14-E6	1,2,3,5-TETRAMETHYL-BENZENE
C10H8	NAPHTHALENE	C10H14-E7	1,2,3,4-TETRAMETHYL-BENZENE
C10H9N	QUINALDINE	C10H14-E8	1-METHYL-2-N-PROPYLBENZENE
C10H10-D1	M-DIVINYLBENZENE	C10H14-E9	1-METHYL-3-N-PROPYLBENZENE
C10H10-D2	1-METHYLINDENE	C10H14O	P-TERT-BUTYLPHENOL
C10H10-D3	2-METHYLINDENE	C10H14O2	P-TERT-BUTYLCATECHOL
C10H10O4-D1	O-DIMETHYL-PHTHALATE	C10H15N	N-BUTYLANILINE
C10H10O4-D2	DIMETHYL-TEREPHTHALATE	C10H15N-E1	N,N-DIETHYLANILINE
C10H10O4-D3	DIMETHYL-ISOPHTHALATE	C10H15N-E2	2,6-DIETHYLANILINE
C10H11NO2	ACETOACETANILIDE	C10H16-D1	D-LIMONENE
C10H12	1,2,3,4-TETRAHYDRONAPHTHALENE	C10H16-D2	ALPHA-PINENE
C10H12-D0	DICYCLOPENTADIENE	C10H16-D3	BETA-PINENE
C10H12-E1	2-PHENYLBUTENE-1	C10H16-D4	TERPINOLENE
C10H12-E2	CIS-2-PHENYLBUTENE-2	C10H16-D5	ADAMANTANE
C10H12-E3	TRANS-2-PHENYLBUTENE-2	C10H16-E1	CAMPHENE
C10H12O	ANETHOLE	C10H16-E2	ALPHA-PHELLANDRENE
C10H12O2	N-PROPYL-BENZOATE	C10H16-E3	BETA-PHELLANDRENE
C10H12O4	DIALLYL-MALEATE	C10H16-E4	ALPHA-TERPINENE
C10H14-1	N-BUTYLBENZENE	C10H16-E5	GAMMA-TERPINENE
C10H14-2	ISOBUTYLBENZENE	C10H16N2O8	ETHYLENEDIAMINETETRAACETIC-ACID
C10H14-3	SEC-BUTYLBENZENE	C10H16O	CAMPHOR
C10H14-4	TERT-BUTYLBENZENE	C10H16O4	DIPROPYL-MALEATE
C10H14-5	1-METHYL-2-ISOPROPYLBENZENE	C10H18-1	CIS-DECALIN
C10H14-6	1-METHYL-3-ISOPROPYLBENZENE	C10H18-2	TRANS-DECALIN
C10H14-7	1-METHYL-4-ISOPROPYLBENZENE	C10H18O4	SEBACIC-ACID
C10H14-8	1,4-DIETHYLBENZENE	C10H19N	CAPRINITRILE
C10H14-9	1,2,4,5-TETRAMETHYLBENZENE	C10H19O6PS2	MALATHION
C10H14-D1	M-DIETHYLBENZENE	C10H20-1	N-BUTYLCYCLOHEXANE
C10H14-D2	O-DIETHYLBENZENE	C10H20-2	ISOBUTYLCYCLOHEXANE
C10H14-D3	1,2-DIMETHYL-3-ETHYLBENZENE	C10H20-3	SEC-BUTYLCYCLOHEXANE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C10H20-4	TERT-BUTYLCYCLOHEXANE	C11H10-2	2-METHYLNAPHTHALENE
C10H20-5	1-DECENE	C11H12	P-ISOPROPENYLSTYRENE
C10H20O	1-DECANAL	C11H14O2	BUTYL-BENZOATE
C10H20O-D1	L-MENTHOL	C11H16	N-PENTYLBENZENE
C10H20O2	P-MENTHANE-HYDROPEROXIDE	C11H16O	P-TERT-AMYLPHENOL
C10H20O2-D1	N-DECANOIC-ACID	C11H20O2	2-ETHYLHEXYL-ACRYLATE
C10H20O2-D2	2-ETHYLHEXYL-ACETATE	C11H22-1	N-HEXYLCYCLOPENTANE
C10H20O2-D3	ISOPENTYL-ISOVALERATE	C11H22-2	1-UNDECENE
C10H20O2-D4	N-OCTYL-ACETATE	C11H22O	1-UNDECANAL
C10H20O2-D5	N-NONYL-FORMATE	C11H22O2	N-NONYL-ACETATE
C10H20O4	DIGLYCOL-MONOBUTYL-ETHER-ACETATE	C11H22O2-D1	N-DECYL-FORMATE
C10H22-1	N-DECANE	C11H22O2-D2	METHYL-DECANOATE
C10H22-2	3,3,5-TRIMETHYLHEPTANE	C11H22O2-D3	N-UNDECANOIC-ACID
C10H22-3	2,2,3,3-TETRAMETHYLHEXANE	C11H24	N-UNDECANE
C10H22-4	2,2,5,5-TETRAMETHYLHEXANE	C11H24O	1-UNDECANOL
C10H22-D1	2,3-DIMETHYLOCTANE	C11H24S	UNDECYL-MERCAPTAN
C10H22-D2	2,4-DIMETHYLOCTANE	C11H25N	UNDECYLAMINE
C10H22-D3	2,5-DIMETHYLOCTANE	C12H6N2O2	1,5-NAPHTHALENE-DIISOCYANATE
C10H22-D4	2,6-DIMETHYLOCTANE	C12H8	ACENAPHTHALENE
C10H22-D5	2,7-DIMETHYLOCTANE	C12H8O	DIBENZOFURAN
C10H22-E1	2,2-DIMETHYL-OCTANE	C12H8S	DIBENZOTHIOPHENE
C10H22-E2	2-METHYLNONANE	C12H9N	DIBENZOPYRROLE
C10H22-E3	3-METHYLNONANE	C12H9N3O4	4,4-DINITRODIPHENYLAMINE
C10H22-E4	4-METHYLNONANE	C12H10	DIPHENYL
C10H22-E5	5-METHYLNONANE	C12H10-D0	ACENAPHTHENE
C10H22O	1-DECANOL	C12H10N2O2-A	O-NITRODIPHENYLAMINE
C10H22O-D0	ISODECANOL	C12H10N2O2-B	P-NITRODIPHENYLAMINE
C10H22O-D1	DI-N-PENTYL-ETHER	C12H10O	DIPHENYL-ETHER
C10H22O4	TRIPROPYLENE-GLYCOL-MONOMETHYL-E	C12H11N	DIPHENYLAMINE
C10H22O5	TETRAETHYLENE-GLYCOL-DIMETHYL-ET	C12H11N-D1	P-AMINODIPHENYL
C10H22S	N-DECYL-MERCAPTAN	C12H11N3-E1	P-AMINOAZOBENZENE
C10H23N	N-DECYLAMINE	C12H11N3-E2	1,3-DIPHENYLTRIAZENE
C10H23N-D1	DIAMYLAMINE	C12H12-E1	2,6-DIMETHYLNAPHTHALENE
C10H30SI4O3	DECAMETHYLTETRASILOXANE	C12H12-E2	2,7-DIMETHYLNAPHTHALENE
C10H30SI5O5	DECAMETHYLCYCLOPENTASILOXANE	C12H12-E3	1-ETHYLNAPHTHALENE
C11H10-1	1-METHYLNAPHTHALENE	C12H12-E4	2-ETHYLNAPHTHALENE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C12H12N2-D1	P-AMINODIPHENYLAMINE	C13H10	FLUORENE
C12H12N2-D2	HYDRAZOBENZENE	C13H10O	BENZOPHENONE
C12H12N2-D3	BENZIDINE	C13H12	DIPHENYLMETHANE
C12H14	1,2,3-TRIMETHYLINDENE	C13H14	1-N-PROPYLNAPHTHALENE
C12H14O4	DIETHYL-PHTHALATE	C13H18O2	IBUPROFEN
C12H14O6	BIS-2-HYDROXYETHYL-TEREPHTHALATE	C13H20	N-HEPTYLBENZENE
C12H16	CYCLOHEXYLBENZENE	C13H26-1	N-OCTYLCYCLOPENTANE
C12H16-D1	P-TERT-BUTYLSTYRENE	C13H26-2	1-TRIDECENE
C12H16-D2	4-ISOBUTYLSTYRENE	C13H26O	1-TRIDECANAL
C12H18-D1	M-DIISOPROPYLBENZENE	C13H26O2	METHYL-DODECANOATE
C12H18-D2	P-DIISOPROPYLBENZENE	C13H26O2-D1	N-BUTYL-NONANOATE
C12H18-D3	N-HEXYLBENZENE	C13H26O2-D2	N-TRIDECANOIC-ACID
C12H18-D4	P-TERT-BUTYL-ETHYLBENZENE	C13H28	N-TRIDECANE
C12H18O2	M-DIISOPROPYL-BENZENE-HYDROPEROX	C13H28O	1-TRIDECANOL
C12H18O2-D1	P-DIISOPROPYLBENZ-HYDROPEROXIDE	C14H8O2	ANTHRAQUINONE
C12H20O	2-CYCLOHEXYL-CYCLOHEXANONE	C14H10	DIPHENYLACETYLENE
C12H20O4	DIBUTYL-MALEATE	C14H10-1	ANTHRACENE
C12H22	BICYCLOHEXYL	C14H10-2	PHENANTHRENE
C12H22O11	SUCROSE	C14H10O4	BENZOYL-PEROXIDE
C12H23N	DICYCLOHEXYLAMINE	C14H12-D1	CIS-STILBENE
C12H24-1	N-HEPTYLCYCLOPENTANE	C14H12-D2	TRANS-STILBENE
C12H24-2	1-DODECENE	C14H12O2	BENZYL-BENZOATE
C12H24O	1-DODECANAL	C14H14-D1	1,1-DIPHENYLETHANE
C12H24O2	N-DODECANOIC-ACID	C14H14-D2	1,2-DIPHENYLETHANE
C12H24O2-E1	N-DECYL-ACETATE	C14H14O	DIBENZYL-ETHER
C12H26	N-DODECANE	C14H16	1-N-BUTYLNAPHTHALENE
C12H26O-1	DIHEXYLETHER	C14H16-D1	2,6-DIETHYLNAPHTHALENE
C12H26O-2	DODECANOL	C14H18O4	DIPROPYL-PHTHALATE
C12H26O3	DIETHYLENE-GLYCOL-DI-N-BUTYL-ETH	C14H20	DIAMANTANE
C12H26S	N-DODECYL-MERCAPTAN	C14H22	N-OCTYLBENZENE
C12H26S-E1	TERT-DODECYL-MERCAPTAN	C14H22O	P-TERT-OCTYLPHENOL
C12H27BO3	TRI-N-BUTYL-BORATE	C14H28-1	N-NONYLCYCLOPENTANE
C12H27N	TRIBUTYLAMINE	C14H28-2	1-TETRADECENE
C12H27N-D0	DODECYLAMINE	C14H28O2	N-TETRADECANOIC-ACID
C12H36SI6O6	DODECAMETHYLCYCLOHEXASILOXANE	C14H30	N-TETRADECANE
C13H9N	ACRIDINE	C14H30O	1-TETRADECANOL

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C14H31N	TETRADECYLAMINE	C17H36O	HEPTADECANOL
C14H42SI6O5	TETRADECAMETHYLHEXASILOXANE	C18H12	CHRYSENE
C15H10N2O2	DIPHENYLMETHANE-4,4-DIISOCYANATE	C18H13N3O4	4,4-DINITROTRIPHENYLAMINE
C15H12	1-PHENYLINDENE	C18H14-1	O-TERPHENYL
C15H16O	P-CUMYLPHENOL	C18H14-2	M-TERPHENYL
C15H16O2	BISPHENOL-A	C18H14-3	P-TERPHENYL
C15H18	1-N-PENTYLNAPHTHALENE	C18H15PO	TRIPHENYLPHOSPHINE-OXIDE
C15H24	N-NONYLBENZENE	C18H15O4P	TRIPHENYL-PHOSPHATE
C15H24O-D1	2,6-DI-TERT-BUTYL-P-CRESOL	C18H15P	TRIPHENYLPHOSPHINE
C15H24O-D2	NONYLPHENOL	C18H16N2	N-N-DIPHENYL-P-PHENYLENEDIAMINE
C15H30-1	N-DECYLCYCLOPENTANE	C18H20	2,4-DIPHENYL-4-METHYLPENTENE-1
C15H30-2	1-PENTADECENE	C18H22	2,3-DIMETHYL-2,3-DIPHENYLBUTANE
C15H30O2	PENTADECANOIC-ACID	C18H22O2	DICUMYLPEROXIDE
C15H32	N-PENTADECANE	C18H30	N-DODECYLBENZENE
C15H32O	1-PENTADECANOL	C18H30O2	LINOLENIC-ACID
C15H33N	TRIAMYLAMINE	C18H32O2	LINOLEIC-ACID
C16H10-D1	FLUORANTHENE	C18H34O2	OLEIC-ACID
C16H10-D2	PYRENE	C18H34O4-D1	DIBUTYL-SEBACATE
C16H12	1-PHENYLNAPHTHALENE	C18H34O4-D2	DIHEXYL-ADIPATE
C16H20	1-N-HEXYLNAPHTHALENE	C18H36-1	1-OCTADECENE
C16H22O4	DIBUTYL-O-PHTHALATE	C18H36-2	N-TRIDECYLCYCLOPENTANE
C16H22O4-D1	DIISOBUTYL-PHTHALATE	C18H36O2	STEARIC-ACID
C16H24	1-N-HEXYL-1,2,3,4-TETRAHYDRONAPH	C18H38	N-OCTADECANE
C16H26	N-DECYLBENZENE	C18H38O	1-OCTADECANOL
C16H32-1	N-DECYLCYCLOHEXANE	C18H38O-D0	DINONYL-ETHER
C16H32-2	1-HEXADECENE	C19H16	TRIPHENYLMETHANE
C16H32O2	N-HEXADECANOIC-ACID	C19H26	1-N-NONYLNAPHTHALENE
C16H34	N-HEXADECANE	C19H32	N-TRIDECYLBENZENE
C16H34O	1-HEXADECANOL	C19H36O2	METHYL-OLEATE
C16H34O-D1	DI-N-OCTYL-ETHER	C19H38	N-TETRADECYLCYCLOPENTANE
C17H28	N-UNDECYLBENZENE	C19H38-D1	1-NONADECENE
C17H34	N-DODECYLCYCLOPENTANE	C19H38O2	NONADECANOIC-ACID
C17H34-D1	1-HEPTADECENE	C19H40	N-NONADECANE
C17H34O2	N-HEPTADECANOIC-ACID	C19H40O	1-NONADECANOL
C17H34O2-D1	ISOPROPYL-MYRISTATE	C20H16	TRIPHENYLETHYLENE
C17H36	N-HEPTADECANE	C20H18	1,1,2-TRIPHENYLETHANE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
C20H28	1-N-DECYLNAPHTHALENE	C30H62	N-TRIACONTANE
C20H30O2	ABIETIC-ACID	C30H62-D1	SQUALANE
C20H31N	DEHYDROABIETYLAMINE	C32H66	N-DOTRIACONTANE
C20H34	N-TETRADECYLBENZENE	C36H74	N-HEXATRIACONTANE
C20H37NAO7S	DIOCTYLSODIUM-SULFOSUCCINATE	CA	CALCIUM
C20H38O2	CETYL-METHACRYLATE	CACL2	CALCIUM-CHLORIDE
C20H40	N-PENTADECYLCYCLOPENTANE	CACL2O2	CALCIUM-HYPOCHLORITE
C20H40-D1	1-EICOSENE	CAF2	CALCIUM-FLUORIDE
C20H40O2	N-EICOSANIC-ACID	CA(OH)2	CALCIUM-HYDROXIDE
C20H42	N-EICOSANE	CAO	CALCIUM-OXIDE
C20H42O	1-EICOSANOL	CASO4	CALCIUM-SULFATE
C21H21O4P	TRI-O-CRESYL-PHOSPHATE	CUCL	CUPROUS-CHLORIDE
C21H36	N-PENTADECYLBENZENE	CLO3F	PERCHLORYL-FLUORIDE
C21H42	N-HEXADECYLCYCLOPENTANE	HCLO	HYPOCHLOROUS-ACID
C21H44	N-HENEICOSANE	CLHO3S	CHLOROSULFONIC-ACID
C22H38	N-HEXADECYLBENZENE	HCLO4	PERCHLORIC-ACID
C22H42O4	DI-2-ETHYLHEXYL-ADIPATE	NH4CL	AMMONIUM-CHLORIDE
C22H44O2	N-BUTYL-STEARATE	CLH4NO	HYDROXYLAMINE-HYDROCHLORIDE
C22H46	N-DOCOSANE	NH4CLO4	AMMONIUM-PERCHLORATE
C23H40	N-HEPTADECYLBENZENE	KCL	POTASSIUM-CHLORIDE
C23H48	N-TRICOSANE	NOCL	NITROSYL-CHLORIDE
C24H38O4	DIOCTYL-PHTHALATE	NACL	SODIUM-CHLORIDE
C24H38O4-D1	DIISOOCTYL-PHTHALATE	NACLO	SODIUM-HYPOCHLORITE
C24H38O4-D2	DIOCTYL-TEREPHTHALATE	NACLO3	SODIUM-CHLORATE
C24H42	N-OCTADECYLBENZENE	CLO2	CHLORINE-DIOXIDE
C24H42O	DINONYLPHENOL	KCLO3	POTASSIUM-CHLORATE
C24H50	N-TETRACOSANE	CL2	CHLORINE
C25H20	TETRAPHENYLMETHANE	CUCL2	CUPRIC-CHLORIDE
C25H52	N-PENTACOSANE	SCL2	SULFUR-DICHLORIDE
C26H20	TETRAPHENYLETHYLENE	GACL3	GALLIUM-TRICHLORIDE
C26H22	1,1,2,2-TETRAPHENYLETHANE	NCL3	NITROGEN-TRICHLORIDE
C26H54	N-HEXACOSANE	POCL3	PHOSPHORUS-OXYCHLORIDE
C27H56	N-HEPTACOSANE	VCL3O	VANADIUM-OXYTRICHLORIDE
C28H46O4	DIISODECYL-PHTHALATE	PCL3	PHOSPHORUS-TRICHLORIDE
C28H58	N-OCTACOSANE	PSCL3	PHOSPHORUS-THIOCHLORIDE
C29H60	N-NONACOSANE	SICL4	SILICON-TETRACHLORIDE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
VCL4	VANADIUM-TETRACHLORIDE	NANH2	SODIUM-AMIDE
PCL5	PHOSPHORUS-PENTACHLORIDE	NAH2PO4	MONOSODIUM-PHOSPHATE
CRO3	CHROMIUM-TRIOXIDE	H2O	WATER
NA2CR2O7	SODIUM-DICHROMATE	H2O2	HYDROGEN-PEROXIDE
CUSO4	CUPRIC-SULFATE	H2SO4	SULFURIC-ACID
D2	DEUTERIUM	H2S	HYDROGEN-SULFIDE
D2O	DEUTERIUM-OXIDE	H2SE	HYDROGEN-SELENIDE
FHO3S	FLUOROSULFONIC-ACID	H3N	AMMONIA
NAF	SODIUM-FLUORIDE	H3NO	HYDROXYLAMINE
F2	FLUORINE	H3NO3S	SULFAMIC-ACID
NF3	NITROGEN-TRIFLUORIDE	H3PO2	HYPOPHOSPHOROUS-ACID
SIF4	SILICON-TETRAFLUORIDE	H3PO3	PHOSPHOROUS-ACID
SF6	SULFUR-HEXAFLUORIDE	H3PO4	ORTHOPHOSPHORIC-ACID
FE	IRON	H4N2	HYDRAZINE
FECL2	FERROUS-CHLORIDE	NH4NO3	AMMONIUM-NITRATE
FECL3	FERRIC-CHLORIDE	NH4OH	AMMONIUM-HYDROXIDE
FEO	FERROUS-OXIDE	NH5SO3	AMMONIUM-BISULFITE
FESO4	FERROUS-SULFATE	NH4HSO4	AMMONIUM-BISULFATE
FE2O3	FERRIC-OXIDE	NH6PO4	AMMONIUM-PHOSPHATE
GE	GERMANIUM	N2H8SO3	AMMONIUM-SULFITE
GEH4	GERMANIUM-TETRAHYDRIDE	(NH4)2SO4	AMMONIUM-SULFATE
HBR	HYDROGEN-BROMIDE	(NH4)2HPO4	DIAMMONIUM-PHOSPHATE
HCL	HYDROGEN-CHLORIDE	HE-3	HELIUM-3
HF	HYDROGEN-FLUORIDE	HE-4	HELIUM-4
HI	HYDROGEN-IODIDE	HG	MERCURY
KOH	POTASSIUM-HYDROXIDE	I2	IODINE
K2HPO4	DIPOTASSIUM-PHOSPHATE	K	POTASSIUM
HNO2	NITROUS-ACID	KI	POTASSIUM-IODIDE
HNO3	NITRIC-ACID	KR	KRYPTON
HNO5S	NITROSYLSULFURIC-ACID	LI	LITHIUM
NAOH	SODIUM-HYDROXIDE	MGN2O6	MAGNESIUM-NITRATE
NAHSO3	SODIUM-BISULFITE	MGO	PERICLASE
NAHSO4	SODIUM-BISULFATE	MGSO4	MAGNESIUM-SULFATE
NA2HPO4	DISODIUM-PHOSPHATE	NANO2	SODIUM-NITRITE
H2	HYDROGEN	NANO3	SODIUM-NITRATE
H2-PARA	HYDROGEN-PARA	NO	NITRIC-OXIDE

continued

Table 1.9B Components Available in the PURE93 Databank (continued)

Alias	Component Name	Alias	Component Name
NO2	NITROGEN-DIOXIDE	SIO2	SILICON-DIOXIDE
N2	NITROGEN	TIO2	TITANIUM-OXIDE(RUTILE)
N2F4	TETRAFLUOROHYDRAZINE	O3	OZONE
N2O	NITROUS-OXIDE	O3S	SULFUR-TRIOXIDE
N2O3	NITROGEN-TRIOXIDE	ZNSO4	ZINC-SULFATE
N2O4	NITROGEN-TETROXIDE	(P2O5)2	PHOSPHORUS-PENTOXIDE(DIMERIC)
N2O5	NITROGEN-PENTOXIDE	P	PHOSPHORUS
NA	SODIUM	PH3	PHOSPHINE
NAI	SODIUM-IODIDE	P4S10	PHOSPHORUS-PENTASULFIDE
NA2O2	SODIUM-PEROXIDE	S	SULFUR
NA2S2O3	SODIUM-THIOSULFATE	SOCL2	THIONYL-CHLORIDE
NA2SIO3	SODIUM-SILICATE	SO2CL2	SULFURYL-CHLORIDE
NA2SO4	SODIUM-SULFATE	SBCL3	ANTIMONY-TRICHLORIDE
NA2S2O4	SODIUM-HYDROSULFITE	SIHCL3	TRICHLOROSILANE
NA2S	SODIUM-SULFIDE	SIH2CL2	DICHLOROSILANE
NA3PO4	TRISODIUM-PHOSPHATE	SIH4	SILANE
NA4P2O7	TETRASODIUM-PYROPHOSPHATE	SI2H6	DISILANE
NA5P3O10	SODIUM-TRIPOLYPHOSPHATE	SI	SILICON
NA6P6O18	SODIUM-HEXAMETAPHOSPHATE	TICL3	TITANIUM-TRICHLORIDE
NE	NEON	TICL4	TITANIUM-TETRACHLORIDE
ZNO	ZINC-OXIDE	V	VANADIUM
O2	OXYGEN	XE	XENON
O2S	SULFUR-DIOXIDE	ZN	ZINC

Table 1.10 Parameters Available in the PURE856 Databank

Parameter Name	Description
AIT†	Auto ignition temperature
ATOMNO ††	Atomic number of each atom in the compound
CPIGDP	DIPPR ideal gas heat capacity coefficients
CPLDIP	DIPPR liquid heat capacity coefficients
CPSDIP	DIPPR solid heat capacity coefficients
DELTA	Solubility parameter at 298.2 K
DGFORM	Standard Gibbs free energy of formation; ideal gas at 298.2 K
DHFORM	Standard heat of formation; ideal gas at 298.2 K
DHVLB	Heat of vaporization at TB
DHVLDP	DIPPR heat of vaporization coefficients
DNLDIP	DIPPR liquid density coefficients
DNSDIP	DIPPR solid density coefficients
ENT†	Absolute entropy of formation at 298.2 K
FLML†	Lower flammability limit
FLMU†	Upper flammability limit
FP	Flash point
GMUQQ	UNIQUAC area parameter
GMUQR	UNIQUAC volume parameter
HCOM	Standard enthalpy of combustion at 298.2 K
HFUS	Enthalpy of fusion at melting point
KLDIP	DIPPR liquid thermal conductivity coefficients
KVDIP	DIPPR vapor thermal conductivity coefficients
MULDIP	DIPPR liquid viscosity coefficients
MUP	Dipole moment
MUVDIP	DIPPR vapor viscosity coefficients
MW	Molecular weight
NOATOM ††	Number of occurrences of each atom
OMEGA	Pitzer acentric factor
OMGCTD	Acentric factor for the COSTALD model
PC	Critical pressure
PLXANT	Extended Antoine vapor pressure coefficients

† *These parameters are not used in Aspen Plus models but can be accessed by user or in-house models.*

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

continued

Table 1.10 Parameters Available in the PURE856 Databank (continued)

Parameter Name	Description
RGYR	Radius of gyration
RI	Refractive index at 298.2 K
RKTZRA	Rackett liquid density parameter
SIGDIP	DIPPR surface tension coefficients
SVRDIP†	Second virial coefficient
TB	Normal boiling point
TC	Critical temperature
TFP	Normal freezing point
TPP†	Triple point pressure
TPT	Triple point temperature
UFGRP†††	Functional group information for the UNIFAC model
VB	Liquid molar volume at TB
VC	Critical volume
VLSTD	Standard liquid volume at 60°F
VSTCTD	Characteristic volume for the COSTALD model
ZC	Critical compressibility factor

† *These parameters are not used in Aspen Plus models but can be accessed by user or in-house models.*

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

††† *Contains UNIFAC functional group number and number of occurrences of each group.*

Table 1.11 Components Available in PURE856 Databank

Alias	Component Name	Alias	Component Name
AIR	AIR	CHN	HYDROGEN-CYANIDE
AG	SILVER	CHNAO2	SODIUM-FORMATE
AL	ALUMINUM	NAHCO3	SODIUM-BICARBONATE
ALCL3	ALUMINUM-CHLORIDE	CH2BRCL	BROMOCHLOROMETHANE
'AL(OH)3'	GIBBSITE	CH2BR2	DIBROMOMETHANE
ALO4P	ALUMINUM-PHOSPHATE--ORTHO-	CH2CL2	DICHLOROMETHANE
AL2O3-2	ALUMINUM-OXIDE	CH2F2	DIFLUOROMETHANE
AL2O12S3	ALUMINUM-SULFATE	CH2I2	DIIODOMETHANE
AR	ARGON	CH2O	FORMALDEHYDE
ASH3	ARSINE	CH2O2	FORMIC-ACID
BCL3	BORON-TRICHLORIDE	CH3BR	METHYL-BROMIDE
BF3	BORON-TRIFLUORIDE	CH3CL	METHYL-CHLORIDE
H3BO3	HYDROGEN-ORTHOBORATE	CH3CL3SI	METHYL-TRICHLOROSILANE
B2H6	DIBORANE	CH3F	METHYL-FLUORIDE
B4H20NA2O17	BORAX	CH3I	METHYL-IODIDE
BRNA	SODIUM-BROMIDE	CH3NO	FORMAMIDE
BR2	BROMINE	CH3NO2	NITROMETHANE
C	'CARBON(GRAPHITE)'	CH4	METHANE
CBAO3	BARIUM-CARBONATE	CH4CL2SI	METHYL-DICHLOROSILANE
CBRCLF2	BROMOCHLORODIFLUOROMETHANE	CH4N2O	UREA
CBRCL3	BROMOTRICHLOROMETHANE	CH4N2S	THIOUREA
CBRF3	TRIFLUOROBROMOMETHANE	CH4O	METHANOL
CBR2F2	DIBROMODIFLUOROMETHANE	CH4O3S	METHANESULFONIC-ACID
CACO3-2	'CALCIUM-CARBONATE(CALCITE)'	CH4S	METHYL-MERCAPTAN
CCLF3	CHLOROTRIFLUOROMETHANE	CH5CLSI	METHYL-CHLOROSILANE
CCLN	CYANOGEN-CHLORIDE	CH5N	METHYL-AMINE
CCL2F2	DICHLORODIFLUOROMETHANE	CH6SI	METHYL-SILANE
CCL2O	PHOSGENE	CK2O3	POTASSIUM-CARBONATE
CCL3F	TRICHLOROFLUOROMETHANE	CNNA	SODIUM-CYANIDE
CCL4	CARBON-TETRACHLORIDE	CN4O8	TETRANITROMETHANE
CF4	CARBONTETRAFLUORIDE	NA2CO3	SODIUM-CARBONATE
CHBR3	TRIBROMOMETHANE	CO	CARBON-MONOXIDE
CHCLF2	CHLORODIFLUOROMETHANE	CF2O	CARBONYL-FLUORIDE
CHCL2F	DICHLOROMONOFLUOROMETHANE	COS	CARBONYL-SULFIDE
CHCL3	CHLOROFORM	CO2	CARBON-DIOXIDE
CHF3	TRIFLUOROMETHANE	CS2	CARBON-DISULFIDE

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
CSI	SILICON-CARBIDE	C2H2O	KETENE
C2BRF3	BROMOTRIFLUOROETHYLENE	C2H2O2	GLYOXAL
C2BR2F4	1,2-DIBROMOTETRAFLUOROETHANE	C2H2O4	OXALIC-ACID
C2CLF3	CHLOROTRIFLUOROETHYLENE	C2H3BR	VINYL-BROMIDE
C2CLF5	CHLOROPENTAFLUOROETHANE	C2H3CL	VINYL-CHLORIDE
C2CL2F4-2	1,2-DICHLORO-1,1,2,2-TETRAFLUORO	C2H3CLF2	1-CHLORO-1,1-DIFLUOROETHANE
C2CL3F3	1,2,2-TRICHLORO-1,1,2-TRIFLUOROE	C2H3CLO	ACETYL-CHLORIDE
C2CL4	TETRACHLOROETHYLENE	C2H3CLO-D0	CHLOROACETALDEHYDE
C2CL4F2	1,1,2,2-TETRACHLORO-1,2-DIFLUORO	C2H3CLO2	CHLOROACETIC-ACID
C2CL4F2-D1	1,1,1,2-TETRACHLORODIFLUOROETHAN	C2H3CLO2-D1	METHYL-CHLOROFORMATE
C2CL4O	TRICHLOROACETYL-CHLORIDE	C2H3CL3	1,1,2-TRICHLOROETHANE
C2CL6	HEXACHLOROETHANE	C2H3CL3-D0	1,1,1-TRICHLOROETHANE
C2F4	PERFLUOROETHENE	C2H3F	VINYL-FLUORIDE
C2F6	PERFLUOROETHANE	C2H3F3	1,1,1-TRIFLUOROETHANE
C2HBRCLF3	HALOTHANE	C2H3N	ACETONITRILE
C2HCLF2	2-CHLORO-1,1-DIFLUOROETHYLENE	C2H3NO	METHYL-ISOCYANATE
C2HCL3	TRICHLOROETHYLENE	C2H4	ETHYLENE
C2HCL3O	DICHLOROACETYL-CHLORIDE	C2H4BR2	1,2-DIBROMOETHANE
C2HCL3O-D1	TRICHLOROACETALDEHYDE	C2H4BR2-D1	1,1-DIBROMOETHANE
C2HCL3O2	TRICHLOROACETIC-ACID	C2H4CL2-1	1,1-DICHLOROETHANE
C2HCL5	PENTACHLOROETHANE	C2H4CL2-2	1,2-DICHLOROETHANE
C2HF3O2	TRIFLUOROACETIC-ACID	C2H4CL2O	BIS-CHLOROMETHYL-ETHER
C2HF5	PENTAFLUOROETHANE	C2H4F2	1,1-DIFLUOROETHANE
C2H2	ACETYLENE	C2H4F2-D1	1,2-DIFLUOROETHANE
C2H2BR4	1,1,2,2-TETRABROMOETHANE	C2H4O-1	ACETALDEHYDE
C2H2CL2-D1	1,1-DICHLOROETHYLENE	C2H4O-2	ETHYLENE-OXIDE
C2H2CL2-D2	CIS-1,2-DICHLOROETHYLENE	C2H4O2-1	ACETIC-ACID
C2H2CL2-D3	TRANS-1,2-DICHLOROETHYLENE	C2H4O2-2	METHYL-FORMATE
C2H2CL2O	CHLOROACETYL-CHLORIDE	C2H4O3-D1	GLYCOLIC-ACID
C2H2CL2O-D1	DICHLOROACETALDEHYDE	C2H4O3-D2	PERACETIC-ACID
C2H2CL2O2	DICHLOROACETIC-ACID	C2H5BR	ETHYL-BROMIDE
C2H2CL3F	1,1,1-TRICHLOROFLUOROETHANE	C2H5CL	ETHYL-CHLORIDE
C2H2CL4-D1	1,1,1,2-TETRACHLOROETHANE	C2H5CLO	2-CHLOROETHANOL
C2H2CL4-D2	1,1,2,2-TETRACHLOROETHANE	C2H5F	ETHYL-FLUORIDE
C2H2F2	1,1-DIFLUOROETHYLENE	C2H5I	ETHYL-IODIDE
C2H2F4	1,1,1,2-TETRAFLUOROETHANE	C2H5N	ETHYLENE-IMINE

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
C2H5NO-D1	ACETAMIDE	C3H4O3	ETHYLENE-CARBONATE
C2H5NO-D2	N-METHYLFORMAMIDE	C3H4O3-D1	PYRUVIC-ACID
C2H5NO2	NITROETHANE	C3H5CL	ALLYL-CHLORIDE
C2H6	ETHANE	C3H5CL-D0	2-CHLOROPROPENE
C2H6ALCL	DIMETHYLALUMINUM-CHLORIDE	C3H5CLO	ALPHA-EPICHLOROHYDRIN
C2H6O-1	DIMETHYL-ETHER	C3H5CLO2	METHYL-CHLOROACETATE
C2H6O-2	ETHANOL	C3H5CLO2-D1	ETHYL-CHLOROFORMATE
C2H6OS	DIMETHYL-SULFOXIDE	C3H5CL3	1,2,3-TRICHLOROPROPANE
C2H6O2	ETHYLENE-GLYCOL	C3H5N	PROPIONITRILE
C2H6O4S	DIMETHYL-SULFATE	C3H5NO	LACTONITRILE
C2H6S-1	ETHYL-MERCAPTAN	C3H5NO-D1	ACRYLAMIDE
C2H6S-2	DIMETHYL-SULFIDE	C3H5NO-D2	HYDRACRYLONITRILE
C2H6S2	DIMETHYL-DISULFIDE	C3H5N3O9	NITROGLYCERINE
C2H7N-1	ETHYL-AMINE	C3H6-1	CYCLOPROPANE
C2H7N-2	DIMETHYLAMINE	C3H6-2	PROPYLENE
C2H7NO	MONOETHANOLAMINE	C3H6CL2	1,2-DICHLOROPROPANE
C2H7NO2	AMMONIUM-ACETATE	C3H6CL2-D1	1,1-DICHLOROPROPANE
C2H8N2	ETHYLENEDIAMINE	C3H6CL2-D2	1,3-DICHLOROPROPANE
C2H8N2O4	AMMONIUM-OXALATE	C3H6O-1	ACETONE
C2H8SI	DIMETHYL-SILANE	C3H6O-2	ALLYL-ALCOHOL
C2N2	CYANOGEN	C3H6O-3	N-PROPIONALDEHYDE
C3F6	HEXAFLUOROPROPYLENE	C3H6O-4	PROPYLENE-OXIDE
C3F6O	HEXAFLUOROACETONE	C3H6O-5	VINYL-METHYL-ETHER
C3F8	OCTAFLUOROPROPANE	C3H6O-D0	1,3-PROPYLENE-OXIDE
C3H2N2	MALONONITRILE	C3H6O2-1	PROPIONIC-ACID
C3H3CL	PROPARGYL-CHLORIDE	C3H6O2-2	ETHYL-FORMATE
C3H3N	ACRYLONITRILE	C3H6O2-3	METHYL-ACETATE
C3H3NO	OXAZOLE	C3H6O2S	3-MERCAPTOPROPIONIC-ACID
C3H4-1	PROPADIENE	C3H6O3	METHOXYACETIC-ACID
C3H4-2	METHYL-ACETYLENE	C3H6O3-D1	LACTIC-ACID
C3H4CL2	2,3-DICHLOROPROPENE	C3H6O3-D2	TRIOXANE
C3H4O	ACROLEIN	C3H7BR-D1	1-BROMOPROPANE
C3H4O-D0	PROPARGYL-ALCOHOL	C3H7BR-D2	2-BROMOPROPANE
C3H4O2-1	ACRYLIC-ACID	C3H7CL-1	PROPYL-CHLORIDE
C3H4O2-2	VINYL-FORMATE	C3H7CL-2	ISOPROPYL-CHLORIDE
C3H4O2-D0	BETA-PROPIOLACTONE	C3H7I-D1	ISOPROPYL-IODIDE

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
C3H7I-D2	N-PROPYL-IODIDE	C4H4O2	DIKETENE
C3H7N	ALLYLAMINE	C4H4O3	SUCCINIC-ANHYDRIDE
C3H7N-D1	PROPYLENEIMINE	C4H4O4-D1	FUMARIC-ACID
C3H7NO	N,N-DIMETHYLFORMAMIDE	C4H4O4-D2	MALEIC-ACID
C3H7NO-D1	N-METHYLACETAMIDE	C4H4S	THIOPHENE
C3H7NO2-D1	1-NITROPROPANE	C4H5CL	CHLOROPRENE
C3H7NO2-D2	2-NITROPROPANE	C4H5N	METHACRYLONITRILE
C3H8	PROPANE	C4H5N-1	ALLYL-CYANIDE
C3H8O-1	1-PROPANOL	C4H5N-2	PYRROLE
C3H8O-2	ISOPROPYL-ALCOHOL	C4H5N-E1	TRANS-CROTONITRILE
C3H8O-3	METHYL-ETHYL-ETHER	C4H5N-E3	CIS-CROTONITRILE
C3H8O2	2-METHOXYETHANOL	C4H5NO2	METHYL-CYANOACETATE
C3H8O2-1	METHYLAL	C4H6-1	1-BUTYNE
C3H8O2-2	PROPANEDIOL-1,2	C4H6-2	2-BUTYNE
C3H8O2-3	1,3-PROPANEDIOL	C4H6-3	1,2-BUTADIENE
C3H8O3	GLYCEROL	C4H6-4	1,3-BUTADIENE
C3H8S-E1	N-PROPYLMERCAPTAN	C4H6CL2	1,4-DICHLORO-TRANS-2-BUTENE
C3H8S-E2	ISOPROPYL-MERCAPTAN	C4H6CL2-E1	1,3-DICHLORO-TRANS-2-BUTENE
C3H9N-1	N-PROPYL-AMINE	C4H6CL2-E2	3,4-DICHLORO-1-BUTENE
C3H9N-2	ISOPROPYL-AMINE	C4H6CL2-E3	1,4-DICHLORO-CIS-2-BUTENE
C3H9N-3	TRIMETHYL-AMINE	C4H6O	2,5-DIHYDROFURAN
C3H9NO	METHYL-ETHANOLAMINE	C4H6O-D1	TRANS-CROTONALDEHYDE
C3H9NO-D1	1-AMINO-2-PROPANOL	C4H6O-D2	DIVINYL-ETHER
C3H9NO-D2	3-AMINO-1-PROPANOL	C4H6O-D3	METHACROLEIN
C3H9O4P	TRIMETHYL-PHOSPHATE	C4H6O2-1	VINYL-ACETATE
C3H10N2	1,2-PROPANEDIAMINE	C4H6O2-2	METHYL-ACRYLATE
C3H10SI	TRIMETHYL-SILANE	C4H6O2-D1	2-BUTYNE-1,4-DIOL
C4CL4S	TETRACHLOROTHIOPHENE	C4H6O2-D2	GAMMA-BUTYROLACTONE
C4CL6	HEXACHLORO-1,3-BUTADIENE	C4H6O2-D3	CIS-CROTONIC-ACID
C4F8-D1	OCTAFLUORO-2-BUTENE	C4H6O2-D4	TRANS-CROTONIC-ACID
C4F8-D2	OCTAFLUOROCYCLOBUTANE	C4H6O2-D5	METHACRYLIC-ACID
C4F10	DECAFLUOROBUTANE	C4H6O3	ACETIC-ANHYDRIDE
C4H2O3	MALEIC-ANHYDRIDE	C4H6O4-2	SUCCINIC-ACID
C4H4	VINYLACETYLENE	C4H6O5	DIGLYCOLIC-ACID
C4H4N2	SUCCINONITRILE	C4H6O5-D1	MALIC-ACID
C4H4O	FURAN	C4H6O6	TARTARIC-ACID

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
C4H7N	BUTYRONITRILE	C4H10-1	N-BUTANE
C4H7N-D0	ISOBUTYRONITRILE	C4H10-2	ISOBUTANE
C4H7NO-D1	ACETONE-CYANOHYDRIN	C4H10N2	PIPERAZINE
C4H7NO-D2	2-PYRROLIDONE	C4H10O-1	N-BUTANOL
C4H7NO-E1	2-METHACRYLAMIDE	C4H10O-2	2-BUTANOL
C4H7NO-E2	3-METHOXYPROPIONITRILE	C4H10O-3	ISOBUTANOL
C4H8-1	1-BUTENE	C4H10O-4	TERT-BUTYL-ALCOHOL
C4H8-2	CIS-2-BUTENE	C4H10O-5	DIETHYL-ETHER
C4H8-3	TRANS-2-BUTENE	C4H10O-D1	METHYL-ISOPROPYL-ETHER
C4H8-4	CYCLOBUTANE	C4H10O2	1,2-DIMETHOXYETHANE
C4H8-5	ISOBUTYLENE	C4H10O2-D1	1,3-BUTANEDIOL
C4H8CL2	1,4-DICHLOROBUTANE	C4H10O2-D2	1,4-BUTANEDIOL
C4H8O	1,2-EPOXYBUTANE	C4H10O2-D3	T-BUTYL-HYDROPEROXIDE
C4H8O-1	N-BUTYRALDEHYDE	C4H10O2-D4	2-ETHOXYETHANOL
C4H8O-2	ISOBUTYRALDEHYDE	C4H10O2-D5	2,3-BUTANEDIOL
C4H8O-3	METHYL-ETHYL-KETONE	C4H10O3	DIETHYLENE-GLYCOL
C4H8O-4	TETRAHYDROFURAN	C4H10O4S	DIETHYL-SULFATE
C4H8O-5	VINYL-ETHYL-ETHER	C4H10S	DIETHYL-SULFIDE
C4H8O2-1	N-BUTYRIC-ACID	C4H10S-D1	N-BUTYL-MERCAPTAN
C4H8O2-2	1,4-DIOXANE	C4H10S-D2	TERT-BUTYL-MERCAPTAN
C4H8O2-3	ETHYL-ACETATE	C4H10S-E1	SEC-BUTYL-MERCAPTAN
C4H8O2-4	ISOBUTYRIC-ACID	C4H10S-E2	ISOBUTYL-MERCAPTAN
C4H8O2-5	METHYL-PROPIONATE	C4H10S2	DIETHYL-DISULFIDE
C4H8O2-6	N-PROPYL-FORMATE	C4H11N-1	N-BUTYL-AMINE
C4H8O2-D2	CIS-2-BUTENE-1,4-DIOL	C4H11N-2	ISOBUTYL-AMINE
C4H8O2-D3	TRANS-2-BUTENE-1,4-DIOL	C4H11N-3	DIETHYL-AMINE
C4H8O2S	SULFOLANE	C4H11N-D1	SEC-BUTYLAMINE
C4H8S	TETRAHYDROTHIOPHENE	C4H11N-D2	TERT-BUTYLAMINE
C4H9BR-D1	1-BROMOBUTANE	C4H11NO	DIMETHYLETHANOLAMINE
C4H9BR-D2	2-BROMOBUTANE	C4H11NO2-1	DIETHANOLAMINE
C4H9CL-1	1-CHLOROBUTANE	C4H11NO2-2	DIGLYCOLAMINE
C4H9CL-2	2-CHLOROBUTANE	C4H12N2O	N-AMINOETHYL-ETHANOLAMINE
C4H9CL-3	TERT-BUTYL-CHLORIDE	C4H12SI	TETRAMETHYLSILANE
C4H9N	PYRROLIDINE	C4H13N3	DIETHYLENE-TRIAMINE
C4H9NO	MORPHOLINE	C5CL6	HEXACHLOROCYCLOPENTADIENE
C4H9NO-D0	N,N-DIMETHYLACETAMIDE	C5H4O2	FURFURAL

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
C5H5N	PYRIDINE	C5H9NO-D2	N-METHYL-2-PYRROLIDONE
C5H6	CYCLOPENTADIENE	C5H9NO4	L-GLUTAMIC-ACID
C5H6-E1	2-METHYL-1-BUTENE-3-YNE	C5H10-1	CYCLOPENTANE
C5H6-E2	1-PENTENE-3-YNE	C5H10-2	1-PENTENE
C5H6-E3	1-PENTENE-4-YNE	C5H10-3	CIS-2-PENTENE
C5H6N2	GLUTARONITRILE	C5H10-4	TRANS-2-PENTENE
C5H6O2	FURFURYL-ALCOHOL	C5H10-5	2-METHYL-1-BUTENE
C5H6O3	GLUTARIC-ANHYDRIDE	C5H10-6	2-METHYL-2-BUTENE
C5H6O4-E1	CITRACONIC-ACID	C5H10-7	3-METHYL-1-BUTENE
C5H6O4-E2	ITACONIC-ACID	C5H10CL2	1,5-DICHLOROPENTANE
C5H7N	N-METHYLPYRROLE	C5H10O-1	VALERALDEHYDE
C5H7NO2	ETHYL-CYANOACETATE	C5H10O-2	METHYL-N-PROPYL-KETONE
C5H8	CIS-1,3-PENTADIENE	C5H10O-3	METHYL-ISOPROPYL-KETONE
C5H8-1	CYCLOPENTENE	C5H10O-4	DIETHYL-KETONE
C5H8-2	1,2-PENTADIENE	C5H10O2-1	N-VALERIC-ACID
C5H8-3	1-TRANS-3-PENTADIENE	C5H10O2-2	ISOBUTYL-FORMATE
C5H8-4	1,4-PENTADIENE	C5H10O2-3	N-PROPYL-ACETATE
C5H8-5	1-PENTYNE	C5H10O2-4	ETHYL-PROPIONATE
C5H8-6	2-METHYL-1,3-BUTADIENE	C5H10O2-5	METHYL-BUTYRATE
C5H8-7	3-METHYL-1,2-BUTADIENE	C5H10O2-D1	N-BUTYL-FORMATE
C5H8-E2	3-METHYL-1-BUTYNE	C5H10O2-D2	ISOPROPYL-ACETATE
C5H8-E4	2,3-PENTADIENE	C5H10O2-D3	ISOVALERIC-ACID
C5H8N4O12	PENTAERYTHRITOL-TETRANITRATE	C5H10O2-D4	2-METHYLBUTYRIC-ACID
C5H8O	CYCLOPENTANONE	C5H10O2-D5	TETRAHYDROFURFURYL-ALCOHOL
C5H8O-D1	METHYL-ISOPROPENYL-KETONE	C5H10O2S	3-METHYL-SULFOLANE
C5H8O2	ETHYL-ACRYLATE	C5H10O3-D1	DIETHYL-CARBONATE
C5H8O2-D1	ACETYLACETONE	C5H10O3-D2	ETHYL-LACTATE
C5H8O2-D2	ALLYL-ACETATE	C5H11CL	1-CHLOROPENTANE
C5H8O2-D3	METHYL-METHACRYLATE	C5H11N	PIPERIDINE
C5H8O2-D5	VINYL-PROPIONATE	C5H11N-D0	N-METHYLPYRROLIDINE
C5H8O3	2-HYDROXYETHYL-ACRYLATE	C5H11NO	TERT-BUTYLFORMAMIDE
C5H8O3-D1	LEVULINIC-ACID	C5H12-1	N-PENTANE
C5H8O3-D2	METHYL-ACETOACETATE	C5H12-2	2-METHYL-BUTANE
C5H8O4	GLUTARIC-ACID	C5H12-3	2,2-DIMETHYL-PROPANE
C5H9N	VALERONITRILE	C5H12O	METHYL-SEC-BUTYL-ETHER
C5H9NO-D1	N-BUTYL-ISOCYANATE	C5H12O-1	1-PENTANOL

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
C5H12O-2	2-METHYL-1-BUTANOL	C6H5CLO-E1	M-CHLOROPHENOL
C5H12O-3	3-METHYL-1-BUTANOL	C6H5CLO-E2	O-CHLOROPHENOL
C5H12O-4	2-METHYL-2-BUTANOL	C6H5CLO-E3	P-CHLOROPHENOL
C5H12O-5	2,2-DIMETHYL-1-PROPANOL	C6H5CL2N	3,4-DICHLOROANILINE
C5H12O-6	ETHYL-PROPYL-ETHER	C6H5F	FLUOROBENZENE
C5H12O-D1	3-METHYL-2-BUTANOL	C6H5I	IODOBENZENE
C5H12O-D2	METHYL-TERT-BUTYL-ETHER	C6H5NO2	NITROBENZENE
C5H12O-D3	2-PENTANOL	C6H6	BENZENE
C5H12O-D4	3-PENTANOL	C6H6CLN-D1	M-CHLOROANILINE
C5H12O-E1	METHYL-ISOBUTYL-ETHER	C6H6CLN-D2	O-CHLOROANILINE
C5H12O2-D1	NEOPENTYL-GLYCOL	C6H6CLN-D3	P-CHLOROANILINE
C5H12O2-D2	1,5-PENTANEDIOL	C6H6N2-E1	CIS-DICYANO-1-BUTENE
C5H12O2-D3	ETHYLENE-GLYCOL-MONOPROPYL-ETHER	C6H6N2-E2	TRANS-DICYANO-1-BUTENE
C5H12O3	2--2-METHOXYETHOXY-ETHANOL	C6H6N2-E3	1,4-DICYANO-2-BUTENE
C5H12O4	PENTAERYTHRITOL	C6H6N2O2-D1	M-NITROANILINE
C5H12S	1-PENTANETHIOL	C6H6N2O2-D2	O-NITROANILINE
C5H13N	N-PENTYLAMINE	C6H6N2O2-D3	P-NITROANILINE
C5H13NO2	METHYL-DIETHANOLAMINE	C6H6O	PHENOL
C6CL6	HEXACHLOROBENZENE	C6H6O2	P-HYDROQUINONE
C6F6	PERFLUOROBENZENE	C6H6O2-E1	1,2-BENZENEDIOL
C6H3CLN2O4	1-CHLORO-2,4-DINITROBENZENE	C6H6O2-E2	1,3-BENZENEDIOL
C6H3CL2NO2	1,2-DICHLORO-4-NITROBENZENE	C6H6O3	1,2,3-BENZENETRIOL
C6H3CL3	1,2,4-TRICHLOROBENZENE	C6H6S	PHENYL-MERCAPTAN
C6H3N3O6	1,3,5-TRINITROBENZENE	C6H7N-1	ANILINE
C6H4BR2	M-DIBROMOBENZENE	C6H7N-2	4-METHYLPYRIDINE
C6H4CLNO2-D1	M-CHLORONITROBENZENE	C6H7N-D1	2-METHYLPYRIDINE
C6H4CLNO2-D2	O-CHLORONITROBENZENE	C6H7N-D2	3-METHYLPYRIDINE
C6H4CLNO2-D3	P-CHLORONITROBENZENE	C6H8-E1	1,3-CYCLOHEXADIENE
C6H4CL2-1	O-DICHLOROBENZENE	C6H8-E2	METHYLCYCLOPENTADIENE
C6H4CL2-2	M-DICHLOROBENZENE	C6H8N2	METHYLGLUTARONITRILE
C6H4CL2-3	P-DICHLOROBENZENE	C6H8N2-D1	ADIPONITRILE
C6H4N2O4-E1	M-DINITROBENZENE	C6H8N2-D2	M-PHENYLENEDIAMINE
C6H4N2O4-E2	O-DINITROBENZENE	C6H8N2-D3	O-PHENYLENEDIAMINE
C6H4N2O4-E3	P-DINITROBENZENE	C6H8N2-D4	P-PHENYLENEDIAMINE
C6H5BR	BROMOBENZENE	C6H8N2-D5	PHENYLHYDRAZINE
C6H5CL	CHLOROBENZENE	C6H8N2O	BIS-CYANOETHYL-ETHER

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
C6H8O4	DIMETHYL-MALEATE	C6H12-7	TRANS-3-HEXENE
C6H8O6	ASCORBIC-ACID	C6H12-8	2-METHYL-2-PENTENE
C6H8O7	CITRIC-ACID	C6H12-9	3-METHYL-CIS-2-PENTENE
C6H10-1	1,5-HEXADIENE	C6H12-D1	2-ETHYL-1-BUTENE
C6H10-2	CYCLOHEXENE	C6H12-D2	2-METHYL-1-PENTENE
C6H10-E2	1-HEXYNE	C6H12-D3	4-METHYL-1-PENTENE
C6H10-E3	2,3-DIMETHYL-1,3-BUTADIENE	C6H12-E3	3-METHYL-1-PENTENE
C6H10-E4	CIS,TRANS-2,4-HEXADIENE	C6H12N2-E2	TRIETHYLENEDIAMINE
C6H10-E5	TRANS,TRANS-2,4-HEXADIENE	C6H12O	3-HEXANONE
C6H10-E6	2-HEXYNE	C6H12O-1	CYCLOHEXANOL
C6H10-E7	3-HEXYNE	C6H12O-2	METHYL-ISOBUTYL-KETONE
C6H10O	CYCLOHEXANONE	C6H12O-D1	BUTYL-VINYL-ETHER
C6H10O-D0	MESITYL-OXIDE	C6H12O-D2	1-HEXANAL
C6H10O2-D1	CAPROLACTONE	C6H12O-D3	2-HEXANONE
C6H10O2-D2	ETHYL-METHACRYLATE	C6H12O-E1	ETHYL-ISOPROPYL-KETONE
C6H10O2-D3	N-PROPYL-ACRYLATE	C6H12O2	TERT-BUTYL-ACETATE
C6H10O3-D1	ETHYLACETOACETATE	C6H12O2-1	N-BUTYL-ACETATE
C6H10O3-D2	PROPIONIC-ANHYDRIDE	C6H12O2-2	ISOBUTYL-ACETATE
C6H10O4	ETHYLIDENE-DIACETATE	C6H12O2-3	ETHYL-BUTYRATE
C6H10O4-D1	ADIPIC-ACID	C6H12O2-4	ETHYL-ISOBUTYRATE
C6H10O4-D2	DIETHYL-OXALATE	C6H12O2-5	N-PROPYL-PROPIONATE
C6H10O4-D3	ETHYLENE-GLYCOL-DIACETATE	C6H12O2-D1	SEC-BUTYL-ACETATE
C6H11N	HEXANENITRILE	C6H12O2-D2	CYCLOHEXYL-PEROXIDE
C6H11NO	EPSILON-CAPROLACTAM	C6H12O2-D3	DIACETONE-ALCOHOL
C6H11NO-D1	CYCLOHEXANONE-OXIME	C6H12O2-D4	2-ETHYL-BUTYRIC-ACID
C6H12-1	CYCLOHEXANE	C6H12O2-D5	N-HEXANOIC-ACID
C6H12-11	4-METHYL-CIS-2-PENTENE	C6H12O2-E1	N-PENTYL-FORMATE
C6H12-12	4-METHYL-TRANS-2-PENTENE	C6H12O3-D1	2-ETHOXYETHYL-ACETATE
C6H12-13	2,3-DIMETHYL-1-BUTENE	C6H12O3-D2	PARALDEHYDE
C6H12-14	2,3-DIMETHYL-2-BUTENE	C6H12O3-E1	HYDROXYCAPROIC-ACID
C6H12-15	3,3-DIMETHYL-1-BUTENE	C6H12O6	DEXTROSE
C6H12-2	METHYLCYCLOPENTANE	C6H13N-D1	CYCLOHEXYLAMINE
C6H12-3	1-HEXENE	C6H13N-D2	HEXAMETHYLENEIMINE
C6H12-4	CIS-2-HEXENE	C6H14-1	N-HEXANE
C6H12-5	TRANS-2-HEXENE	C6H14-2	2-METHYL-PENTANE
C6H12-6	CIS-3-HEXENE	C6H14-3	3-METHYL-PENTANE

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
C6H14-4	2,2-DIMETHYL-BUTANE	C6H18N3OP	HEXAMETHYL-PHOSPHORAMIDE
C6H14-5	2,3-DIMETHYL-BUTANE	C6H18N4	TRIETHYLENE-TETRAMINE
C6H14N2O2	LYSINE	C6H18OSI2	HEXAMETHYLDISILOXANE
C6H14O-1	1-HEXANOL	C6H18O3SI3	HEXAMETHYLCYCLOTRISILOXANE
C6H14O-2	ETHYL-BUTYL-ETHER	C6H19NSI2	HEXAMETHYLDISILAZANE
C6H14O-3	DIISOPROPYL-ETHER	C7H3CLF3NO2	4-CHLORO-3-NITROBENZOTRIFLUORIDE
C6H14O-D1	DI-N-PROPYL-ETHER	C7H3CL2F3	2,4-DICHLOROBENZOTRIFLUORIDE
C6H14O-D2	2-ETHYL-1-BUTANOL	C7H3CL2NO	3,4-DICHLOROPHENYL-ISOCYANATE
C6H14O-D3	2-METHYL-1-PENTANOL	C7H4CLF3	P-CHLOROBENZOTRIFLUORIDE
C6H14O-D4	4-METHYL-2-PENTANOL	C7H4CL2O	M-CHLOROBENZOYL-CHLORIDE
C6H14O-E1	2-HEXANOL	C7H4F3NO2	3-NITROBENZOTRIFLUORIDE
C6H14O-E2	METHYL-TERT-PENTYL-ETHER	C7H5CLO	BENZOYL-CHLORIDE
C6H14O2-D1	ACETAL	C7H5CLO2	O-CHLOROBENZOIC-ACID
C6H14O2-D2	2-BUTOXYETHANOL	C7H5CL3	BENZOTRICHLORIDE
C6H14O2-D3	1,6-HEXANEDIOL	C7H5F3	BENZOTRIFLUORIDE
C6H14O2-D4	HEXYLENE-GLYCOL	C7H5N	BENZONITRILE
C6H14O2S	DI-N-PROPYL-SULFONE	C7H5NO	PHENYL-ISOCYANATE
C6H14O3-D1	DIETHYLENE-GLYCOL-DIMETHYL-ETHER	C7H5N3O6	2,4,6-TRINITROTOLUENE
C6H14O3-D2	DIPROPYLENE-GLYCOL	C7H6CL2	2,4-DICHLOROTOLUENE
C6H14O3-D3	2--2-ETHOXYETHOXY-ETHANOL	C7H6CL2-D1	BENZYL-DICHLORIDE
C6H14O3-D4	TRIMETHYLOLPROPANE	C7H6N2O4-E1	2,4-DINITROTOLUENE
C6H14O4	TRIETHYLENE-GLYCOL	C7H6N2O4-E2	2,5-DINITROTOLUENE
C6H14O6	SORBITOL	C7H6N2O4-E3	2,6-DINITROTOLUENE
C6H14S	N-HEXYLMERCAPTAN	C7H6N2O4-E4	3,4-DINITROTOLUENE
C6H15AL	TRIETHYL-ALUMINUM	C7H6N2O4-E5	3,5-DINITROTOLUENE
C6H15AL2CL3	ETHYL-ALUMINUM-SESQUICHLORIDE	C7H6O	BENZALDEHYDE
C6H15N-1	DIPROPYLAMINE	C7H6O2	BENZOIC-ACID
C6H15N-2	TRIETHYLAMINE	C7H6O2-D0	SALICYLALDEHYDE
C6H15N-D1	DIISOPROPYLAMINE	C7H6O2-E1	P-HYDROXY-BENZALDEHYDE
C6H15N-D2	N-HEXYLAMINE	C7H6O3	SALICYLIC-ACID
C6H15NO	6-AMINOHEXANOL	C7H7BR	P-BROMOTOLUENE
C6H15NO2	DIISOPROPANOLAMINE	C7H7CL-D1	BENZYL-CHLORIDE
C6H15NO3	TRIETHANOLAMINE	C7H7CL-D2	O-CHLOROTOLUENE
C6H15N3	N-AMINOETHYL-PIPERAZINE	C7H7CL-D3	P-CHLOROTOLUENE
C6H15O4P	TRIETHYL-PHOSPHATE	C7H7NO	FORMANILIDE
C6H16N2	HEXAMETHYLENEDIAMINE	C7H7NO2-D1	M-NITROTOLUENE

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
C7H7NO2-D2	O-NITROTOLUENE	C7H14-E3	TRANS-1,3-DIMETHYLCYCLOPENTANE
C7H7NO2-D3	P-NITROTOLUENE	C7H14-E4	TRANS-2-HEPTENE
C7H7NO3	O-NITROANISOLE	C7H14-E5	TRANS-3-HEPTENE
C7H8	TOLUENE	C7H14-E6	4-METHYL-1-HEXENE
C7H8O-1	METHYL-PHENYL-ETHER	C7H14-E7	2-ETHYL-1-PENTENE
C7H8O-2	BENZYL-ALCOHOL	C7H14-E8	3-ETHYL-1-PENTENE
C7H8O-3	O-CRESOL	C7H14-E9	2-METHYL-1-HEXENE
C7H8O-4	M-CRESOL	C7H14O	DIISOPROPYL-KETONE
C7H8O-5	P-CRESOL	C7H14O-D1	1-HEPTANAL
C7H8O2	P-METHOXYPHENOL	C7H14O-D10	5-METHYL-2-HEXANONE
C7H8O2-E1	GUAIACOL	C7H14O-D2	2-HEPTANONE
C7H9N-5	METHYLPHENYLAMINE	C7H14O-D3	1-METHYLCYCLOHEXANOL
C7H9N-6	O-TOLUIDINE	C7H14O-D4	CIS-2-METHYLCYCLOHEXANOL
C7H9N-7	M-TOLUIDINE	C7H14O-D5	TRANS-2-METHYLCYCLOHEXANOL
C7H9N-8	P-TOLUIDINE	C7H14O-D6	CIS-3-METHYLCYCLOHEXANOL
C7H9N-D1	BENZYLAMINE	C7H14O-D7	TRANS-3-METHYLCYCLOHEXANOL
C7H9N-D2	2,6-DIMETHYLPYRIDINE	C7H14O-D8	CIS-4-METHYLCYCLOHEXANOL
C7H10	2-NORBORNENE	C7H14O-D9	TRANS-4-METHYLCYCLOHEXANOL
C7H10N2	TOLUENEDIAMINE	C7H14O2-D1	N-BUTYL-PROPIONATE
C7H11NO	CYCLOHEXYL-ISOCYANATE	C7H14O2-D2	ETHYL-ISOVALERATE
C7H12O2-D1	N-BUTYL-ACRYLATE	C7H14O2-D3	N-HEPTANOIC-ACID
C7H12O2-D2	ISOBUTYL-ACRYLATE	C7H14O2-D4	ISOPENTYL-ACETATE
C7H12O2-D3	N-PROPYL-METHACRYLATE	C7H14O2-D5	N-PENTYL-ACETATE
C7H12O4	DIETHYL-MALONATE	C7H14O2-D6	N-PROPYL-N-BUTYRATE
C7H14-1	CYCLOHEPTANE	C7H14O3	ETHYL-3-ETHOXYPROPIONATE
C7H14-2	1,1-DIMETHYLCYCLOPENTANE	C7H15BR	1-BROMOHEPTANE
C7H14-3	CIS-1,2-DIMETHYLCYCLOPENTANE	C7H15N	N-METHYLCYCLOHEXYLAMINE
C7H14-4	TRANS-1,2-DIMETHYLCYCLOPENTANE	C7H16-1	N-HEPTANE
C7H14-5	ETHYLCYCLOPENTANE	C7H16-2	2-METHYLHEXANE
C7H14-6	METHYLCYCLOHEXANE	C7H16-3	3-METHYLHEXANE
C7H14-7	1-HEPTENE	C7H16-4	2,2-DIMETHYLPENTANE
C7H14-8	2,3,3-TRIMETHYL-1-BUTENE	C7H16-5	2,3-DIMETHYLPENTANE
C7H14-D1	CIS-2-HEPTENE	C7H16-6	2,4-DIMETHYLPENTANE
C7H14-D2	CIS-3-HEPTENE	C7H16-7	3,3-DIMETHYLPENTANE
C7H14-E10	3-METHYL-1-HEXENE	C7H16-8	3-ETHYLPENTANE
C7H14-E2	CIS-1,3-DIMETHYLCYCLOPENTANE	C7H16-9	2,2,3-TRIMETHYLBUTANE

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
C7H16O	1-HEPTANOL	C8H11N-D0	O-ETHYLANILINE
C7H16O-D0	2-HEPTANOL	C8H11N-D1	2,4,6-TRIMETHYLPYRIDINE
C7H16O-E1	ISOHEPTANOL	C8H11NO	P-PHENETIDINE
C7H16S	N-HEPTYL-MERCAPTAN	C8H12	VINYLCYCLOHEXENE
C7H17N	1-AMINOHEPTANE	C8H12-D1	1,5-CYCLOOCTADIENE
C8H4CL2O2	ISOPHTHALOYL-CHLORIDE	C8H12O4-E1	1,4-CYCLOHEXANEDICARBOXYLIC-ACID
C8H4O3	PHTHALIC-ANHYDRIDE	C8H12O4-E2	DIETHYL-MALEATE
C8H6O4-D1	ISOPHTHALIC-ACID	C8H14O2	N-BUTYL-METHACRYLATE
C8H6O4-D2	PHTHALIC-ACID	C8H14O3	BUTYRIC-ANHYDRIDE
C8H6O4-D3	TEREPHTHALIC-ACID	C8H14O4	DIETHYL-SUCCINATE
C8H6S	BENZOTHIOPHENE	C8H16-1	1,1-DIMETHYLCYCLOHEXANE
C8H7N	INDOLE	C8H16-13	1-METHYL-1-ETHYLCYCLOPENTANE
C8H8	STYRENE	C8H16-14	N-PROPYLCYCLOPENTANE
C8H8O	METHYL-PHENYL-KETONE	C8H16-16	1-OCTENE
C8H8O-D0	P-TOLUALDEHYDE	C8H16-17	TRANS-2-OCTENE
C8H8O2	METHYL-BENZOATE	C8H16-2	CIS-1,2-DIMETHYLCYCLOHEXANE
C8H8O2-D1	O-TOLUIC-ACID	C8H16-3	TRANS-1,2-DIMETHYLCYCLOHEXANE
C8H8O2-D2	P-TOLUIC-ACID	C8H16-4	CIS-1,3-DIMETHYLCYCLOHEXANE
C8H8O3	METHYL-SALICYLATE	C8H16-5	TRANS-1,3-DIMETHYLCYCLOHEXANE
C8H8O3-D1	VANILLIN	C8H16-6	CIS-1,4-DIMETHYLCYCLOHEXANE
C8H9NO	ACETANILIDE	C8H16-7	TRANS-1,4-DIMETHYLCYCLOHEXANE
C8H10-1	O-XYLENE	C8H16-8	ETHYLCYCLOHEXANE
C8H10-2	M-XYLENE	C8H16-D1	2-ETHYL-1-HEXENE
C8H10-3	P-XYLENE	C8H16-D2	TRANS-3-OCTENE
C8H10-4	ETHYLBENZENE	C8H16-D3	TRANS-4-OCTENE
C8H10N4O2	CAFFEINE	C8H16-D4	2,4,4-TRIMETHYL-1-PENTENE
C8H10O	2-PHENYLETHANOL	C8H16-D5	2,4,4-TRIMETHYL-2-PENTENE
C8H10O-10	3,5-XYLENOL	C8H16O	2-ETHYLHEXANAL
C8H10O-3	P-ETHYLPHENOL	C8H16O-E1	1-OCTANAL
C8H10O-4	PHENETOLE	C8H16O-E2	2-OCTANONE
C8H10O-5	2,3-XYLENOL	C8H16O2-D1	N-BUTYL-N-BUTYRATE
C8H10O-6	2,4-XYLENOL	C8H16O2-D2	ISOBUTYL-ISOBUTYRATE
C8H10O-7	2,5-XYLENOL	C8H16O2-D3	N-OCTANOIC-ACID
C8H10O-8	2,6-XYLENOL	C8H16O2-D4	N-HEXYL-ACETATE
C8H10O-9	3,4-XYLENOL	C8H16O4	2--2-ETHOXYETHOXY-ETHYL-ACETATE
C8H11N	N,N-DIMETHYLANILINE	C8H18-1	N-OCTANE

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
C8H18-10	3,4-DIMETHYLHEXANE	C9H6N2O2	TOLUENE-DIISOCYANATE
C8H18-11	3-ETHYLHEXANE	C9H7N-D1	ISOQUINOLINE
C8H18-12	2,2,3-TRIMETHYLPENTANE	C9H7N-D2	QUINOLINE
C8H18-13	2,2,4-TRIMETHYLPENTANE	C9H7NO	8-HYDROXYQUINOLINE
C8H18-14	2,3,3-TRIMETHYLPENTANE	C9H8	INDENE
C8H18-15	2,3,4-TRIMETHYLPENTANE	C9H8O	2-METHYLBENZOFURAN
C8H18-16	2-METHYL-3-ETHYLPENTANE	C9H10	ALPHA-METHYL-STYRENE
C8H18-17	3-METHYL-3-ETHYLPENTANE	C9H10-E1	INDANE
C8H18-2	2-METHYLHEPTANE	C9H10-E2	M-METHYL-STYRENE
C8H18-3	3-METHYLHEPTANE	C9H10-E3	O-METHYL-STYRENE
C8H18-4	4-METHYLHEPTANE	C9H10-E4	P-METHYL-STYRENE
C8H18-5	2,2-DIMETHYLHEXANE	C9H10O2	ETHYL-BENZOATE
C8H18-6	2,3-DIMETHYLHEXANE	C9H10O2-D0	BENZYL-ACETATE
C8H18-7	2,4-DIMETHYLHEXANE	C9H10O3	ETHYL-VANILLIN
C8H18-8	2,5-DIMETHYLHEXANE	C9H11NO	P-DIMETHYLAMINOBENZALDEHYDE
C8H18-9	3,3-DIMETHYLHEXANE	C9H12-1	N-PROPYLBENZENE
C8H18O	DI-TERT-BUTYL-ETHER	C9H12-2	ISOPROPYLBENZENE
C8H18O-1	1-OCTANOL	C9H12-3	1-METHYL-2-ETHYLBENZENE
C8H18O-2	2-OCTANOL	C9H12-4	1-METHYL-3-ETHYLBENZENE
C8H18O-3	2-ETHYLHEXANOL	C9H12-5	1-METHYL-4-ETHYLBENZENE
C8H18O-4	BUTYL-ETHER	C9H12-6	1,2,3-TRIMETHYLBENZENE
C8H18O-D1	DI-SEC-BUTYL-ETHER	C9H12-7	1,2,4-TRIMETHYLBENZENE
C8H18O2	DI-T-BUTYL-PEROXIDE	C9H12-8	1,3,5-TRIMETHYLBENZENE
C8H18O2S	DI-N-BUTYL-SULFONE	C9H12O	BENZYL-ETHYL-ETHER
C8H18O3	DIETHYLENE-GLYCOL-MONOBUTYL-ETHE	C9H12O-E1	DIMETHYL-PHENYL-CARBINOL
C8H18O3-D1	DIETHYLENE-GLYCOL-DIETHYL-ETHER	C9H12O2	CUMENE-HYDROPEROXIDE
C8H18O4	TRIETHYLENE-GLYCOL-DIMETHYL-ETHE	C9H14O	ISOPHORONE
C8H18O5	TETRAETHYLENE-GLYCOL	C9H14O6	GLYCERYL-TRIACETATE
C8H18S	TERT-OCTYLMERCAPTAN	C9H16O4	AZELAIC-ACID
C8H18S-D1	N-OCTYL-MERCAPTAN	C9H18-1	N-PROPYLCYCLOHEXANE
C8H19N	DIBUTYLAMINE	C9H18-2	ISOPROPYLCYCLOHEXANE
C8H19N-D0	N-OCTYLAMINE	C9H18-3	1-NONENE
C8H19N-D1	DIISOBUTYLAMINE	C9H18O	1-NONANAL
C8H23N5	TETRAETHYLENEPENTAMINE	C9H18O-D1	DIISOBUTYL-KETONE
C8H24O4SI4	OCTAMETHYLCYCLOTETRASILOXANE	C9H18O2	N-NONANOIC-ACID
C9H4O5	TRIMELLITIC-ANHYDRIDE	C9H18O2-D1	N-BUTYL-VALERATE

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
C9H18O2-D2	N-OCTYL-FORMATE	C10H14-2	ISOBUTYLBENZENE
C9H20-1	N-NONANE	C10H14-3	SEC-BUTYLBENZENE
C9H20-4	2,2,5-TRIMETHYLHEXANE	C10H14-4	TERT-BUTYLBENZENE
C9H20-5	3,3-DIETHYLPENTANE	C10H14-5	1-METHYL-2-ISOPROPYLBENZENE
C9H20-6	2,2,3,3-TETRAMETHYLPENTANE	C10H14-6	1-METHYL-3-ISOPROPYLBENZENE
C9H20-7	2,2,3,4-TETRAMETHYLPENTANE	C10H14-7	1-METHYL-4-ISOPROPYLBENZENE
C9H20-8	2,2,4,4-TETRAMETHYLPENTANE	C10H14-8	1,4-DIETHYLBENZENE
C9H20-D1	2-METHYLOCTANE	C10H14-9	1,2,4,5-TETRAMETHYLBENZENE
C9H20-D2	3-METHYLOCTANE	C10H14-D1	M-DIETHYLBENZENE
C9H20-D3	4-METHYLOCTANE	C10H14-D2	O-DIETHYLBENZENE
C9H20-E1	2,2-DIMETHYLHEPTANE	C10H14-D3	1,2-DIMETHYL-3-ETHYLBENZENE
C9H20-E2	2,6-DIMETHYLHEPTANE	C10H14-E1	2-ETHYL-M-XYLENE
C9H20-E3	2,2-DIMETHYL-3-ETHYLPENTANE	C10H14-E2	2-ETHYL-P-XYLENE
C9H20-E4	2,4-DIMETHYL-3-ETHYLPENTANE	C10H14-E3	4-ETHYL-M-XYLENE
C9H20-E5	3-ETHYLHEPTANE	C10H14-E4	4-ETHYL-O-XYLENE
C9H20O-D1	2,6-DIMETHYL-4-HEPTANOL	C10H14-E5	5-ETHYL-M-XYLENE
C9H20O-D2	1-NONANOL	C10H14-E6	1,2,3,5-TETRAMETHYL-BENZENE
C9H20O-E1	2-NONANOL	C10H14O	P-TERT-BUTYLPHENOL
C9H20S	N-NONYL-MERCAPTAN	C10H14O2	P-TERT-BUTYLCATECHOL
C9H21N-D1	N-NONYLAMINE	C10H15N-E1	N,N-DIETHYLANILINE
C9H21N-D2	TRIPROPYLAMINE	C10H15N-E2	2,6-DIETHYLANILINE
C10H6O8	PYROMELLITIC-ACID	C10H16-D1	D-LIMONENE
C10H7BR	1-BROMONAPHTHALENE	C10H16-D2	ALPHA-PINENE
C10H7CL	1-CHLORONAPHTHALENE	C10H16-D3	BETA-PINENE
C10H8	NAPHTHALENE	C10H16-D4	TERPINOLENE
C10H9N	QUINALDINE	C10H16-E1	CAMPHENE
C10H10-D1	M-DIVINYLBENZENE	C10H16-E2	ALPHA-PHELLANDRENE
C10H10-D2	1-METHYLINDENE	C10H16-E3	BETA-PHELLANDRENE
C10H10-D3	2-METHYLINDENE	C10H16-E4	ALPHA-TERPINENE
C10H10O4-D1	O-DIMETHYL-PHTHALATE	C10H16-E5	GAMMA-TERPINENE
C10H10O4-D2	DIMETHYL-TEREPHTHALATE	C10H16O	CAMPHOR
C10H12	1,2,3,4-TETRAHYDRONAPHTHALENE	C10H18-1	CIS-DECALIN
C10H12-D0	DICYCLOPENTADIENE	C10H18-2	TRANS-DECALIN
C10H12O	ANETHOLE	C10H18O4	SEBACIC-ACID
C10H12O4	DIALLYL-MALEATE	C10H20-1	N-BUTYLCYCLOHEXANE
C10H14-1	N-BUTYLBENZENE	C10H20-5	1-DECENE

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
C10H20O	1-DECANAL	C12H12-E1	2,6-DIMETHYLNAPHTHALENE
C10H20O2-D1	N-DECANOIC-ACID	C12H12-E2	2,7-DIMETHYLNAPHTHALENE
C10H20O2-D2	2-ETHYLHEXYL-ACETATE	C12H12-E3	1-ETHYLNAPHTHALENE
C10H20O2-D3	ISOPENTYL-ISOVALERATE	C12H12N2-D1	P-AMINODIPHENYLAMINE
C10H22-1	N-DECANE	C12H12N2-D2	HYDRAZOBENZENE
C10H22-E1	2,2-DIMETHYL-OCTANE	C12H14	1,2,3-TRIMETHYLINDENE
C10H22-E2	2-METHYLNONANE	C12H14O4	DIETHYL-PHTHALATE
C10H22-E3	3-METHYLNONANE	C12H16	CYCLOHEXYLBENZENE
C10H22-E4	4-METHYLNONANE	C12H18-D1	M-DIISOPROPYLBENZENE
C10H22-E5	5-METHYLNONANE	C12H18-D2	P-DIISOPROPYLBENZENE
C10H22O	1-DECANOL	C12H18-D3	N-HEXYLBENZENE
C10H22O-D0	ISODECANOL	C12H20O4	DIBUTYL-MALEATE
C10H22O-D1	DI-N-PENTYL-ETHER	C12H22	BICYCLOHEXYL
C10H22O5	TETRAETHYLENE-GLYCOL-DIMETHYL-ET	C12H23N	DICYCLOHEXYLAMINE
C10H22S	N-DECYL-MERCAPTAN	C12H24-2	1-DODECENE
C10H23N	N-DECYLAMINE	C12H24O	1-DODECANAL
C11H10-1	1-METHYLNAPHTHALENE	C12H24O2	N-DODECANOIC-ACID
C11H10-2	2-METHYLNAPHTHALENE	C12H26	N-DODECANE
C11H14O2	BUTYL-BENZOATE	C12H26O-1	DIHEXYLETHER
C11H16	N-PENTYLBENZENE	C12H26O-2	DODECANOL
C11H16O	P-TERT-AMYLPHENOL	C12H26O3	DIETHYLENE-GLYCOL-DI-N-BUTYL-ETH
C11H20O2	2-ETHYLHEXYLACRYLATE	C12H26S	N-DODECYL-MERCAPTAN
C11H22-2	1-UNDECENE	C12H27BO3	TRI-N-BUTYL-BORATE
C11H22O	1-UNDECANAL	C12H27N	TRIBUTYLAMINE
C11H24	N-UNDECANE	C12H27N-D0	DODECYLAMINE
C11H24O	1-UNDECANOL	C13H10	FLUORENE
C11H24S	UNDECYL-MERCAPTAN	C13H10O	BENZOPHENONE
C12H8O	DIBENZOFURAN	C13H12	DIPHENYLMETHANE
C12H9N	DIBENZOPYRROLE	C13H20	N-HEPTYLBENZENE
C12H10	DIPHENYL	C13H26-2	1-TRIDECENE
C12H10-D0	ACENAPHTHENE	C13H26O	1-TRIDECANAL
C12H10O	DIPHENYL-ETHER	C13H26O2	METHYL-DODECANOATE
C12H11N	DIPHENYLAMINE	C13H26O2-D1	N-BUTYL-NONANOATE
C12H11N-D1	P-AMINODIPHENYL	C13H28	N-TRIDECANE
C12H11N3-E1	P-AMINOAZOBENZENE	C13H28O	1-TRIDECANOL
C12H11N3-E2	1,3-DIPHENYLTRIAZENE	C14H8O2	ANTHRAQUINONE

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
C14H10	DIPHENYLACETYLENE	C16H34O	1-HEXADECANOL
C14H10-1	ANTHRACENE	C16H34O-D1	DI-N-OCTYL-ETHER
C14H10-2	PHENANTHRENE	C17H28	N-UNDECYLBENZENE
C14H12-D1	CIS-STILBENE	C17H34-D1	1-HEPTADECENE
C14H12-D2	TRANS-STILBENE	C17H36	N-HEPTADECANE
C14H12O2	BENZYL-BENZOATE	C17H36O	HEPTADECANOL
C14H14-D1	1,1-DIPHENYLETHANE	C18H12	CHRYSENE
C14H14-D2	1,2-DIPHENYLETHANE	C18H14-1	O-TERPHENYL
C14H14O	DIBENZYL-ETHER	C18H14-2	M-TERPHENYL
C14H16	1-N-BUTYLNAPHTHALENE	C18H14-3	P-TERPHENYL
C14H22	N-OCTYLBENZENE	C18H15O4P	TRIPHENYL-PHOSPHATE
C14H22O	P-TERT-OCTYLPHENOL	C18H15P	TRIPHENYLPHOSPHINE
C14H28-2	1-TETRADECENE	C18H16N2	N-N--DIPHENYL-P-PHENYLENEDIAMINE
C14H28O2	N-TETRADECANOIC-ACID	C18H22	2,3-DIMETHYL-2,3-DIPHENYLBUTANE
C14H30	N-TETRADECANE	C18H22O2	DICUMYLPEROXIDE
C14H30O	1-TETRADECANOL	C18H30	N-DODECYLBENZENE
C14H31N	TETRADECYLAMINE	C18H32O2	LINOLEIC-ACID
C15H10N2O2	DIPHENYLMETHANE-4,4--DIISOCYANAT	C18H34O2	OLEIC-ACID
C15H16O	P-CUMYLPHENOL	C18H34O4-D1	DIBUTYL-SEBACATE
C15H16O2	BISPHENOL-A	C18H34O4-D2	DIHEXYL-ADIPATE
C15H24	N-NONYLBENZENE	C18H36-1	1-OCTADECENE
C15H24O-D1	2,6-DI-TERT-BUTYL-P-CRESOL	C18H36O2	STEARIC-ACID
C15H24O-D2	NONYLPHENOL	C18H38	N-OCTADECANE
C15H30-2	1-PENTADECENE	C18H38O	1-OCTADECANOL
C15H30O2	PENTADECANOIC-ACID	C18H38O-D0	DINONYL-ETHER
C15H32	N-PENTADECANE	C19H26	1-N-NONYLNAPHTHALENE
C16H10-D1	FLUORANTHENE	C19H32	N-TRIDECYLBENZENE
C16H10-D2	PYRENE	C19H36O2	METHYL-OLEATE
C16H12	1-PHENYLNAPHTHALENE	C19H38-D1	1-NONADECENE
C16H20	1-N-HEXYLNAPHTHALENE	C19H38O2	NONADECANOIC-ACID
C16H22O4	DIBUTYL-O-PHTHALATE	C19H40	N-NONADECANE
C16H26	N-DECYLBENZENE	C20H16	TRIPHENYLETHYLENE
C16H32-1	N-DECYLCYCLOHEXANE	C20H28	1-N-DECYLNAPHTHALENE
C16H32-2	1-HEXADECENE	C20H30O2	ABIETIC-ACID
C16H32O2	N-HEXADECANOIC-ACID	C20H31N	DEHYDROABIETYLAMINE
C16H34	N-HEXADECANE	C20H40-D1	1-EICOSENE

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
C20H42	N-EICOSANE	CRO3	CHROMIUM-TRIOXIDE
C20H42O	1-EICOSANOL	CR2NA2O7	SODIUM-DICHROMATE
C21H21O4P	TRI-O-CRESYL-PHOSPHATE	CUO4S	CUPRIC-SULFATE
C22H44O2	N-BUTYL-STEARATE	D2	DEUTERIUM
C24H38O4	DIOCTYL-PHTHALATE	D2O	DEUTERIUM-OXIDE
C24H38O4-D1	DIISOOCTYL-PHTHALATE	NAF	VILLIAUMITE
C24H42O	DINONYLPHENOL	F2	FLUORINE
C26H20	TETRAPHENYLETHYLENE	F3N	NITROGEN-TRIFLUORIDE
C28H46O4	DIISODECYL-PHTHALATE	F4SI	SILICON-TETRAFLUORIDE
CACL2	CALCIUM-CHLORIDE	F6S	SULFUR-HEXAFLUORIDE
CAF2	CALCIUM-FLUORIDE	FE	IRON
'CA(OH)2'	CALCIUM-HYDROXIDE	FEO	FERROUS-OXIDE
CAO	CALCIUM-OXIDE	FEO4S	FERROUS-SULFATE
CASO4	CALCIUM-SULFATE	FE2O3	FERRIC-OXIDE
CLCU	CUPROUS-CHLORIDE	GEH4	GERMANIUM-TETRAHYDRIDE
CLFO3	PERCHLORYL-FLUORIDE	HBR	HYDROGEN-BROMIDE
CLHO3S	CHLOROSULFONIC-ACID	HCL	HYDROGEN-CHLORIDE
CLHO4	PERCHLORIC-ACID	HF	HYDROGEN-FLUORIDE
NH4CL	SALAMMONIAC	HI	HYDROGEN-IODIDE
CLK	POTASSIUM-CHLORIDE	KOH	POTASSIUM-HYDROXIDE
CLNO	NITROSYL-CHLORIDE	HNO3	NITRIC-ACID
NACL	SODIUM-CHLORIDE	NAOH	SODIUM-HYDROXIDE
CLNAO3	SODIUM-CHLORATE	NAHSO4	SODIUM-BISULFATE
CLO2	CHLORINE-DIOXIDE	H2	HYDROGEN
CLO3K	POTASSIUM-CHLORATE	H2NNA	SODIUM-AMIDE
CL2	CHLORINE	H2O	WATER
CL2CU	CUPRIC-CHLORIDE	H2O2	HYDROGEN-PEROXIDE
CL3GA	GALLIUM-TRICHLORIDE	H2SO4	SULFURIC-ACID
CL3N	NITROGEN-TRICHLORIDE	H2S	HYDROGEN-SULFIDE
CL3OP	PHOSPHORUS-OXYCHLORIDE	H3N	AMMONIA
CL3OV	VANADIUM-OXYTRICHLORIDE	H3NO	HYDROXYLAMINE
CL3P	PHOSPHORUS-TRICHLORIDE	H3NO3S	SULFAMIC-ACID
CL3PS	PHOSPHORUS-THIOCHLORIDE	H3O2P	HYPOPHOSPHOROUS-ACID
CL4SI	SILICON-TETRACHLORIDE	H3O3P	PHOSPHOROUS-ACID
CL4V	VANADIUM-TETRACHLORIDE	H3PO4	ORTHOPHOSPHORIC-ACID
CL5P	PHOSPHORUS-PENTACHLORIDE	H4N2	HYDRAZINE

continued

Table 1.11 Components Available in PURE856 Databank (continued)

Alias	Component Name	Alias	Component Name
NH4NO3	AMMONIUM-NITRATE	NA2S	SODIUM-SULFIDE
NH4OH	NH4OH	NA3O4P	TRISODIUM-PHOSPHATE
H5NO3S	AMMONIUM-BISULFITE	NA4O7P2	TETRASODIUM-PYROPHOSPHATE
H8N2O3S	AMMONIUM-SULFITE	NA6O18P6	SODIUM-HEXAMETAPHOSPHATE
H8N2O4S	AMMONIUM-SULFATE	NE	NEON
HE	HELIUM-3	OZN	ZINC-OXIDE
HE-4	HELIUM-4	O2	OXYGEN
HG	MERCURY	O2S	SULFUR-DIOXIDE
I2	IODINE	SIO2	SILICON-DIOXIDE
K	POTASSIUM	TIO2	'TITANIUM-OXIDE(RUTILE)'
KR	KRYPTON	O3	OZONE
LI	LITHIUM	O3S	SULFUR-TRIOXIDE
MGO	PERICLASE	O4SZN	ZINC-SULFATE
MGO4S	MAGNESIUM-SULFATE	'(P2O5)2'	'PHOSPHORUS-PENTOXIDE(DIMERIC)'
NNAO2	SODIUM-NITRITE	P	PHOSPHORUS
NANO3	SODA-NITER	PH3	PH3
NO	NITRIC-OXIDE	P4S10	PHOSPHORUS-PENTASULFIDE
NO2	NITROGEN-DIOXIDE	S	SULFUR
N2	NITROGEN	CL2OS	THIONYL-CHLORIDE
F4N2	TETRAFLUOROHYDRAZINE	CL2O2S	SULFURYL-CHLORIDE
N2O	NITROUS-OXIDE	CL3SB	ANTIMONY-TRICHLORIDE
N2O3	NITROGEN-TRIOXIDE	CL3HSI	TRICHLOROSILANE
N2O4	NITROGEN-TETROXIDE	CL2H2SI	DICHLOROSILANE
N2O5	NITROGEN-PENTOXIDE	H4SI	SILANE
NA	SODIUM	H6SI2	DISILANE
NA2O2	SODIUM-PEROXIDE	SI	SILICON
NA2O3S2	SODIUM-THIOSULFATE	CL3TI	TITANIUM-TRICHLORIDE
NA2O3SI	SODIUM-SILICATE	CL4TI	TITANIUM-TETRACHLORIDE
NA2SO4	SODIUM-SULFATE	XE	XENON
NA2O4S2	SODIUM-HYDROSULFITE	ZN	ZINC

Table 1.12 Parameters Available in the SOLIDS Databank

Parameter Name	Description
ATOMNO †	Atomic number of each atom in the compound
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†	Number of occurrences of each atom
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
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 compute molecular weight and are used in RGIBBS.*

†† *Ideal gas at 25°C*

Table 1.13 Components Available in SOLIDS Databank

Alias	Component Name	Alias	Component Name
(AS2O5)3*5W	(AS2O5)3*5H2O	3BAO*4C2H6O	(BAO)3*4C2H5OH
(BAO)2*3SIO2	(BAO)2*3SIO2	3BAO*4CH4O	(BAO)3*4CH3OH
(BAO)2*GEO2	(BAO)2*GEO2	3KBR*2SBBR3	3KBR*2SBBR3
(BAO)2*SIO2	(BAO)2*SIO2	3NA2O*NB2O5	3NA2O*NB2O5
(BAO)3*AL2O3	(BAO)3*AL2O3	3NAI*8SO2	3NAI*8SO2
(BAO)3*GEO2	(BAO)3*GEO2	7RBBR*3SBBR3	7RBBR*3SBBR3
(NAPO3)3	(NAPO3)3	AG	SILVER
(NH4)2HASO4	DIAMMONIUM	AG2C2	AG2C2
(NH4)2HPO4	DIAMMONIUM	AG2C2O4	AG2C2O4
(NH4)2S2O8	(NH4)2S2O8	AG2H3IO6	AG2H3IO6
(NH4)2S4	(NH4)2S4	AG2HGI4	AG2HGI4
(NH4)2S5	(NH4)2S5	AG2HVO4	AG2HVO4
(NH4)2S8	(NH4)2S8	AG2MOO4	AG2MOO4
(NH4)2SEO4	AMMONIUM	AG2N2O2	AG2N2O2
(NH4)2SIF6-C	(NH4)2SIF6-CUBIC	AG2PTBR6	AG2PTBR6
(NH4)2SIF6-H	(NH4)2SIF6-HEXAGONAL	AG2PTCL6	AG2PTCL6
(NH4)2SNBR6	(NH4)2SNBR6	AG2S2O6*2W	AG2S2O6*2H2O
(NH4)2SNCL6	(NH4)2SNCL6	AG2SEO3	AG2SEO3
(NH4)2SO3	AMMONIUM	AG2SEO4	AG2SEO4
(NH4)2SO3*W	AMMONIUM	AG2SO3	AG2SO3
(NH4)2SO4	AMMONIUM-SULFATE	AG3C2CL	AG2C2*AGCL
(NH4)2SO4*3N	(NH4)2SO4*3NH3	AG3C2I	AG2C2*AGI
(NH4)3ASO4	AMMONIUM	AG3C2NO3	AG2C2*AGNO3
(NH4)3ASO4*3	AMMONIUM	AG3H2VO5	AG2HVO4*AGOH
(NH4)3PO4	AMMONIUM	AG3I4H*7W	(AGI)3*HI*7H2O
(NH4)3PO4*3W	AMMONIUM	AG3IN2O6	AG3I(NO3)2
(P2O5)2	PHOSPHORUS-PENTOXIDE(DIMERIC)	AG3N	AG3N
(TEO2)2SO3	(TEO2)2SO3	AG3P3O9*W	(AGPO3)3*H2O
2(CASO4)*W	2(CASO4)*H2O	AG3PO4	AG3PO4
2LIBH4*C2H6O	(LIBH4)2*(CH3)2O	AG4C2I2	AG2C2*2AGI
2NACL*BACL2	2NACL*BACL2	AG4C2SO4	AG2C2*AG2SO4
2NACL*MGCL2	2NACL*MGCL2	AG4FEC6N6*W	AG4FE(CN)6*H2O
2NACL*SRCL2	2NACL*SRCL2	AG4P2O7	AG4P2O7
2NAHSO3CHO*W	(CHO)2*2NAHSO3*H2O	AG5C4CL	(AG2C2)2*AGCL
2NH4NASO4*W	NA2SO4*(NH4)2SO4*H2O	AG6C4SO4	(AG2C2)2*AG2SO4

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
AGAUF4	AGAUF4	AGREO4	AGREO4
AGBR	SILVER-BROMIDE	AGSCN	AGSCN
AGBR*1.5NH3	AGBR*1.5NH3	AGVO3	AGVO3
AGBR4AL	AGBR*ALBR3	AL	ALUMINUM
AGBR7AL2	AGBR*2ALBR3	AL(OH)3	ALUMINUM-HYDROXIDE
AGBRCH5N	AGBR*CH3NH2	AL2CL9ZN1.5	AL2CL6*1.5ZNCL2
AGBRNH3	AGBR*NH3	AL2NABR6CL	(ALBR3)2*NACL
AGCH3CO2	AGCH3CO2	AL2NABR7	(ALBR3)2*NABR
AGCL	SILVER-CHLORIDE	AL2O3-1	ALUMINUM-OXIDE(CORUNDUM)
AGCL*1.5NH3	AGCL*1.5NH3	AL2O3-2	ALUMINUM-OXIDE(ALUMINA)
AGCL*NH3	AGCL*NH3	AL2S3O12*18W	AL2(SO4)3*18H2O
AGCL4AL	AGCL*ALCL3	AL2S3O12*6W	ALUMINUM
AGCLCH5N	AGCL*CH3NH2	AL2SI2O7*2W	AL2SI2O7*2H2O
AGCLO2	AGCLO2	AL2SI4O12H2	AL2SI4O10(OH)2
AGCLO4	AGCLO4	AL2SIO5-S	AL2SIO5-SILLIMANITE
AGCN2	SILVER	AL6SI2O13	AL6SI2O13
AGCN2H3	AGCN*NH3	ALB12-A	ALB12-ALPHA
AGF*2W	AGF*2H2O	ALBR3*14NH3	ALBR3*14NH3
AGF*4W	AGF*4H2O	ALBR3*3NH3	ALBR3*3NH3
AGF2	AGF2	ALBR3*5NH3	ALBR3*5NH3
AGI	SILVER-IODIDE	ALBR3*6NH3	ALBR3*6NH3
AGI*0.5NH3	AGI*0.5NH3	ALBR3*7NH3	ALBR3*7NH3
AGI*0.5PH3	AGI*0.5PH3	ALBR3*9NH3	ALBR3*9NH3
AGINH3	AGI*NH3	ALBR3*H2S	ALBR3*H2S
AGIO3	AGIO3	ALBR3*NABR	ALBR3*NABR
AGN2H6CLO4	AG(NH3)2CLO4	ALBR3*NACL	ALBR3*NACL
AGN3	AGN3	ALBR3*NH3	ALBR3*NH3
AGN3H6O3	AG(NH3)2NO3	ALBR3*PH3	ALBR3*PH3
AGN3H9BR	AG(NH3)3BR	ALC3H9	AL(CH3)3
AGN3H9CL	AG(NH3)3CL	ALC6H9O6	ALUMINUM
AGN3H9CLO4	AG(NH3)3CLO4	ALCL3*0.5SO2	ALCL3*0.5SO2
AGN4H9O3	AG(NH3)3NO3	ALCL3*14NH3	ALCL3*14NH3
AGNO2	AGNO2	ALCL3*3NH3	ALCL3*3NH3
AGOCN	SILVER	ALCL3*5NH3	ALCL3*5NH3
AGONC	SILVER	ALCL3*6NH3	ALCL3*6NH3

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
ALCL3*7NH3	ALCL3*7NH3	AUI*3NH3	AUI*3NH3
ALCL3*H2S	ALCL3*H2S	AUI*6NH3	AUI*6NH3
ALCL3*NABR	ALCL3*NABR	AUI*NH3	AUI*NH3
ALCL3*NACL	ALCL3*NACL	AUI*PH3	AUI*PH3
ALCL3*NH3	ALCL3*NH3	AUIN	AUIN
ALCL3*NH4CL	ALCL3*NH4CL	AUIN2	AUIN2
ALCL3*PH3	ALCL3*PH3	AUPB2	AUPB2
ALCL3*SO2	ALCL3*SO2	B	BORON
ALCL4N7H22	ALCL3*NH4CL*6NH3	B10H14	DECABORANE
ALI3*13NH3	ALI3*13NH3	B13P2	B13P2
ALI3*20NH3	ALI3*20NH3	B2O3	BORON-OXIDE
ALI3*2H2S	ALI3*2H2S	B3N3H3CL3	TRICHLOROBORAZOLE-BETA
ALI3*3NH3	ALI3*3NH3	BA	BARIUM
ALI3*5NH3	ALI3*5NH3	BA(C2H5O)2	BA(C2H5O)2
ALI3*6NH3	ALI3*6NH3	BA(CH3CO2)2	BA(CH3CO2)2
ALI3*7NH3	ALI3*7NH3	BA(CH3CO3)2	BA(CH2OHCO2)2
ALI3*9NH3	ALI3*9NH3	BA(CN)2	BA(CN)2
ALI3*NH3	ALI3*NH3	BA(CN)2*2W	BA(CN)2*2H2O
ALN3O9*6W	ALUMINUM	BA(CN)2*W	BA(CN)2*H2O
ALN3O9*9W	ALUMINUM	BA(CNO)2	BA(CNO)2
ALO(OH)	BOEHMITE	BA(H2PO2)2*W	BA(H2PO2)2*H2O
AS	ARSENIC	BA(H2PO4)2	BA(H2PO4)2
AS2O3*SO3	AS2O3*SO3	BA(HCO2)2	BA(HCO2)2
AU	GOLD	BA(IO3)2	BA(IO3)2
AU2PB	AU2PB	BA(IO3)2*W	BA(IO3)2*H2O
AUBR*2NH3	AUBR*2NH3	BA(NH2)2	BA(NH2)2
AUBR*3NH3	AUBR*3NH3	BA(NH3)6	BA(NH3)6
AUBR*4NH3	AUBR*4NH3	BA(NO2)2	BA(NO2)2
AUBR*6NH3	AUBR*6NH3	BA(NO2)2*W	BA(NO2)2*H2O
AUBR*NH3	AUBR*NH3	BA(REO4)2*4W	BA(REO4)2*4H2O
AUBR3	AUBR3	BA2AL2O5*5W	(BAO)2*AL2O3*5H2O
AUCL*2NH3	AUCL*2NH3	BA2N	BA2N
AUCL*NH3	AUCL*NH3	BA2NBR	BA2NBR
AUCL3*2W	AUCL3*2H2O	BA2NCL	BA2NCL
AUI*2NH3	AUI*2NH3	BA2TL(NO2)5	(BA(NO2)2)2*TLNO2

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
BA3(ASO4)2	BA3(ASO4)2-HYDRATED,PRECIPITATE	BACL2O8	BA(CLO4)2
BA3(RHCL6)2	BA3(RHCL6)2	BACL2O8*2NH3	BA(CLO4)2*2NH3
BA3AL4CL18	(BACL2)3*2AL2CL6	BACL2O8*3W	BA(CLO4)2*3H2O
BA3P2O8	BA3(PO4)2-COLLOIDAL	BACL2O8*6NH3	BA(CLO4)2*6NH3
BA3WO6	BA3WO6	BACLF	BACLF
BA6NI9	BA6NI9	BACLH	BACLH
BAAL4	BAAL4	BACN2	BACN2
BABR2*2NH3	BABR2*2NH3	BACO3	BARIUM-CARBONATE
BABR2*2W	BABR2*2H2O	BACS3	BACS3
BABR2*4NH3	BABR2*4NH3	BAF2	BAF2
BABR2*8NH3	BABR2*8NH3	BAH4AS2O8*2W	BA(H2ASO4)2*2H2O
BABR2*BAO*2W	BABR2*BAO*2H2O	BAH4P2O4	BA(H2PO2)2
BABR2*BAO*5W	BABR2*BAO*5H2O	BAH4S3O12*W	BASO4*2H2SO4*H2O
BABR2*NH3	BABR2*NH3	BAHASO4*W	BAHASO4*H2O
BABR2*W	BABR2*H2O	BAHPO4	BAHPO4
BABR2O6	BA(BRO3)2	BAI2*10NH3	BAI2*10NH3
BABR2O6*W	BA(BRO3)2*H2O	BAI2*2.5W	BAI2*2.5H2O
BAC2O4	BAC2O4	BAI2*2NH3	BAI2*2NH3
BAC2O4*0.5W	BAC2O4*0.5H2O	BAI2*2PBI	BAI2*2PBI2
BAC2O4*2W	BAC2O4*2H2O	BAI2*2SO2	BAI2*2SO2
BAC2O4*3.5W	BAC2O4*3.5H2O	BAI2*2W	BAI2*2H2O
BAC4H14S2O10	BA(C2H5SO4)2*2H2O	BAI2*4NH3	BAI2*4NH3
BAC4H6O4*3W	BA(CH3CO2)2*3H2O	BAI2*4SO2	BAI2*4SO2
BACA(CO3)2	BACA(CO3)2	BAI2*6NH3	BAI2*6NH3
BACL2*2W	BACL2*2H2O	BAI2*7W	BAI2*7H2O
BACL2*8NH3	BACL2*8NH3	BAI2*8NH3	BAI2*8NH3
BACL2*AL2CL6	BACL2*AL2CL6	BAI2*9NH3	BAI2*9NH3
BACL2*BAO*3W	BACL2*BAO*3H2O	BAI2*BAO*2W	BAI2*BAO*2H2O
BACL2*BAO*5W	BACL2*BAO*5H2O	BAI2*BAO*9W	BAI2*BAO*9H2O
BACL2*BAO*8W	BACL2*BAO*8H2O	BAI2*W	BAI2*H2O
BACL2*W	BACL2*H2O	BAIH	BAIH
BACL2O4	BA(CLO2)2	BAMG2	BAMG2
BACL2O4*3.5W	BA(CLO2)2*3.5H2O	BAMNO4	BAMNO4
BACL2O6	BA(CLO3)2	BAMOO3	BAMOO3
BACL2O6*W	BA(CLO3)2*H2O	BAN2	BAN2

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
BAN6*W	BA(N3)2*H2O	BEBR2*10NH3	BEBR2*10NH3
BANH	BANH	BEBR2*2H2S	BEBR2*2H2S
BAO*2SIO2	BAO*2SIO2	BEBR2*4NH3	BEBR2*4NH3
BAO*AL2O3	BAO*AL2O3	BEBR2*6NH3	BEBR2*6NH3
BAO*AL2O3*2W	BAO*AL2O3*2H2O	BECL2*12NH3	BECL2*12NH3
BAO*AL2O3*4W	BAO*AL2O3*4H2O	BECL2*2NH3	BECL2*2NH3
BAO*AL2O3*7W	BAO*AL2O3*7H2O	BECL2*4NH3	BECL2*4NH3
BAO*AL2O3*W	BAO*AL2O3*H2O	BECL2*4W	BECL2*4H2O
BAO*GEO2	BAO*GEO2	BECL2*6NH3	BECL2*6NH3
BAO*SIO2	BAO*SIO2	BECO3	BECO3
BAO2H2*3W	BA(OH)2*3H2O	BEH2	BEH2
BAO2H2*8W	BA(OH)2*8H2O	BEI2*13NH3	BEI2*13NH3
BAO2H2*W	BA(OH)2*H2O	BEI2*2H2S	BEI2*2H2S
BAOSCL6	BAOSCL6	BEI2*4NH3	BEI2*4NH3
BAPB2I6*7W	BAI2*2PBI2*7H20	BEI2*6NH3	BEI2*6NH3
BAPDCL4	BAPDCL4	BEMOO4	BEMOO4
BAPTCL6	BAPTCL6	BEO*3AL2O3	BEO*3AL2O3
BAPTCL6*6W	BAPTCL6*6H2O	BEO*AL2O3	BEO*AL2O3
BARUO4*W	BARUO4*H2O	BESEO4	BESEO4
BAS2O3	BAS2O3	BESEO4*2W	BESEO4*2H2O
BAS2O6*2W	BAS2O6*2H2O	BESEO4*4W	BESEO4*4H2O
BAS2O8*4W	BAS2O8*4H2O	BESO4	BESO4
BAS4O6*2W	BAS4O6*2H2O	BESO4*W	BESO4*H2O
BASE	BASE	BF3*PC3H9	BF3*P(CH3)3
BASEO3	BASEO3	BH3NH2CH3	BH3NH2CH3
BASEO4	BASEO4	BI	BISMUTH
BASIF6	BASIF6	BI(OH)2CL	BI(OH)2CL
BASO3	BASO3	BI(OH)3	BISMUTH
BASO4	BARIUM-SULFATE	BIOBR	BIOBR
BASO4*H2SO4	BASO4*H2SO4	BIONO3	BIONO3
BASRTIO4	BASRTIO4	BIOOH	BIOOH
BC4H12NH2	B(CH3)3*NH2CH3	BO3C3H9*NH3	B(OCH3)3*NH3
BE	BERYLLIUM	BO3C6H12N	TRIETHANOLAMINE
BE2SIO4	BE2SIO4	C	CARBON(GRAPHITE)
BE3B2O6	BE3B2O6	C2H4O8S2K2	C2H2O2*2KHSO3

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
C2H5OK	C2H5OK	CA2V2O7	(CAO)2*V2O5
C2O3.5H4NA	CH2OHCOONA*0.5H2O	CA3AL2O6	(CAO)3*AL2O3
C2O4H3NA	CH(OH)2COONA	CA3AL2O6*6W	(CAO)3*AL2O3*6H2O
C3H9AS*BC3H9	(CH3)3AS*B(CH3)3	CA3AL2SI2O10	(CAO)3*AL2O3*2SIO2
C3H9AS*BF3	(CH3)3AS*BF3	CA3AL4CL18	(CACL2)3*4ALCL3
C3H9B*NH3	(CH3)3B*BH3	CA3B2O6	(CAO)3*B2O3
C3H9N*ALBR3	(CH3)3N*ALBR3	CA3BI2	CA3BI2
C3H9N*ALCL3	(CH3)3N*ALCL3	CA3CL2O2	CACL2*2CAO
C3H9N*BC3H9	(CH3)3N*B(CH3)3	CA3GEO5	(CAO)3*GEO2
C3H9N*BH3	(CH3)3N*BH3	CA3MGSI2O8	(CAO)3*MGO*2SIO2
C3H9NB3H7	(CH3)3NB3H7	CA3O7C8H24	(CAO)3*4C2H5OH
C3H9P*BC3H9	(CH3)3P*B(CH3)3	CA3P2O8-A	CA3(PO4)2-ALPHA
C4H11N*BC3H9	(C2H5)2NH*B(CH3)3	CA3P2O8-B	CA3(PO4)2-BETA
C4H11O2CS	C2H5OCS*C2H5OH	CA3TI2O7	(CAO)3*2TIO2
C4H11O2K	C2H5OK*C2H5OH	CA3V2O8	(CAO)3*V2O5
C4H12N*BH4	(CH3)4N*BH4	CA4AL2O7	(CAO)4*AL2O3
CA	CALCIUM	CA4BR2O19H32	CABR2*3CAO*16H2O
CA(OH)2	CALCIUM-HYDROXIDE	CA4CL2O3	CACL2*3CAO
CA10P6O24F2	CA10(PO4)6F2	CA4CL2O3*16W	CACL2*3CAO*16H2O
CA10P6O26H2	CA10(PO4)6(OH)2	CA4CL2O3*3W	CACL2*3CAO*3H2O
CA12AL14O33	(CAO)12*7AL2O3	CA4I2O19H32	CAI2*3CAO*16H2O
CA2AL2O5	(CAO)2*AL2O3	CA4SI2O7F2	(CAO)3*2SIO2*CAF2
CA2AL2O5*5W	(CAO)2*AL2O3*5H2O	CA5I2O12	CA5(IO6)2
CA2AL2SIO7	(CAO)2*AL2O3*SIO2	CA8H12P6O29	CA8H2(PO4)6*5H2O
CA2B2O5	(CAO)2*B2O3	CAAL2	CAAL2
CA2B2SI2O9	(CAO)2*B2O3*2SIO2	CAAL2O4	CAO*AL2O3
CA2B2SI2O9*W	(CAO)2*B2O3*2SIO2*H2O	CAAL2SI2O8	CAO*AL2O3*2SIO2
CA2B6O11	(CAO)2*3B2O3	CAAL2SI6O16	CAO*AL2O3*6SIO2
CA2B6O11*13W	(CAO)2*3B2O3*13H2O	CAAL2SIO6	CAO*AL2O3*SIO2
CA2FE2O5	(CAO)2*FE2O3	CAAL4	CAAL4
CA2GEO4	(CAO)2*GEO2	CAAL4O7	CAO*2AL2O3
CA2MGSI2O7	(CAO)2*MGO*2SIO2	CAALGASI2O8	CAALGASI2O8
CA2N2O10.5H7	CA(NO3)2*CA(OH)2*2.5H2O	CAB2F8	CA(BF4)2
CA2N2O8H2	CA(NO3)2*CA(OH)2	CAB2O4	CAO*B2O3
CA2SIO4-B	(CAO)2*SIO2-BETA	CAB4O7	CAO*2B2O3

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
CABR2*2NH3	CABR2*2NH3	CAFESIO4	CAFESIO4
CABR2*6NH3	CABR2*6NH3	CAGEO3	CAO*GEO2
CABR2*6W	CABR2*6H2O	CAH12P2O9N2	CA(H2PO4)2*H2O*2NH3
CABR2*8NH3	CABR2*8NH3	CAH18P2O9N4	CA(H2PO4)2*H2O*4NH3
CABR2*NH3	CABR2*NH3	CAH2	CAH2
CABR2O6	CA(BRO3)2	CAH2C2O4	CA(HCOO)2
CABRH	CABRH	CAH4P2O4	CA(H2PO2)2
CAC2N2	CA(CN)2	CAH4P2O8	CA(H2PO4)2
CAC2O4	CAC2O4	CAH6P2O9	CA(H2PO4)2*H2O
CAC2O4*W	CAC2O4*H2O	CAH9P2O9N	CA(H2PO4)2*H2O*NH3
CAC4H10O2	CA(C2H5O)2	CAI2*2NH3	CAI2*2NH3
CAC4H6O4	CA(CH3CO2)2	CAI2*6NH3	CAI2*6NH3
CAC4H6O4*W	CA(CH3CO2)2*H2O	CAI2*8NH3	CAI2*8NH3
CAC4H6O6	CA(CH2OHCO2)2	CAI2*8W	CAI2*8H2O
CAC4H6O6*3W	CA(CH2OHCO2)2*3H2O	CAI2*NH3	CAI2*NH3
CAC4H6O6*5W	CA(CH2OHCO2)2*5H2O	CAI2O6	CA(IO3)2
CAC8H22O4	CA(C2H5O)2*2C2H5OH	CAI2O6*6W	CA(IO3)2*6H2O
CACL2	CALCIUM-CHLORIDE	CAI2O6*W	CA(IO3)2*H2O
CACL2*2NH3	CACL2*2NH3	CAIH	CAIH
CACL2*2W	CACL2*2H2O	CAMG(CO3)2	CALCIUM-MAGNESIUM-CARBONATE
CACL2*4NH3	CACL2*4NH3	CAMG2CL6*2W	CACL2*2MGCL2*2H2O
CACL2*4W	CACL2*4H2O	CAMOO3	CAMOO3
CACL2*6W	CACL2*6H2O	CAN2H4	CA(NH2)2
CACL2*8NH3	CACL2*8NH3	CAN2O2*4W	CAN2O2*4H2O
CACL2*NH3	CACL2*NH3	CAN2O4	CA(NO2)2
CACL2*W	CACL2*H2O	CAN2O4*4W	CA(NO2)2*4H2O
CACL2C6H18O3	CACL2*3C2H5OH	CAN2O8C2H8	CA(NO3)2*2CH3OH
CACL2C8H24O4	CACL2*4C2H5OH	CAN6	CA(N3)2
CACL2O4	CA(CLO2)2	CAN6*0.5W	CA(N3)2*0.5H2O
CACL2O8	CA(CLO4)2	CAN6*1.5W	CA(N3)2*1.5H2O
CACL2O8*4W	CA(CLO4)2*4H2O	CAN6*2N2H4	CA(N3)2*2N2H4
CACL2O8*6NH3	CA(CLO4)2*6NH3	CAN6*4W	CA(N3)2*4H2O
CACLH	CACLH	CAN6*N2H4	CA(N3)2*N2H4
CACO3-1	CALCIUM-CARBONATE(ARAGONITE)	CAO	CALCIUM-OXIDE
CACO3-2	CALCIUM-CARBONATE(CALCITE)	CAO*FE2O3	CAO*FE2O3

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
CAO4H4	CA(OH)2*H2O2	CDBR3NH5O0.5	CDBR2*NH4BR*0.5H2O
CAOCL2	CA(OCL)CL	CDBROH	CDBROH
CAP2O6-B	CA(PO3)2-BETA	CDC2N2	CADMIUM
CAPB2I6	CAI2*2PBI2	CDC2N2S2	CD(CNS)2
CAPB2I6*7W	CAI2*2PBI2*7H2O	CDC2O4	CADMIUM
CAPB3	CAPB3	CDC2O7H6	CADMIUM
CAS2O6*4W	CAS2O6*4H2O-DITHIONATE	CDCL2*2.5W	CDCL2*2.5H2O
CASEO3*2W-1	CASEO3*2H2O	CDCL2*W	CADMIUM
CASEO3*2W-2	CASEO3*2H2O-PRECIPITATED	CDCL2N10H30	CDCL2*10NH3
CASEO4	CASEO4	CDCL2N2H6	CDCL2*2NH3
CASEO4*2W	CASEO4*2H2O	CDCL2N4H12	CDCL2*4NH3
CASO4	CALCIUM-SULFATE	CDCL2N6H18	CDCL2*6NH3
CASO4*0.5W-B	CASO4*0.5H2O-BETA	CDCL2NH3	CDCL2*NH3
CASO4-A	CASO4-SOLUBLE-ALPHA	CDCL2O8*6W	CADMIUM
CASO4-B	CASO4-SOLUBLE-BETA	CDCL3NH5O0.5	CDCL2*NH4CL*0.5H2O
CATIO3	CAO*TIO2	CDCL4H2*7W	CDCL2*2HCL*7H2O
CATL	CATL	CDCL6N4H16	CDCL2*4NH4CL
CAV2O6	CAO*V2O5	CDH5S3.5O14	CDSO4*2.5H2SO4
CCL3COONA	CCL3COONA	CDI2N2H6	CDI2*2NH3
CD	CADMIUM	CDI2N6H18	CDI2*6NH3
CD2I6PB	(CDI2)2*PBI2	CDI2O6	CADMIUM
CD3C4N4O6H10	(CD(CN)2)2*CDO*5H2O	CDI3NH5O0.5	CDI2*NH4I*0.5H2O
CD3N2	CADMIUM	CDIOH	CDIOH
CD3P2	CADMIUM	CDN2H4	CACMIUM
CD3P2O8	CD3(PO4)2	CDN2O6	CADMIUM
CD3S2O10H2	(CDSO4)2*CD(OH)2	CDN2O6*2W	CADMIUM
CD3SB2	CD3SB2	CDN2O6*4W	CADMIUM
CD3SO8H4	CDSO4*2CD(OH)2	CDN6	CADMIUM
CDAS2	CDAS2	CDO2N2C2	CADMIUM
CDB2O4	CD(BO2)2	CDOHCL	CD(OH)CL
CDBR2*4W	CADMIUM	CDSEO4	CADMIUM
CDBR2N12H36	CDBR2*12NH3	CDSEO4*W	CADMIUM
CDBR2N2H6	CDBR2*2NH3	CDSO4*W	CADMIUM
CDBR2N6H18	CDBR2*6NH3	CE	CERIUM
CDBR2NH3	CDBR2*NH3	CE2C6O12*10W	CE2(C2O4)3*10H2O

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
CE2S3O12*5W	CE2(SO4)3*5H2O	CO2SI	CO2SI
CE2S3O12*8W	CE2(SO4)3*8H2O	CO2SIO4	CO2SIO4
CE2SE3O9*10W	CE2(SEO3)3*10H2O	CO3AS2	CO3AS2
CE3AL	CE3AL	CO3N18H27O18	(CO(NH3)5NO2)(CO(NH3)2(NO2)4)2
CEAL2	CEAL2	CO3P2O8	CO3(PO4)2
CEAL4	CEAL4	CO3TE4	CO3TE4
CEAS	CEAS	CO3W	CO3W
CECL3*12NH3	CECL3*12NH3	CO4N24H36O24	(CO(NH3)6)(CO(NH3)2(NO2)4)3
CECL3*20NH3	CECL3*20NH3	CO4SO10H6	COSO4*3CO(OH)2
CECL3*2NH3	CECL3*2NH3	CO5AS2	CO5AS2
CECL3*4NH3	CECL3*4NH3	CO5N30H45O30	(CO(NH3)5NO2)3(CO(NO2)6)2
CECL3*7W	CECL3*7H2O	CO5TE6	CO5TE6
CECL3*8NH3	CECL3*8NH3	COAL	COAL
CEF3*W	CEF3*H2O	COAL2	COAL2
CEHG4	CEHG4	COAL4	COAL4
CEI3O9	CE(IO3)3	COAS	COAS
CEI3O9*2W	CE(IO3)3*2H2O	COAS2	COAS2
CEN3O9	CE(NO3)3	COB2O4	CO(BO2)2
CEN3O9*3W	CE(NO3)3*3H2O	COBALT	COBALT
CEN3O9*4W	CE(NO3)3*4H2O	COBR2*2N2H4	COBR2*2N2H4
CEN3O9*6W	CE(NO3)3*6H2O	COBR2*2NH3	COBR2*2NH3-ROSE
CEOCL	CEOCL	COBR2*6W	COBR2*6H2O
CES2	CES2	COBR2*NH3	COBR2*NH3
CEZN	CEZN	COBR2C2H8O2	COBR2*2CH3OH
CH2OHCOONA	CH2OHCOONA	COBR2C4H12O2	COBR2*2C2H5OH
CH2SO4	METHYLENE	COBR2C4H12O4	COBR2*2C2H4(OH)2
CH3COOK	CH3COOK	COBR2C6H18O3	COBR2*3C2H5OH
CH3COONH4	AMMONIUM	COBR2C6H18O6	COBR2*3C2H4(OH)2
CO2AL5	CO2AL5	COC2N2O2	CO(CNO)2
CO2AS	CO2AS	COC2N2S2	CO(CNS)2
CO2AS3	CO2AS3	COC2O4	COC2O4
CO2C	CO2C	COCL2	COCL2
CO2N11H17O13	(CO(NH3)5H2O)(CO(NO2)6)	COCL2*2N2H4	COCL2*2N2H4
CO2N12H18O12	(CO(NH3)6)(CO(NO2)6)	COCL2*2NH3	COCL2*2NH3-ROSE
CO2S3	CO2S3	COCL2*2W	COCL2*2H2O

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
COCL2*6W	COCL2*6H2O	CON5H17OBR3	(CO(NH3)5H2O)BR3
COCL2*NH3	COCL2*NH3	CON5H17OCL3	(CO(NH3)5H2O)CL3
COCL2*W	COCL2*H2O	CON5H17OF3	(CO(NH3)5H2O)F3
COCL2C4H12O2	COCL2*2C2H5OH	CON5H17OI3	(CO(NH3)5H2O)I3
COCL2C6H18O3	COCL2*3C2H5OH	CON5H19C4CL3	(CO(C2H4(NH2)2)2CL2)CL*NH3
COCL2C6H18O6	COCL2*3C2H4(OH)2	CON6H11C2O6	(CO(C2H4(NH2)2)(NH3)(NO2)3
COCL2O8*6W	CO(CLO4)2*6H2O	CON6H12O4CL	(CO(NH3)4(NO2)2)CL
COH2C2O4	CO(HCO2)2	CON6H12O4I-C	(CO(NH3)4(NO2)2)I-CIS
COHPO4	COHPO4	CON6H12O4I-T	(CO(NH3)4(NO2)2)I-TRANS
COI2*2NH3	COI2*2NH3-BLUE	CON6H12O8S	(CO(NH3)4(NO2)2)SO4-CIS
COI2O6*2W	CO(IO3)2*2H2O	CON6H15C2O6	(CO(NH3)5NO2)C2O4
CON12H9	(CO(NH3)3(N3)3)	CON6H15O2BR2	(CO(NH3)5NO2)BR2
CON13H12-C	(CO(NH3)4(N3)2)N3-CIS	CON6H15O2CL2	(CO(NH3)5NO2)CL2
CON13H12-T	(CO(NH3)4(N3)2)N3-TRANS	CON6H15O2I2	(CO(NH3)5NO2)I2
CON14H15	(CO(NH3)5N3)(N3)2	CON6H15O3CL2	(CO(NH3)5NO3)CL2
CON15H18	(CO(NH3)6)(N3)3	CON6H15O3I2	(CO(NH3)5NO3)I2
CON2H8C2CL2	(CO(C2H4(NH2)2))CL2	CON6H15O7S	(CO(NH3)5SO4)NO3
CON2O6*2W	CO(NO3)2*2H2O	CON6H17CO7	(CO(NH3)5CO3)NO3*H2O
CON2O6*3W	CO(NO3)2*3H2O	CON6H18BR2	(CO(NH3)6)BR2
CON2O6*4W	CO(NO3)2*4H2O	CON6H18BR3	(CO(NH3)6)BR3
CON2O6*6W	CO(NO3)2*6H2O	CON6H18CL2	(CO(NH3)6)CL2
CON3H12C3CL2	COCL2*1.5C2H4(NH2)2	CON6H18CL3	(CO(NH3)6)CL3
CON4H12CL3	(CO(NH3)4CL2)CL-CIS	CON6H18I2	(CO(NH3)6)I2
CON4H16C4CL3	(CO(C2H4(NH2)2)2CL2)CL	CON6H18I3	(CO(NH3)6)I3
CON4H16O2CL3	(CO(NH3)4(H2O)2)CL3	CON6H24C6BR2	(CO(C2H4(NH2)2)3)BR2
CON5H10C2O8	NH4(CO(NH3)2(NO2)2C2O4)	CON6H24C6CL2	(CO(C2H4(NH2)2)3)CL2
CON5H15BR3	(CO(NH3)5BR)BR2	CON6H24C6I2	(CO(C2H4(NH2)2)3)I2
CON5H15CL3	(CO(NH3)5CL)CL2	CON6H24C6I3	(CO(C2H4(NH2)2)3)I3
CON5H15CLBR2	(CO(NH3)5CL)BR2	CON6H9O6	(CO(NH3)3(NO2)3)
CON5H15CLC2O	(CO(NH3)5CL)C2O4	CON7H10O8	NH4(CO(NH3)2(NO2)4)
CON5H15CLI2	(CO(NH3)5CL)I2	CON7H12O7	(CO(NH3)4(NO2)2)NO3
CON5H15I3	(CO(NH3)5I)I2	CON7H14O10	(CO(NH3)4(NO3)H2O)(NO3)2
CON5H15ICL2	(CO(NH3)5I)CL2	CON7H15IO6	(CO(NH3)5I)(NO3)2
CON5H15SO4I	(CO(NH3)5SO4)I	CON7H16C4O7	(CO(C2H4(NH2)2)2(NO2)2)NO3-CIS
CON5H16CO2I2	(CO(NH3)5HCO2)I2	CON7H16CO8	(CO(NH3)5HCO2)(NO3)2

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
CON8H15CSO6	(CO(NH3)5CNS)(NO3)2	CRCL2N3H9	CRCL2*3NH3
CON8H15O8	(CO(NH3)5NO2)(NO3)2	CRCL2N6H18	CRCL2*6NH3
CON8H15O9	(CO(NH3)5NO3)(NO3)2	CRH11O7	(CR(H2O)4(OH)2)OH
CON8H17O10	(CO(NH3)5H2O)(NO3)3	CRH12O6BR3	(CR(H2O)6)BR3-PURPLE
CON9H18O9	(CO(NH3)6)(NO3)3	CRH12O6BR3-G	(CR(H2O)4BR2)BR*2H2O-GREEN
CON9H24C6O9	(CO(C2H4(NH2)2)3)(NO3)3	CRH12O6CL3	(CR(H2O)4CL2)CL*2H2O-GREEN
CONH2COOK	CONH2COOK	CRH12O6CL3-V	(CR(H2O)6)CL3-VIOLET
COO2H2-B	CO(OH)2-BLUE,PRECIPITATED	CRH13O8	(CR(H2O)5OH)(OH)2
COO2H2-P1	CO(OH)2-PINK,PRECIPITATED	CRH20O10CL3	(CR(H2O)4CL2)CL*6H2O-GREEN
COO2H2-P2	CO(OH)2-PINK,PRECIPITATED,AGED	CRH8O4CL3	(CR(H2O)4CL2)CL-GREEN
COO3H3	CO(OH)3-PRECIPITATED	CRIBR2	CRIBR2
COSB	COSB	CRICL2	CRICL2
COSE	COSE	CRN3O18H18	CR(NO3)3*9H2O
COSEO3*2W	COSEO3*2H2O	CRO3H3	CR(OH)3-PRECIPITATED
COSI	COSI	CRSB	CRSB
COSI2	COSI2	CRSB2	CRSB2
COSI3	COSI3	CS	CESIUM
COSO4*6W	COSO4*6H2O	CS(UO2)2F5	CS(UO2)2F5
COSO4*7W	COSO4*7H2O	CS12H22C7O31	5CS2CO3*2CSHCO3*10H2O
COTE2	COTE2	CS2BAN4O8	BA(NO2)2*2CSNO2
CR	CHROMIUM	CS2C2O4	CS2C2O4
CR2H16O20S3	(CR2(H2O)6(SO4)3)*2H2O-GREEN	CS2CO3	CS2CO3
CR2H28O26S3	(CR(H2O)6)2(SO4)3*2H2O	CS2CO3*3W	CS2CO3*3H2O
CR2H30O27S3	(CR(H2O)6)2(SO4)3*3H2O	CS2COCL4	CS2COCL4
CR2H32O28S3	(CR(H2O)6)2(SO4)3*4H2O	CS2CR2O7	CS2CR2O7
CR2H34O29S3	(CR(H2O)6)2(SO4)3*5H2O	CS2CRO4	CS2CRO4
CR2O3	ESKOLAITE	CS2CUCL4	CS2CUCL4
CR2S3O12*18W	CR2(SO4)3*18H2O	CS2CUCL4*2W	CS2CUCL4*2H2O
CR2TE3	CR2TE3	CS2FECL4	CS2FECL4
CR3TE4	CR3TE4	CS2GECL6	CS2GECL6
CR5TE6	CR5TE6	CS2HFCL6	CS2HFCL6
CR7H2	CR7H2	CS2I8	CS2I8
CRCL2*2W	CRCL2*2H2O-LIGHT	CS2MNCL4	CS2MNCL4
CRCL2*3W	CRCL2*3H2O-PALE	CS2MO2O7	CS2MO2O7
CRCL2*4W	CRCL2*4H2O-DARK	CS2MOO4	CS2MOO4

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
CS2NACECL6	CS2NACECL6	CS2ZNCL4	CS2ZNCL4
CS2NADYCL6	CS2NADYCL6	CS2ZNI4	CS2ZNI4
CS2NAERCL6	CS2NAERCL6	CS2ZRBR6	CS2ZRBR6
CS2NAGDCL6	CS2NAGDCL6	CS2ZRCL6	CS2ZRCL6
CS2NALACL6	CS2NALACL6	CS3COCL5	CS3COCL5
CS2NALUCL6	CS2NALUCL6	CS3CR2CL9	CS3CR2CL9
CS2NANDCL6	CS2NANDCL6	CS3CRCL6	CS3CRCL6
CS2NAPUCL6	CS2NAPUCL6	CS3CUCL5	CS3CUCL5
CS2NAYCL6	CS2NAYCL6	CS3FECL5	CS3FECL5
CS2NBOCL5	CS2NBOCL5	CS3MNCL5	CS3MNCL5
CS2NPBR6	CS2NPBR6	CS3NICL5	CS3NICL5
CS2NPCL6	CS2NPCL6	CS3TI2BR9	CS3TI2BR9
CS2PACL6	CS2PACL6	CS3TIBR6	CS3TIBR6
CS2PTCL4	CS2PTCL4	CS3UO2F5	CS3UO2F5
CS2PUCL6	CS2PUCL6	CS3V2CL9	CS3V2CL9
CS2RECL6	CS2RECL6	CS3VCL6	CS3VCL6
CS2S	CS2S	CS4THCL8	CS4THCL8
CS2S2O5	CS2S2O5	CS5U2O4F9	CS5(UO2)2F9
CS2SEO3*W	CS2SEO3*H2O	CSALH4	CSALH4
CS2SEO4	CS2SEO4	CSALS2O8*12W	CSAL(SO4)2*12H2O
CS2SNCL6	CS2SNCL6	CSB(CLO4)4	CSB(CLO4)4
CS2SO3	CS2SO3	CSBA2N5O10	CSNO2*2BA(NO2)2
CS2TEBR6	CS2TEBR6	CSBCL4	CSBCL4
CS2TEO3	CS2TEO3	CSBF4	CSBF4
CS2TEO3*5W	CS2TEO3*5H2O	CSBO2	CSBO2
CS2THCL6	CS2THCL6	CSBR2CL	CSBR2CL
CS2THCL6*8W	CS2THCL6*8H2O	CSBR3	CSBR3
CS2TIBR6	CS2TIBR6	CSBRCL2	CSBRCL2
CS2TICL4	CS2TICL4	CSBRO3	CSBRO3
CS2TICL6	CS2TICL6	CSC10	CSC10
CS2U2O7	CS2U2O7	CSC24	CSC24
CS2UBR6	CS2UBR6	CSC36	CSC36
CS2UCL6	CS2UCL6	CSC48	CSC48
CS2UO4	CS2UO4	CSC60	CSC60
CS2ZNBR4	CS2ZNBR4	CSC72	CSC72

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
CSC8	CSC8	CSNB2OCL9	CSNB2OCL9
CSCACL3	CSCACL3	CSNBCL6	CSNBCL6
CSCL*ZNSO4	CSCL*ZNSO4	CSNBO3	CSNBO3
CSCLO3	CSCLO3	CSNH2	CSNH2-TETRAGONAL
CSCLO4	CSCLO4	CSNICL3	CSNICL3
CSCN	CSCN	CSNO3	CSNO3
CSCOCL3	CSCOCL3	CSOH*W	CSOH*H2O
CSCUCL3	CSCUCL3	CSPF6	CSPF6
CSF*1.5W	CSF*1.5H2O	CSPO3	CSPO3
CSFECL3	CSFECL3	CSPTNH3CL3	CSPTNH3CL3
CSGDFEC6N6	CSGD(FE(CN)6)	CSREO4	CSREO4
CSH	CSH	CSSO2F	CSSO2F
CSH2PO4	CSH2PO4	CSTACL6	CSTACL6
CSHC2	CSHC2	CSTIBR3	CSTIBR3
CSHCO3	CSHCO3	CSTICL3	CSTICL3
CSHF2	CSHF2	CSU2CL9	CSU2CL9
CSHS	CSHS	CSUCL5	CSUCL5
CSHSE	CSHSE	CSUCL6	CSUCL6
CSHSO4	CSHSO4	CSUF6	CSUF6
CSI*3SO2	CSI*3SO2	CSWF6	CSWF6
CSI2BR	CSI2BR	CSYFEC6N6*2W	CSY(FE(CN)6)*2H2O
CSI3	CSI3	CU	COPPER
CSI4	CSI4	CU2AL	CU2AL
CSIBR2	CSIBR2	CU2AL2O4	CU2AL2O4
CSIBRCL	CSIBRCL	CU2CD3	CU2CD3
CSIBRF	CSIBRF	CU2CL2*C2H2	(CUCL)2*C2H2
CSICL2	CSICL2	CU2CL2*CO*2W	(CUCL)2*CO*2H2O
CSICL4	CSICL4	CU2CO5H2	CUCO3*CU(OH)2
CSIO3	CSIO3	CU2FEC6N6	CU2FE(CN)6
CSIO4	CSIO4	CU2O	COPPER-OXIDE(CUPRITE)
CSKCLI	CSKCLI	CU2OCL2	CU2OCL2
CSMNCL3	CSMNCL3	CU2S	COPPER-SULFIDE(CHALCOCITE)
CSMOF6	CSMOF6	CU3AL	CU3AL
CSN3	CSN3	CU3AL2	CU3AL2
CSNACLI	CSNACLI	CU3C2O8H2	(CUCO3)2*CU(OH)2

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
CU3CL3*C2H2	(CUCL)3*C2H2	CUC4H24O6N6	CU(CH2OHCOO)2*6NH3
CU3N	CU3N	CUC4H6O4	CU(CH3COO)2
CU3P2O8	CU3(PO4)2	CUC4H6O4*W	CU(CH3COO)2*H2O
CU3SB	CU3SB	CUC4H6O6	CU(CH2OHCOO)2
CU3SN	CU3SN	CUCL*1.5NH3	CUCL*1.5NH3
CU3SO8H4	CUSO4*2CU(OH)2	CUCL*2PH3	CUCL*2PH3
CU4BR2O12H6	CU(BRO3)2*3CU(OH)2	CUCL*3NH3	CUCL*3NH3
CU4BR2O6H6	CUBR2*3CU(OH)2	CUCL*NH3	CUCL*NH3
CU4CL2O3	CUCL2*3CUO	CUCL*PH3	CUCL*PH3
CU4CL2O3*4W	CUCL2*3CUO*4H2O	CUCL2*10NH3	CUCL2*10NH3
CU4CL2O6H6	CUCL2*3CU(OH)2	CUCL2*2NH3	CUCL2*2NH3
CU4I2O12H6	CU(IO3)2*3CU(OH)2	CUCL2*2W	CUCL2*2H2O
CU4N2O12H6	CU(NO3)2*3CU(OH)2	CUCL2*4NH3W2	CUCL2*4NH3*2H2O
CU4SO10H6	CUSO4*3CU(OH)2	CUCL2*5NH3	CUCL2*5NH3
CU4SO10H6*W	CUSO4*3CU(OH)2*H2O	CUCL2*6NH3	CUCL2*6NH3
CUAL	CUAL	CUCL2C2H8O2	CUCL2*2CH3OH
CUAL2	CUAL2	CUCL2C4H12O2	CUCL2*2C2H5OH
CUAL2O4	CUAL2O4	CUCL2O8*6W	CU(CLO4)2*6H2O
CUBR*1.5NH3	CUBR*1.5NH3	CUCL4N2H8	CUCL2*2NH4CL
CUBR*2PH3	CUBR*2PH3	CUCL4N2H8*2W	CUCL2*2NH4CL*2H2O
CUBR*3NH3	CUBR*3NH3	CUCNS	CUCNS
CUBR*NH3	CUBR*NH3	CUH	CUH
CUBR*PH3	CUBR*PH3	CUH14C2O4N4	CU(HCOO)2*4NH3
CUBR2*10NH3	CUBR2*10NH3	CUH20C2O4N6	CU(HCOO)2*6NH3
CUBR2*2NH3	CUBR2*2NH3	CUH8C2O4N2	CU(HCOO)2*2NH3
CUBR2*4W	CUBR2*4H2O	CUI*0.5NH3	CUI*0.5NH3
CUBR2*5NH3	CUBR2*5NH3	CUI*2NH3	CUI*2NH3
CUBR2*6NH3	CUBR2*6NH3	CUI*2PH3	CUI*2PH3
CUC2H2O4	CU(CHO2)2	CUI*3NH3	CUI*3NH3
CUC2H2O4*4W	CU(CHO2)2*4H2O	CUI*NH3	CUI*NH3
CUC2O4	CUC2O4-OXALATE	CUI*PH3	CUI*PH3
CUC4H12O4N2	CU(CH3COO)2*2NH3	CUI2O6*W	CU(IO3)2*H2O
CUC4H12O6N2	CU(CH2OHCOO)2*2NH3	CUN2H8C4O4*W	CU(NH2CH2COO)2*H2O
CUC4H14N4O4	CU(CH2NH2COO)2*2NH3	CUN2H8C4O4-A	CU(NH2CH2COO)2-ALPHA
CUC4H24O4N6	CU(CH3COO)2*6NH3	CUN2H8C4O4-B	CU(NH2CH2COO)2-BETA

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
CUN2O6	CU(NO3)2	DYCO5	DYCO5
CUN2O6*3W	CU(NO3)2*3H2O	DYI3O9	DY(IO3)3
CUN2O6*6W	CU(NO3)2*6H2O	DYOCL	DYOCL
CUN3	CUN3	ER2C6O12*6W	ER2(C2O4)3*6H2O
CUN4H12SO4	(CU(NH3)4)SO4	ERBR3O9*9W	ER(BRO3)3*9H2O
CUN4H15SO5.5	(CU(NH3)4)SO4*1.5H2O	ERH2	ERH2
CUN4H18C4O4	CU(NH3)4(CH3COO)2	ERH3	ERH3
CUN4H18C4O6	CU(NH3)4(CH2OHCOO)2	ERI3O9	ER(IO3)3
CUN6	CU(N3)2	EROCL	EROCL
CUN6H12O6	CU(NH3)4(NO3)2	EU2S3O12*8W	EU2(SO4)3*8H2O
CUN6H20C4O4	CU(NH3)4(CH2NH2COO)2	EUBR3O9*9W	EU(BRO3)3*9H2O
CUO	COPPER-OXIDE(TENORITE)	EUC2	EUC2
CUO*CUSO4	CUO*CUSO4	EUCL2	EUCL2
CUONC	CUONC	EUF3*H2O	EUF3*H2O
CURB2CL4	CUCL2*2RBCL	EUI3O9	EU(IO3)3
CURB2CL4*4W	CUCL2*2RBCL*4H2O	EUN3O9*6W	EU(NO3)3*6H2O
CUS2O10N2H12	CUSO4*(NH4)2SO4*2H2O	EUO3H3	EU(OH)3
CUS2O14N2H20	CUSO4*(NH4)2SO4*6H2O	FE	IRON
CUS2O6*5W	CUS2O6*5H2O	FE1.042SE	FE1.042SE
CUS2O8N2H8	CUSO4*(NH4)2SO4	FE1.111TE	FE1.111TE
CUSE2	CUSE2	FE2(WO4)3*8W	FE2(WO4)3*8H2O
CUSEO4	CUSEO4	FE2CDO4	CDFE2O4
CUSEO4*5W	CUSEO4*5H2O	FE2I6PB	(FEI2)2*PBI2
CUSO4	COPPER-SULFATE(CHALCOCYANITE)	FE2MO3O12	FE2(MOO4)3
CUSO4*2CH3OH	CUSO4*2CH3OH	FE2O3	IRON-OXIDE(HEMATITE)
CUSO4*2NH3	CUSO4*2NH3	FE2OC6N5	FE2CO(CN)5
CUSO4*5NH3	CUSO4*5NH3	FE2P	FE2P
CUSO4*NH3	CUSO4*NH3	FE2ZNO4	ZNFE2O4
CUWO4	CUWO4	FE3C	FE3C
CUWO4*2H2O	CUWO4*2H2O	FE3O4	IRON-OXIDE(MAGNETITE)
DY2C6O12*10W	DY2(C2O4)3*10H2O	FE3P	FE3P
DY2O3*CO2	DY2O3*CO2	FE3SE4	FE3SE4
DYAS	DYAS	FE3SI	FE3SI
DYBR3O9*9W	DY(BRO3)3*9H2O	FE5SI3	FE5SI3
DYC6H9O6	DY(CH3CO2)3	FE7C18N18	FE4(FE(CN)6)3

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
FE7S8	FE7S8-SULPHUR-RICH	FEN3O9*9W	FE(NO3)3*9H2O
FE7SE8	FE7SE8	FEO	FERROUS-OXIDE
FE7W6	FE7W6	FEO2H	FEO(OH)
FEAL	FEAL	FEP	FEP
FEAL2	FEAL2	FEP2	FEP2
FEAL3	FEAL3	FEPB2C6N6*3W	PB2FE(CN)6*3H2O
FEASS	FEASS	FEPO4*2W	FEPO4*2H2O
FEBR2*2NH3	FEBR2*2NH3	FES	IRON-SULFIDE
FEBR2*6NH3	FEBR2*6NH3	FES2-1	IRON-SULFIDE(PYRITE)
FEBR2*NH3	FEBR2*NH3	FES2-2	IRON-SULFIDE(MARCASITE)
FEBR3*6NH3	FEBR3*6NH3	FESB	FESB
FEBRCL2	FEBRCL2	FESB2	FESB2
FEC2O4*2W	FEC2O4*2H2O	FESE	FESE
FEC4O4BR2	FE(CO)4BR2	FESE2	FESE2
FEC4O4I2	FE(CO)4I2	FESIO3	FESIO3
FEC6N5H5O2	H3FECO(CN)5*H2O	FESO4*2NH3	FESO4*2NH3
FECD2C6N6*7W	CD2FE(CN)6*7H2O	FESO4*3NH3	FESO4*3NH3
FECL2	IRON-CHLORIDE(LAWRENCITE)	FESO4*4NH3	FESO4*4NH3
FECL2*10NH3	FECL2*10NH3	FESO4*4W	FESO4*4H2O
FECL2*2NH3	FECL2*2NH3	FESO4*6NH3	FESO4*6NH3
FECL2*2W	FECL2*2H2O	FESO4*7W	FESO4*7H2O
FECL2*4W	FECL2*4H2O	FESO4*NH3	FESO4*NH3
FECL2*6NH3	FECL2*6NH3	FESO4*W	FESO4*H2O
FECL2*NH3	FECL2*NH3	FETE	FETE
FECL2O8*6W	FE(CLO4)2*6H2O	FETL4C6N6*2W	TL4FE(CN)6*2H2O
FECL3	IRON-CHLORIDE(MELYSITE)	FEWO4*3H2O	FEWO4*3H2O
FECL3*6NH3	FECL3*6NH3	FEZN2C6N6*2W	ZN2FE(CN)6*2H2O
FECL3*6W	FECL3*6H2O	GA2BR6*CH3BR	(GABR3)2*CH3BR
FECO2O4	FECO2O4	GA2CL6*CH3CL	(GACL3)2*CH3CL
FECO3	FECO3	GA2CL7C2H5	(GACL3)2*C2H5CL
FECR2O4	FECR2O4	GA2S3O12	GALLIUM
FEH4C6N6	H4FE(CN)6	GABR3*14NH3	GABR3*14NH3
FEI2*2NH3	FEI2*2NH3	GABR3*5NH3	GABR3*5NH3
FEI2*6NH3	FEI2*6NH3	GABR3*6NH3	GABR3*6NH3
FEN10H28C6O6	(NH4)4FE(CN)6*6H2O	GABR3*7NH3	GABR3*7NH3

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
GABR3*9NH3	GABR3*9NH3	GDF3*W	GDF3*H2O
GABR3*CH3BR	GABR3*CH3BR	GDH2	GDH2
GABR3*NH3	GABR3*NH3	GDI3O9	GD(IO3)3
GACH3I2	GACH3I2	GDN3O9*6W	GD(NO3)3*6H2O
GACL3*14NH3	GACL3*14NH3	GDPO4*W	GDPO4*H2O
GACL3*3NH3	GACL3*3NH3	GE3N4	GERMANIUM
GACL3*5NH3	GACL3*5NH3	GEI2	GERMANIUM
GACL3*6NH3	GACL3*6NH3	H2MOO4	H2MOO4-WHITE
GACL3*7NH3	GACL3*7NH3	H2MOO4*W	H2MOO4*H2O-YELLOW
GACL3*CH3CL	GACL3*CH3CL	H2O	WATER
GACL3*NH3	GACL3*NH3	H2PTBR6*9W	H2PTBR6*9H2O
GACL3*PCL3	GACL3*PCL3	H2PTCL6*6W	H2PTCL6*6H2O
GACL3*POCL3	GACL3*POCL3	H2RECL4	H2RECL4
GACL3C3H6O	GACL3*(CH3)2CO	H2S2O7	H2S2O7
GACL3C4H10O	GACL3*(C2H5)2O	H2SEO3	SELENOUS
GACL3C8H20O	GACL3*2(C2H5)2O	H2SEO4	SELENIC
GACL4C2H3O	GACL3*CH3COCL	H2SEO4*W	SELENIC
GAF3*3LIF	GAF3*3LIF	H2SI2O5	DISILICIC
GAI3*13NH3	GAI3*13NH3	H2SIO3	METASILICIC
GAI3*20NH3	GAI3*20NH3	H3BO3	ORTHOBORIC
GAI3*5NH3	GAI3*5NH3	H3PO2	HYPOPHOSPHOROUS
GAI3*6NH3	GAI3*6NH3	H3PO3	ORTHOPHOSPHOROUS
GAI3*7NH3	GAI3*7NH3	H3PO4	ORTHOPHOSPHORIC-ACID
GAI3*9NH3	GAI3*9NH3	H3PO4*0.5W	H3PO4*0.5H2O
GAI3*NH3	GAI3*NH3	H3PO4*HCLO4	H3PO4*HCLO4
GAN	GALLIUM	H3PO4*W	ORTHOPHOSPHORIC
GAO3H3	GALLIUM	H4P2O7	PYROPHOSPHORIC
GAPO4	GALLIUM	H4P2O7*1.5W	H4P2O7*1.5H2O
GD2C6O12*10W	GD2(C2O4)3*10H2O	H4SIO4	H4SIO4
GD2S3O12*8W	GD2(SO4)3*8H2O	H6SI2O7	H6SI2O7
GDAL2	GDAL2	H6TEO6	H6TEO6
GDAS	GDAS	HAUBR4*5W	HAUBR4*5H2O
GDBR3O9*9W	GD(BRO3)3*9H2O	HAUCL4*3W	HAUCL4*3H2O
GDC2	GDC2	HAUCL4*4W	HAUCL4*4H2O
GDCL3*6W	GDCL3*6H2O	HBO2-C	METABORIC

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
HBO2-M	METABORIC	HG5BR2O4	HGBR2*4HGO
HCLO4*W	PERCHLORIC	HG5BR4N2	(NHG2BR)2*HGBR2
HCO2NH4	AMMONIUM	HG5CL4N2	(NHG2CL)2*HGCL2
HCOOK	HCOOK	HG5TL2	HG5TL2
HCOONA	HCOONA	HG9BR6N4	(NHG2BR)4*HGBR2
HCOONA*2W	HCOONA*2H2O	HGBR2*2NH3	HGBR2*2NH3
HCOONA*3W	HCOONA*3H2O	HGBR2*8NH3	HGBR2*8NH3
HFB	HFB	HGBR2C2N2H8	HGBR2*C2H4(NH2)2
HG	MERCURY	HGC2H2CL2	HGCLCHCHCL
HG2BR2N2H4	NHG2BR*NH4BR	HGC2H5BR	HGC2H5BR
HG2BR2O	HGBR2*HGO	HGC2H5CL	HGC2H5CL
HG2BR4N4H12	NHG2BR*3NH4BR	HGC2H5I	HGC2H5I
HG2C2N2O	HG(CN)2*HGO	HGC2N2	HG(CN)2
HG2C2N2S2	HG2(CNS)2	HGC2N3H4BR*W	HG(CN)2*NH4BR*H2O
HG2C2O4	HG2C2O4	HGC2O4	HGC2O4
HG2C4H6O4	HG2(CH3COO)2	HGC4H6O4	HG(CH3COO)2
HG2CL2*2NH3	HG2CL2*2NH3	HGCH3BR	HGCH3BR
HG2CL2N2H4	NHG2CL*NH4CL	HGCH3CL	HGCH3CL
HG2CL4N4H12	NHG2CL*3NH4CL	HGCH3I	HGCH3I
HG2CO3	HG2CO3	HGCL2*2:3NH3	HGCL2*2:3NH3
HG2N2O6*2W	HG2(NO3)2*2H2O	HGCL2*2NH3	HGCL2*2NH3
HG2N6	HG2(N3)2	HGCL2*8NH3	HGCL2*8NH3
HG2SEO3	HG2SEO3	HGCL2*9.5NH3	HGCL2*9.5NH3
HG3BR2O2	HGBR2*2HGO	HGCL2C2N2H8	HGCL2*C2H4(NH2)2
HG3N2O8*W	HG(NO3)2*2HGO*H2O	HGCL2CH3OH	HGCL2CH3OH
HG3SO6	HGSO4*2HGO	HGCL3NO	HGCL2*NOCL
HG4BR2O3	HGBR2*3HGO	HGI2*2NH3	HGI2*2NH3
HG4C6N6O	(HG(CN)2)3*HGO	HGI2*4:3NH3	HGI2*4:3NH3
HG4CL2N2*2W	(NHG2CL)2*2H2O	HGI2*6NH3	HGI2*6NH3
HG4CL2N2*W	(NHG2CL)2*H2O	HGI2*C2H8N2	HGI2*C2H4(NH2)2
HG4CL2N3H3	(NHG2CL)2*NH3	HGINO3	HGINO3
HG4CL2N4H6	(NHG2CL)2*2NH3	HGN2O6*0.5W	HG(NO3)2*0.5H2O
HG4N2O	(HG2N)2O	HGO2N2C2	HG(ONC)2
HG4N2O*4W	(HG2N)2O*4H2O	HIO3	IODIC
HG4N2O*W	(HG2N)2O*H2O	HO2C3	HO2C3

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
HOAS	HOAS	K	POTASSIUM
HOBR3O9*9W	HO(BRO3)3*9H2O	K(UO2)2F5	K(UO2)2F5
HOC2	HOC2	K2AL(NO3)5	K2AL(NO3)5
HOI3	HOI3	K2B3F4O3OH	K2B3F4O3OH
HOI3O9	HO(IO3)3	K2B4O7*4W	K2B4O7*4H2O
HOOCL	HOOCL	K2BA(CO3)2	K2CO3*BACO3-AGED
HPO3	METAPHOSPHORIC	K2BA(NO2)4	2KNO2*BA(NO2)2
HPTCL5*2W	HPTCL5*2H2O	K2BA(NO3)4	2KNO3*BA(NO3)2
I2	IODINE	K2BA(SO4)2-A	K2SO4*BASO4-AGED
I2O5*HIO3	I2O5*HIO3	K2BA(SO4)2-F	K2SO4*BASO4-FUSE
ICL-A	ICL-ALPHA	K2BACL4	K2BACL4-FUSE
ICL3	ICL3	K2BECL4	K2BECL4
IN3S4	IN3S4	K2BEF4	K2BEF4
IN4S5	IN4S5	K2C2O4	K2C2O4
INBR3*15NH3	INBR3*15NH3	K2C2O4*W	K2C2O4*H2O
INBR3*3NH3	INBR3*3NH3	K2CA(SO4)2*W	K2SO4*CASO4*H2O
INBR3*5NH3	INBR3*5NH3	K2CA5S6O24*W	K2SO4*5CASO4*H2O
INBR3*7NH3	INBR3*7NH3	K2CAP2O7	K2CAP2O7
INBR3C4H12S	INBR3*2(CH3)2S	K2CDFEC6N6	K2CDFE(CN)6
INCL3*15NH3	INCL3*15NH3	K2CDI4*2W	K2CDI4*2H2O
INCL3*2NH3	INCL3*2NH3	K2CDS2O9.5H3	K2CD(SO4)2*1.5H2O
INCL3*3NH3	INCL3*3NH3	K2CO3	POTASSIUM-CARBONATE
INCL3*5NH3	INCL3*5NH3	K2CO3*1.5W	K2CO3*1.5H2O
INCL3*7NH3	INCL3*7NH3	K2CO3*COCO3	K2CO3*COCO3
INCL3*NH3	INCL3*NH3	K2COC2O6*4W	K2CO3*COCO3*4H2O
INCL3C4H12S	INCL3*2(CH3)2S	K2CR2O7	K2CR2O7
INI3*13NH3	INI3*13NH3	K2CR3O10	K2CR3O10
INI3*21NH3	INI3*21NH3	K2CRCL4	K2CRCL4
INI3*2NH3	INI3*2NH3	K2CU(CO3)2	K2CU(CO3)2
INI3*5NH3	INI3*5NH3	K2CU(HCO3)4	K2CU(HCO3)4
INI3*7NH3	INI3*7NH3	K2CU(SO4)2	K2CU(SO4)2-BLUE
INI3*9NH3	INI3*9NH3	K2CU2FEC6N6	K2CU2FE(CN)6
INI3C4H12S	INI3*2(CH3)2S	K2CUCL3	K2CUCL3
IRCL	IRCL	K2CUCL4	K2CUCL4
IRCL3C12H30S	IRCL3*3(C2H5)2S	K2CUCL4*2W	K2CUCL4*2H2O

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
K2CUS2O8*.5W	K2CU(SO4)2*0.5H2O	K2MOCL6	K2MOCL6
K2CUS2O8*2W	K2CU(SO4)2*2H2O	K2MOO4	K2MOO4
K2CUS2O8*6W	K2CU(SO4)2*6H2O	K2NA2B12O20	K2O*NA2O*6B2O3
K2GEF6	K2GEF6	K2NA2B16O26	K2O*NA2O*8B2O3
K2H2P2O7	K2H2P2O7	K2NA2B8O14	K2O*NA2O*4B2O3
K2HFCL6	K2HFCL6	K2NA6B16O28	K2O*3NA2O*8B2O3
K2HG(CN)4	K2HG(CN)4	K2NA6B24O40	K2O*3NA2O*12B2O3
K2HGBR4	K2HGBR4	K2NA6B32O52	K2O*3NA2O*16B2O3
K2HGCL4	K2HGCL4	K2NBOBR5	K2NBOBR5
K2HGCL4*W	K2HGCL4*H2O	K2NBOCL5	K2NBOCL5
K2HGI4	K2HGI4	K2O	POTASSIUM-OXIDE
K2IRCL6	K2IRCL6	K2O*3B2O3	K2O*3B2O3
K2LACL5	K2LACL5	K2O*4B2O3	K2O*4B2O3
K2LI2(SO4)2	K2SO4*LI2SO4	K2O*B2O3	K2O*B2O3
K2LI2B12O20	K2O*LI2O*6B2O3	K2OSCL6	K2OSCL6
K2LI2B16O26	K2O*LI2O*8B2O3	K2PB(SO4)2	K2PB(SO4)2
K2LI2B8O14	K2O*LI2O*4B2O3	K2PBI4	K2PBI4
K2LI6B16O28	K2O*3LI2O*8B2O3	K2PBI4*2W	K2PBI4*2H2O
K2LI6B24O40	K2O*3LI2O*12B2O3	K2PDBR4	K2PDBR4
K2LI6B32O52	K2O*3LI2O*16B2O3	K2PDCL4	K2PDCL4
K2MG(SEO4)2	K2MG(SEO4)2	K2PDCL6	K2PDCL6
K2MG2(SO4)3	K2SO4*2MGSO4	K2PRCL5	K2PRCL5
K2MGCL4*2KCL	K2MGCL4*2KCL	K2PT(NO2)4	K2PT(NO2)4
K2MGCL4-A	K2MGCL4-AGED,2	K2PTBR4	K2PTBR4
K2MGCL4-F	K2MGCL4-FUSED	K2PTBR6	K2PTBR6
K2MGS2O8	K2MG(SO4)2-AGED	K2PTCL4	K2PTCL4
K2MGS2O8*2W	K2MG(SO4)2*2H2O	K2PTCL6	K2PTCL6
K2MGS2O8*4W	K2MG(SO4)2*4H2O	K2PTI6	K2PTI6
K2MGS2O8*6W	K2MG(SO4)2*6H2O	K2PTN2O4CL2	K2PT(NO2)2CL2
K2MNS2O8	K2MN(SO4)2	K2PTN3O6CL	K2PT(NO2)3CL
K2MNS2O8*2W	K2MN(SO4)2*2H2O	K2PTNO2CL3	K2PT(NO2)CL3
K2MNS2O8*4W	K2MN(SO4)2*4H2O	K2REBR6	K2REBR6
K2MO2O7	K2MO2O7	K2RECL6	K2RECL6
K2MO3O10	K2MO3O10	K2S*2W	K2S*2H2O
K2MO4O13	K2MO4O13	K2S*5W	K2S*5H2O

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
K2S2	K2S2	K2TE4O9*4W	K2TE4O9*4H2O
K2S2O3	K2S2O3	K2TEBR6	K2TEBR6
K2S2O3*W	K2S2O3*H2O	K2TEO3	K2TEO3
K2S2O5	K2S2O5	K2TEO3*3W	K2TEO3*3H2O
K2S2O5*0.5W	K2S2O5*0.5H2O	K2THCL6	K2THCL6
K2S2O6	K2S2O6	K2TICL6	K2TICL6
K2S2O7	K2S2O7	K2TIO3	K2TIO3
K2S2O8	K2S2O8	K2UCL6	K2UCL6
K2S3	K2S3	K2UO4	K2UO4
K2S3O6	K2S3O6	K2WCL7	K2WCL7
K2S4	K2S4	K2WO4	K2WO4
K2S4*0.5W	K2S4*0.5H2O	K2ZN(CN)4	K2ZN(CN)4
K2S4*2W	K2S4*2H2O	K2ZN(SO4)2	K2ZN(SO4)2
K2S4O6	K2S4O6	K2ZNS2O8*2W	K2ZN(SO4)2*2H2O
K2S5	K2S5	K2ZNS2O8*6W	K2ZN(SO4)2*6H2O
K2S5O6*1.5W	K2S5O6*1.5H2O	K2ZRBR6	K2ZRBR6
K2S6	K2S6	K2ZRCL6	K2ZRCL6
K2SE	K2SE	K3AG2I5*W	K3AG2I5*H2O
K2SE*14W	K2SE*14H2O	K3AGBR4*0.5W	K3AGBR4*0.5H2O
K2SE*19W	K2SE*19H2O	K3AGI4	K3AGI4
K2SE*9W	K2SE*9H2O	K3AGI4*0.5W	K3AGI4*0.5H2O
K2SEO3	K2SEO3	K3AL(NO3)6	K3AL(NO3)6
K2SEO4	K2SEO4	K3AL2CL9	K3AL2CL9
K2SIF6	K2SIF6	K3ALF6*3.5W	K3ALF6*3.5H2O
K2SMCL5	K2SMCL5	K3AS	K3AS
K2SNBR6	K2SNBR6	K3BI	K3BI
K2SNCL6	K2SNCL6	K3CE2CL9	K3CE2CL9
K2SNCL6*W	K2SNCL6*H2O	K3CECL6	K3CECL6
K2SNOCL4	K2SNOCL4	K3CO(C2O4)3	K3(CO(C2O4)3)
K2SO4	POTASSIUM-SULFATE	K3CO(CN)6	K3CO(CN)6
K2SR(SO4)2	K2SO4*SRSO4-FUSED	K3COC6O12*3W	K3(CO(C2O4)3)*3H2O
K2SRCL4	K2SRCL4-FUSED	K3CR2CL9	K3CR2CL9
K2TACL6	K2TACL6	K3CRC6O12	K3CR(C2O4)3
K2TE2O5	K2TE2O5	K3CRC6O12*3W	K3CR(C2O4)3*3H2O
K2TE4O9	K2TE4O9	K3CRCL6	K3CRCL6

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
K3CRO4F	K3CRO4F	KAL(SO4)2	KAL(SO4)2
K3FE(CN)6	K3FE(CN)6	KAL(SO4)2*3W	KAL(SO4)2*3H2O
K3FEC6N5O	K3FECO(CN)5	KAL2BR7	KAL2BR7
K3IRCL6	K3IRCL6	KAL2H5P2O11	KAL2(PO4)2OH*2H2O
K3ND2CL9	K3ND2CL9	KALBR4	KALBR4
K3NDCL6	K3NDCL6	KALCL4*6NH3	KALCL4*6NH3
K3OSCL6	K3OSCL6	KALH4	KALH4
K3PR2CL9	K3PR2CL9	KALS2O8*12W	KAL(SO4)2*12H2O
K3PRCL6	K3PRCL6	KALSE2O8*12W	KAL(SEO4)2*12H2O
K3SB	K3SB	KAS	KAS
K3SMCL6	K3SMCL6	KAS2	KAS2
K3TICL6	K3TICL6	KB5O8*4W	KB5O8*4H2O
K3UO2F5	K3UO2F5	KBA2(NO2)5	KNO2*2BA(NO2)2
K3V2CL9	K3V2CL9	KBCL4	KBCL4
K3VCL6	K3VCL6	KBF3OH	KBF3OH
K4BA(SO4)3	2K2SO4*BASO4-FUSED	KBF4	KBF4
K4CA(NO3)6	4KNO3*CA(NO3)2	KBH4	KBH4
K4CDCL6	K4CDCL6	KBR	POTASSIUM-BROMIDE
K4FE(CN)6	K4FE(CN)6	KBR*ALCL3	KBR*ALCL3
K4FEC6N6*3W	K4FE(CN)6*3H2O	KBR*ZNSO4	KBR*ZNSO4
K4PB3I10	4KI*3PBI2	KBRO3	KBRO3
K4PB3I10*6W	4KI*3PBI2*6H2O	KBRO4	KBRO4
K4SR(SO4)3	2K2SO4*SRSO4-FUSED	KC10	KC10
K5AS4	K5AS4	KC24	KC24
K5SB4	K5SB4	KC36	KC36
K6EU4S9O36	3K2SO4*2EU2(SO4)3	KC4	KC4
K6EU4S9O36W8	3K2SO4*2EU2(SO4)3*8H2O	KC48	KC48
K6NA2B16O28	3K2O*NA2O*8B2O3	KC60	KC60
K6NA2B24O40	3K2O*NA2O*12B2O3	KC8	KC8
K6NA2B32O52	3K2O*NA2O*16B2O3	KCACL3	KCACL3
KAG(CN)2	KAG(CN)2	KCAFEC6N6*5W	KCAFE(CN)6*5H2O
KAGBR2	KAGBR2	KCD3BR7*4W	KBR*3CDBR2*4H2O
KAGCL2	KAGCL2	KCD3CL7*4W	KCL*3CDCL2*4H2O
KAGI2	KAGI2	KCDBR3*W	KCDBR3*H2O
KAL(SEO4)2	KAL(SEO4)2	KCDCL3	KCDCL3

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
KCDCL3*W	KCDCL3*H2O	KGDFEC6N6	KGDFE(CN)6
KCDI3*W	KCDI3*H2O	KH2ASO4	KH2ASO4
KCE3CL10	KCE3CL10	KH3C2O3	CH2OHCOOK
KCECL4	KCECL4	KH3C2O3*0.5W	CH2OHCOOK*0.5H2O
KCEFEC6N6*2W	KCEFE(CN)6*2H2O	KH3C4O8	KHC2HO4*H2C2O4
KCL	POTASSIUM-CHLORIDE	KH3C4O8*2W	KHC2O4*H2C2O4*2H2O
KCL*2ALBR3	KCL*2ALBR3	KHCO3	POTASSIUM-BICARBONATE
KCL*2PBCL2	KCL*2PBCL2	KHF2	KHF2
KCL*ALBR3	KCL*ALBR3	KHG(CN)2BR	KBR*HG(CN)2
KCL*MGSO4*3W	KCL*MGSO4*3H2O	KHG(CN)2CL	KCL*HG(CN)2
KCL*ZNSO4	KCL*ZNSO4	KHG(CN)2CL*W	KCL*HG(CN)2*H2O
KCLBRI	KCLBRI	KHG(CN)2I	KI*HG(CN)2
KCLO3	KCLO3	KHGBR3	KHGBR3
KCNO	KCNO	KHGBR3*W	KHGBR3*H2O
KCNS	KCNS	KHGCL3	KHGCL3
KCNS*0.5SO2	KCNS*0.5SO2	KHGCL3*W	KHGCL3*H2O
KCNS*2SO2	KCNS*2SO2	KHGI3	KHGI3
KCOF3	KCOF3	KHGI3*W	KHGI3*H2O
KCON4C2O8H6	K(CO(NH3)2(NO2)2C2O4)	KHS	KHS
KCOO8N6H6	K(CO(NH3)2(NO2)4)	KHS*0.25W	KHS*0.25H2O
KCRCL3	KCRCL3	KHSE	KHSE
KCRO3CL	KOCRO2CL	KHSO4	KHSO4
KCRS2O8*1.5W	KCR(SO4)2*1.5H2O	KI*4SO2	KI*4SO2
KCRS2O8*12W	KCR(SO4)2*12H2O	KI*ZNSO4	KI*ZNSO4
KCRS2O8*6W	KCR(SO4)2*6H2O	KI3	KI3
KCUCL3	KCUCL3	KIBR2	KIBR2
KCUF3	KCUF3	KIBR2*W	KIBR2*H2O
KERCL4	KERCL4	KIO2F2	KIO2F2
KEUS2O8	KEU(SO4)2	KIO3	KIO3
KEUS2O8*W	KEU(SO4)2*H2O	KIO4	KIO4
KF*2HF	KF*2HF	KLA3CL10	KLA3CL10
KF*2W	KF*2H2O	KLACL4	KLACL4
KF*3HF	KF*3HF	KLAFE(CN)6	KLAFE(CN)6
KF*BRF3	KF*BRF3	KLICLI	KLICLI
KFECL4	KFECL4	KMGCL3	KMGCL3

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
KMGCL3*2W	KMGCL3*2H2O	KREO4	KREO4
KMGCL3*6W	KMGCL3*6H2O	KSB	KSB
KMGPO4*6W	KMGPO4*6H2O	KSB2	KSB2
KMNCL3	KMNCL3	KSO2F	KSO2F
KMNF3	KMNF3	KSO3F	KSO3F
KMNO4	KMNO4	KSR2CL5	KSR2CL5
KMOF6	KMOF6	KTACL6	KTACL6
KNABR2	KNABR2	KTBS2O8	KTB(SO4)2
KNACL2	KNACL2	KTBS2O8*W	KTB(SO4)2*H2O
KNACLI	KNACLI	KTCO4	KTCO4
KNAI2	KNAI2	KTHCL5*9W	KTHCL5*9H2O
KNAUCL6	KNAUCL6	KTICL3	KTICL3
KNB2OCL9	KNB2OCL9	KUCL5	KUCL5
KNBCL6	KNBCL6	KUCL6	KUCL6
KNBO3	KNBO3	KUF6	KUF6
KNBOCL4	KNBOCL4	KVCL3	KVCL3
KNDCL4	KNDCL4	KVO3	KVO3
KNH2	KNH2	KVO4	KVO4
KNH3	KNH3	KWCL6	KWCL6
KNH4CRO4	KNH4CRO4	KWF6	KWF6
KNICL3	KNICL3	KYCL4	KYCL4
KNIF3	KNIF3	KZNF3	KZNF3
KNO2	KNO2	LA2C3N6	LA2(CN2)3
KNO2*KOH	KNO2*KOH	LA2C3O9	LA2(CO3)3
KNO3	POTASSIUM-NITRATE	LA2C6O12*10W	LA2(C2O4)3*10H2O
KNO3*KOH	KNO3*KOH	LA2S3O12	LA2(SO4)3
KOH	POTASSIUM-HYDROXIDE	LA2S3O12*9W	LA2(SO4)3*9H2O
KOH*2W	KOH*2H2O	LA2SE3O9	LA2(SEO3)3
KOH*W	KOH*H2O	LAAL2	LAAL2
KPBCL3*1:3W	KPBCL3*1:3H2O	LAB6	LAB6
KPF6	KPF6	LABI	LABI
KPO3	KPO3	LABR3O9*9W	LA(BRO3)3*9H2O
KPRCL4	KPRCL4	LABSALT	NA4CA(SO4)3*2H2O
KPTNH3CL3	KPT(NH3)CL3	LAC2	LAC2
KPTNH3CL5	KPTNH3CL5	LACL3*7W	LACL3*7H2O

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
LAF3*W	LAF3*H2O	LI2SO3	LI2SO3
LAH3C3O6	LA(HCO2)3	LI2SO4*W	LI2SO4*H2O
LAI3O9	LA(IO3)3	LI2THCL6	LI2THCL6
LAINTE3	LAINTE3	LI2UCL6	LI2UCL6
LAN3O9	LA(NO3)3	LI2UO4	LI2UO4
LAN3O9*3W	LA(NO3)3*3H2O	LI2WO4	LI2WO4
LAN3O9*4W	LA(NO3)3*4H2O	LI3ALH6	LI3ALH6
LAN3O9*6W	LA(NO3)3*6H2O	LI3BI	LI3BI
LASB	LASB	LI3PO4	LI3PO4
LI	LITHIUM	LI3SB	LI3SB
LI.05ZN.9F-A	LI0.05ZN0.9FE2.05O4-ANNEALED	LI3SB2	LI3SB2
LI.05ZN.9F-Q	LI0.05ZN0.9FE2.05O4-QUENCHED	LI4P2O7	LI4P2O7
LI0.5FE2.5O4	LI0.5FE2.5O4	LI4PUF8	LI4PUF8
LI22SN5	LI22SN5	LI4ZRO4	LI4ZRO4
LI2AL2SI8O20	LI2AL2SI8O20	LI5I2O12	LI5(IO6)2
LI2B2C4H18O	(LIBH4)2*(C2H5)2O	LI7PB2	LI7PB2
LI2BECL4	LI2BECL4	LI7SN2	LI7SN2
LI2C2	LI2C2	LI8ZRO6	LI8ZRO6
LI2CRO4	LI2CRO4	LIAL	LIAL
LI2CRO4*2W	LI2CRO4*2H2O	LIAL5O8	LIAL5O8
LI2HFO3	LI2HFO3	LIALBR4	LIALBR4
LI2K6B16O28	LI2O*3K2O*8B2O3	LIALCL4	LIALCL4
LI2K6B24O40	LI2O*3K2O*12B2O3	LIALH4	LIALH4
LI2K6B32O52	LI2O*3K2O*16B2O3	LIALO2	LITHIUM-ALUMINATE
LI2MOO4	LI2MOO4	LIBC4H16O2	LIBH4*2((CH3)2O)
LI2NH	LI2NH	LIBC6H22N2	LIBH4*2N(CH3)3
LI2O*2BEO	LI2O*2BEO	LIBF4	LIBF4
LI2PBI4*4W	LI2PBI4*4H2O	LIBH4	LIBH4
LI2PTCL6	LI2PTCL6	LIBH4*2NH3	LIBH4*2NH3
LI2S2	LI2S2	LIBH4*3NH3	LIBH4*3NH3
LI2SE*9W	LI2SE*9H2O	LIBH4*4NH3	LIBH4*4NH3
LI2SEO3*W	LI2SEO3*H2O	LIBH4*C2H6O	LIBH4*(CH3)2O
LI2SEO4	LI2SEO4	LIBH4*C4H8O	LIBH4*(CH2)4O
LI2SEO4*W	LI2SEO4*H2O	LIBH4*C6H14O	LIBH4*(CH(CH3)2)2O
LI2SIF6	LI2SIF6	LIBH4*NC3H9	LIBH4*N(CH3)3

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
LIBH4*NH3	LIBH4*NH3	LII*W	LII*H2O
LIBR*2NH3	LIBR*2NH3	LIIO3	LIIO3
LIBR*2W	LIBR*2H2O	LIN3	LIN3
LIBR*3NH3	LIBR*3NH3	LINBO3	LINBO3
LIBR*5NH3	LIBR*5NH3	LINH2	LINH2
LIBR*NH3	LIBR*NH3	LINO2	LINO2
LIBR*W	LIBR*H2O	LINO2*0.5W	LINO2*0.5H2O
LIBRO3	LIBRO3	LINO2*W	LINO2*H2O
LICL*2W	LICL*2H2O	LINO3	LINO3
LICL*3NH3	LICL*3NH3	LINO3*3W	LINO3*3H2O
LICL*3W	LICL*3H2O	LIOC2H5	LIOC2H5
LICL*4NH3	LICL*4NH3	LIOH	LITHIUM-HYDROXIDE
LICL*NH3	LICL*NH3	LIOH*W	LIOH*H2O
LICL*W	LICL*H2O	LIPB	LIPB
LICLO3	LICLO3	LIPO3	LIPO3
LICLO3*0.25W	LICLO3*0.25H2O	LIREO4	LIREO4
LICLO4*2N2H4	LICLO4*2N2H4	LIREO4*2W	LIREO4*2H2O
LICLO4*3W	LICLO4*3H2O	LIREO4*W	LIREO4*H2O
LICLO4*W	LICLO4*H2O	LISN	LISN
LICSCLI	LICSCLI	LITHCL5*8W	LITHCL5*8H2O
LIH	LIH	LITL	LITL
LIH2PO4	LIH2PO4	LIUO2ASO4	LIUO2ASO4
LIHF2	LIHF2	LIUO5	LI4UO5
LIHG	LIHG	LIWF6	LIWF6
LIHG2	LIHG2	LTAO2CL2	KTAO2CL2
LIHG3	LIHG3	LUAS	LUAS
LIHS	LIHS	LUBR3O9*9W	LU(BRO3)3*9H2O
LII*2NH3	LII*2NH3	LUCL3	LUCL3
LII*2SO2	LII*2SO2	LUCL3*6W	LUCL3*6H3O
LII*2W	LII*2H2O	LUI3	LUI3
LII*3NH3	LII*3NH3	LUI3O9	LU(IO3)3
LII*3W	LII*3H2O	LUN3O9*5W	LU(NO3)3*5H2O
LII*4NH3	LII*4NH3	LUOCL	LUOCL
LII*NH3	LII*NH3	MG	MAGNESIUM
LII*SO2	LII*SO2	MG(OH)2	MAGNESIUM-HYDROXIDE

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
MG17Y3	MG17Y3	MGC2O4	MGC2O4
MG2AL4SI5O18	MG2AL4SI5O18-CORDIERITE	MGC2O4*2W	MGC2O4*2H2O
MG2CU-G	MG2CU-GAMMA	MGC4H6O6	MG(CH2OHCO2)2
MG2GE	MG2GE	MGC4H6O6*2W	MG(CH2OHCO2)2*2H2O
MG2NI	MG2NI	MGCD	MGCD
MG2OCL2*16W	MGO*MGCL2*16H2O	MGCD3	MGCD3
MG2OCL2*6W	MGO*MGCL2*6H2O	MGCE	MGCE
MG2P2O7-A	MG2P2O7-ALPHA	MGCL2	MAGNESIUM-CHLORIDE
MG2PB	MG2PB	MGCL2*2NH3	MGCL2*2NH3
MG2SN	MG2SN	MGCL2*2W	MGCL2*2H2O
MG2TIO4	MG2TIO4	MGCL2*4W	MGCL2*4H2O
MG2ZN11	MG2ZN11	MGCL2*6C2OH6	MGCL2*6C2H5OH
MG3AS2	MG3AS2	MGCL2*6COH4	MGCL2*6CH3OH
MG3AS2O8	MG3(ASO4)2	MGCL2*6W	MGCL2*6H2O
MG3BI2-B	MG3BI2-BETA	MGCL2*NH3	MGCL2*NH3
MG3CD	MG3CD	MGCL2*W	MGCL2*H2O
MG3CE	MG3CE	MGCL2O8	MG(CLO4)2
MG3LA	MG3LA	MGCL2O8*2W	MG(CLO4)2*2H2O
MG3P2O8	MG3(PO4)2	MGCL2O8*4W	MG(CLO4)2*4H2O
MG3PR	MG3PR	MGCL2O8*6NH3	MG(CLO4)2*6NH3
MG3SB2-A	MG3SB2-ALPHA	MGCL2O8*6W	MG(CLO4)2*6H2O
MG3SI2O9H4	MG3SI2O5(OH)4	MGCN2	MGCN2
MG4C3O14H8	(MGCO3)3*MG(OH)2*3H2O	MGCO3	MAGNESIUM-CARBONATE
MG4O10H14CL2	(MG(OH)2)3*MGCL2*4H2O	MGCO3*3W	MGCO3*3H2O
MG4O13H20CL2	(MG(OH)2)3*MGCL2*7H2O	MGCO3*5W	MGCO3*5H2O
MG4O14H22CL2	(MG(OH)2)3*MGCL2*8H2O	MGCR2O4	MGCR2O4
MG4O18H22S	(MG(OH)2)3*MGSO4*8H2O	MGCRO4	MGCRO4
MG4O6H6CL2	(MG(OH)2)3*MGCL2	MGCU2-B	MGCU2-BETA
MG5Y2	MG5Y2	MGFE2O4	MGFE2O4
MG6O18H26CL2	(MG(OH)2)5*MGCL2*8H2O	MGH2C2O4	MG(HCO2)2
MGAS4	MGAS4	MGI2*2NH3	MGI2*2NH3
MGB12	MGB12	MGLA	MGLA
MGBR2*2NH3	MGBR2*2NH3	MGN2O6*2W	MG(NO3)2*2H2O
MGBR2*6W	MGBR2*6H2O	MGN2O6*6COH4	MG(NO3)2*6CH3OH
MGBR2*NH3	MGBR2*NH3	MGN2O6*6W	MG(NO3)2*6H2O

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
MGNH4ASO4*6W	MGNH4ASO4*6H2O	MN2O3	MANGANESE-OXIDE(BRAUNITE)
MGO	MAGNESIUM-OXIDE	MN3O4	MANGANESE-OXIDE(HAUSMANNITE)
MGO*AL2O3-S	MGO*AL2O3-SPINEL	MN3P2O8	MN3(PO4)2
MGO*MGCL2	MGO*MGCL2	MN8N2	MN8N2
MGOHCL	MGOHCL	MNBI	MNBI
MGPR	MGPR	MNBR2	MNBR2
MGS2O3*3W	MGS2O3*3H2O	MNBR2*2NH3	MNBR2*2NH3
MGS2O3*6W	MGS2O3*6H2O	MNBR2*4W	MNBR2*4H2O
MGSEO3	MGSEO3	MNBR2*6NH3	MNBR2*6NH3
MGSEO3*6W	MGSEO3*6H2O	MNBR2*C2H5OH	MNBR2*C2H5OH
MGSEO4	MGSEO4	MNBR2*NH3	MNBR2*NH3
MGSEO4*4W	MGSEO4*4H2O	MNBR2*W	MNBR2*H2O
MGSEO4*6W	MGSEO4*6H2O	MNC2H2O4	MN(CHO2)2
MGSEO4*W	MGSEO4*H2O	MNC2H2O4*2W	MN(CHO2)2*2H2O
MGSO3	MGSO3	MNC2O4	MNC2O4
MGSO3*3W	MGSO3*3H2O	MNC2O4*2W	MNC2O4*2H2O
MGSO3*6W	MGSO3*6H2O	MNC2O4*3W	MNC2O4*3H2O
MGSO4*2W	MGSO4*2H2O	MNC4H6O4	MN(CH3CO2)2
MGSO4*4W	MGSO4*4H2O	MNC4H6O4*4W	MN(CH3CO2)2*4H2O
MGSO4*6W	MGSO4*6H2O	MNCL2	MANGANESE-CHLORIDE
MGSO4*7W	MGSO4*7H2O	MNCL2*2CH3OH	MNCL2*2CH3OH
MGSO4*W	MGSO4*H2O	MNCL2*2W	MNCL2*2H2O
MGTIO3	MGTIO3	MNCL2*3CH3OH	MNCL2*3CH3OH
MGTL	MGTL	MNCL2*4W	MNCL2*4H2O
MGU3O10	MGU3O10	MNCL2*CH3OH	MNCL2*CH3OH
MGUO4	MGUO4	MNCL2*W	MNCL2*H2O
MGV2O6	MGV2O6	MNCL4N2H12O2	MNCL2*2NH4CL*2H2O
MGWO4	MGWO4	MNCO3	MANGANESE-CARBONATE
MGY	MGY	MNCO3-N	MNCO3-NATURAL
MGZN	MGZN	MNCO3-P	MNCO3-PRECIPITATED
MGZN2	MGZN2	MNFE2O4	MNFE2O4
MN	MANGANESE	MNHASO4	MNHASO4
MN2C10O10	MN2(CO)10	MNHPO4	MNHPO4
MN2FEC6N6	MN2FE(CN)6	MNI2*2W	MNI2*2H2O
MN2O11PB4	PB(MNO4)2*3PBO	MNI2*4W	MNI2*4H2O

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
MNI2O6	MN(IO3)2	N2H8CRO4	(NH4)2CRO4
MNN2O6	MN(NO3)2	N2H8PTCL4	(NH4)2PTCL4
MNN6	MN(N3)2-MANGANESE	N3H12UO2F5	(NH4)3UO2F5
MNO	MANGENESE-OXIDE(MANGANOSITE)	NA	SODIUM
MNO2	MANGANESE-OXIDE(PYROLUSITE)	NA(UO2)2F5	NA(UO2)2F5
MNO2H2	MN(OH)2-PRECIPITATED	NA2AG2O3	NA2AG2O3
MNS-P	MNS-PRECIPITATED	NA2B4O7*10W	NA2B4O7*10H2O
MNS2O14H20N2	(NH4)2MN(SO4)2*6H2O	NA2B4O7*4W	NA2B4O7*4H2O
MNS2O6*2W	MNS2O6*2H2O	NA2B4O7*5W	NA2B4O7*5H2O
MNS2O6*6W	MNS2O6*6H2O	NA2BA(CO3)2	NA2CO3*BACO3
MNSO4*4W	MNSO4*4H2O	NA2BA(SO4)2	NA2SO4*BASO4
MNSO4*5W	MNSO4*5H2O	NA2BECL4	NA2BECL4
MNSO4*7W	MNSO4*7H2O	NA2C2	SODIUM
MNSO4*W-A	MNSO4*H2O-ALPHA	NA2C2H2O3	DISODIUM
MNSO4*W-B	MNSO4*H2O-BETA	NA2C2H2O3*2W	NAOCH2CO2NA*2H2O
MNV2O6	MN(VO3)2	NA2C2O4	NA2C2O4
MO	MOLYBDENUM	NA2CA(SO4)2	NA2CA(SO4)2
MO2B	MO2B	NA2CACL4	NA2CACL4
MO3GE	MO3GE	NA2CO3	SODIUM-CARBONATE
MOB	MOB	NA2CO3.10H2O	SODIUM-CARBONATE-
MOBR2	MOBR2	NA2CO3.3NAHC	WEGSCHEIDER
MOBR4	MOBR4	NA2CO3.7H2O	SODIUM-CARBONATE-
MOCL2	MOCL2	NA2CO3.H2O	SODIUM-CARBONATE-
MOCL3	MOCL3	NA2CO3.NAHCO	TRONA
MOCL4	MOCL4	NA2COO3	NA2COO3
MOCL5	MOCL5	NA2CR2O7	NA2CR2O7
MOO2BR2	MOO2BR2	NA2CR2O7*2W	NA2CR2O7*2H2O
MOO2CL2*W	MOO2CL2*H2O	NA2CRO4*10W	NA2CRO4*10H2O
MOOCL4	MOOCL4	NA2CRO4*4NAO	NA2CRO4*4NAOH
N2H6*B2H6	(NH3)2*B2H6	NA2CRO4*4W	NA2CRO4*4H2O
N2H6U3O9*4W	(NH3)2(UO3)3*4H2O	NA2CUC2O6	NA2CU(CO3)2
N2H7PTCL3	NH4(PT(NH3)CL3)	NA2CUC2O6*3W	NA2CU(CO3)2*3H2O
N2H8CD2S3O12	(NH4)2CD2(SO4)3	NA2CUO3	NA2CUO3
N2H8CR2O7	(NH4)2CR2O7	NA2H2P2O5	NA2H2P2O5
N2H8CR3O10	(NH4)2CR3O10	NA2H2P2O7	NA2H2P2O7

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
NA2H2P2O7*6W	NA2H2P2O7*6H2O	NA2PBI4*6W	(NAI)2PBI2*6H2O
NA2HFCL6	NA2HFCL6	NA2PBO3	NA2PBO3
NA2HPO4	NA2HPO4	NA2PTCL6	NA2PTCL6
NA2HPO4*12W	NA2HPO4*12H2O	NA2PTCL6*2W	NA2PTCL6*2H2O
NA2HPO4*2W	NA2HPO4*2H2O	NA2PTCL6*6W	NA2PTCL6*6H2O
NA2HPO4*7W	NA2HPO4*7H2O	NA2S*4.5W	NA2S*4.5H2O
NA2HSEO3	NAHSEO3	NA2S*5W	NA2S*5H2O
NA2HSEO4	NAHSEO4	NA2S*9W	NA2S*9H2O
NA2IRCL6	NA2IRCL6	NA2S2O3	NA2S2O3
NA2K2(CO3)2	NA2CO3*K2CO3-AGED	NA2S2O3*5W	NA2S2O3*5H2O
NA2K2(SO4)2	NA2SO4*K2SO4-AGED	NA2S2O4	NA2S2O4
NA2K4(CO3)3	NA2CO3*2K2CO3-AGED	NA2S2O5	NA2S2O5
NA2K4(SO4)3	NA2SO4*2K2SO4-AGED	NA2S2O6	NA2S2O6
NA2K6(CO3)4	NA2CO3*3K2CO3-AGED	NA2S2O6*2W	NA2S2O6*2H20
NA2K6(SO4)4	NA2SO4*3K2SO4-GLASERITE	NA2S2O7	NA2S2O7
NA2K8(CO3)5	NA2CO3*4K2CO3-AGED	NA2S3O6*3W	NA2S3O6*3H2O
NA2MG(SO4)2	NA2MG(SO4)2	NA2S4O6*2W	NA2S4O6*2H2O
NA2MGS2O8*2W	NA2MG(SO4)2*2H2O	NA2S5	NA2S5
NA2MN(SO4)2	NA2MN(SO4)2	NA2SE	NA2SE
NA2MNO4	NA2MNO4	NA2SE*16W	NA2SE*16H2O
NA2MNS2O8*2W	NA2MN(SO4)2*2H2O	NA2SE*4.5W	NA2SE*4.5H2O
NA2MO2O7	NA2MO2O7	NA2SE*9W	NA2SE*9H2O
NA2MOCL6	NA2MOCL6	NA2SE2	NA2SE2
NA2MOF8	NA2MOF8	NA2SEO3	NA2SEO3
NA2MOO4*2W	NA2MOO4*2H2O	NA2SEO3*5W	NA2SEO3*5H2O
NA2MOO6*W	NA2MOO6*H2O	NA2SEO4	NA2SEO4
NA2MOO8*2W	NA2MOO8*2H2O	NA2SEO4*10W	NA2SEO4*10H2O
NA2MOO8*4W	NA2MOO8*4H2O	NA2SIF6	NA2SIF6
NA2N2O3	NA2N2O3	NA2SIO3*5W	NA2SIO3*5H2O
NA2NBF7	NA2NBF7	NA2SIO3*9W	NA2SIO3*9H2O
NA2O	SODIUM-OXIDE	NA2SNO3	NA2SNO3
NA2O*3B2O3	NA2O*3B2O3	NA2SO3*7W	NA2SO3*7H2O
NA2O*4B2O3	NA2O*4B2O3	NA2SO4	SODIUM-SULFATE
NA2OSCL6	NA2OSCL6	NA2SO4*SRSO4	NA2SO4*SRSO4
NA2PBI4*4W	(NAI)2PBI2*4H2O	NA2SO4.10H2O	GLAUBER

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
NA2SO4.NAOH	DOUBLE	NA3HP2O7*W	NA3HP2O7*H2O
NA2TAF7	NA2TAF7	NA3IRCL6	NA3IRCL6
NA2TE2	NA2TE2	NA3P	NA3P
NA2TEO3	NA2TEO3	NA3PW3O13*4W	NA3PW3O13*4H2O
NA2TEO3*5W	NA2TEO3*5H2O	NA3RHCL6	NA3RHCL6
NA2THCL6	NA2THCL6	NA3RHCL6*12W	NA3RHCL6*12H2O
NA2U2O7	NA2U2O7	NA3SB	NA3SB
NA2U2O7*1.5W	NA2U2O7*1.5H2O	NA3SCF6	NA3SCF6
NA2UCL6	NA2UCL6	NA3TICL6	NA3TICL6
NA2UO4-A	NA2UO4-ALHPA	NA3UO2F5	NA3UO2F5
NA2UO4-B	NA2UO4-BETA	NA3UO4	NA3UO4
NA2V3F11	NA2V3F11	NA3VCL6	NA3VCL6
NA2W2O7	NA2W2O7	NA3VF6	NA3VF6
NA2W4O13	NA2W4O13	NA3VO4*.5W-O	NA3VO4*0.5H2O-ORTHO
NA2WF8	NA2WF8	NA3VO4*.5W-P	NA3VO4*0.5H2O-PSEUDOSALT
NA2WO4*2W	NA2WO4*2H2O	NA3VO4*10W-O	NA3VO4*10H2O-ORTHO
NA2WO6*W	NA2WO6*H2O	NA3VO4*10W-P	NA3VO4*10H2O-PSEUDOSALT
NA2WO8*2W	NA2WO8*2H2O	NA3VO4*12W	NA3VO4*12H2O-ORTHO
NA2ZN(SO4)2	NA2ZN(SO4)2	NA3VO4*2W	NA3VO4*2H2O-ORTHO
NA2ZNO2	NA2ZNO2	NA3VO4*3.5W	NA3VO4*3.5H2O-PSEUDOSALT
NA2ZNS2O8*2W	NA2ZN(SO4)2*2H2O	NA3VO4*7W	NA3VO4*7H2O-ORTHO
NA2ZNS2O8*4W	NA2ZN(SO4)2*4H2O	NA3VO4*8W	NA3VO4*8H2O-PSEUDOSALT
NA2ZRCL6	NA2ZRCL6	NA4BA(SO4)3	2NA2SO4*BASO4
NA3ALF6	SODIUM-HEXAFLUOROALUMINATE	NA4CA(SO4)3	NA4CA(SO4)3
NA3ALF6*3.5W	NA3ALF6*3.5H2O	NA4CEO4	NA4CEO4
NA3ASO4*12W	NA3ASO4*12H2O	NA4K2(CO3)3	2NA2CO3*K2CO3-AGED
NA3BI	NA3BI	NA4K2(SO4)3	2NA2SO4*K2SO4-AGED
NA3BIO4	NA3BIO4	NA4O4UO4	NA4O4UO4
NA3CON6O12	NA3(CO(NO2)6)	NA4O4UO4*9W	NA4O4UO4*9H2O
NA3CRCL6	NA3CRCL6	NA4P2O7	NA4P2O7
NA3FECO(CN)5	NA3FECO(CN)5	NA4P2O7*10W	NA4P2O7*10H2O
NA3HG	NA3HG	NA4P4O12	NA4P4O12
NA3HG2	NA3HG2	NA4SN	NA4SN
NA3HP2O7	NA3HP2O7	NA4SO4CLOH	TRIPLE
NA3HP2O7*6W	NA3HP2O7*6H2O	NA4SR(SO4)3	2NA2SO4*SRSO4

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
NA4UO2(CO3)3	NA4UO2(CO3)3	NABO2*4W	NABO2*4H2O
NA4UO5	NA4UO5	NABO3*4W	NABO3*4H2O
NA4V2O7*10W	NA4V2O7*10H2O	NABR*2W	NABR*2H2O
NA4V2O7*12W	NA4V2O7*12H2O	NABR*5.25NH3	NABR*5.25NH3
NA4V2O7*18W	NA4V2O7*18H2O	NABR*5.75NH3	NABR*5.75NH3
NA4V2O7*2W	NA4V2O7*2H2O	NABRF4	NABRF4
NA5H3(CO3)4	3NAHCO3*NA2CO3	NABRO3	NABRO3
NA5HG2	NA5HG2	NAC2H5O2	SODIUM
NA5P3O10*6W	NA5P3O10*6H2O	NAC3H9O3	NAC2H5O2*CH3OH
NA5P3O10-1	NA5P3O10-FORM	NAC4H11O3	NAC2H5O2*C2H5OH
NA5P3O10-2	NA5P3O10-FORM	NAC4H11O4	NAC2H5O2*(CH2OH)2
NA5PB2	NA5PB2	NAC4H7O6	CH2OHCOONA*CH2OHCOOH
NA5V3F14	NA5V3F14	NAC6H17O3	NAOC2H5*2C2H5OH
NA6K2(CO3)4	3NA2CO3*K2CO3-AGED	NACH3CO2	NACH3CO2
NA6U7O24	NA6U7O24	NACH3CO2*3W	NACH3CO2*3H2O
NA6ZR2SI4O15	NA6ZR2SI4O15	NACL	SODIUM-CHLORIDE
NA7HG8	NA7HG8	NACL*5NH3	NACL*5NH3
NA8K2(CO3)5	4NA2CO3*K2CO3-AGED	NACLO2	NACLO2
NAALH4	NAALH4	NACLO2*3W	NACLO2*3H2O
NAALS2O8*12W	NAAL(SO4)2*12H2O	NACLO3	NACLO3
NAALS2O8*2W	NAAL(SO4)2*2H2O	NACLO4*W	NACLO4*H2O
NAALS2O8*5W	NAAL(SO4)2*5H2O	NACN*0.5W	NACN*0.5H2O
NAALS2O8*6W	NAAL(SO4)2*6H2O	NACN*2W	NACN*2H2O
NAALSI2O6*W	NAALSI2O6*H2O	NACN-c	NACN-CUBIC
NAAS	NAAS	NACN-o	NACN-ORTHORHOMBIC
NAAS2	NAAS2	NACNO	NACNO
NAASO2	NAASO2	NACNS	NACNS
NAB(OCH3)4	NAB(OCH3)4	NACNS*2SO2	NACNS*2SO2
NAB5O8*5W	NAB5O8*5H2O	NACOO8N4C2H6	NA(CO(NH3)2(NO2)2C2O4)
NABF4	NABF4	NACRO2	NACRO2
NABH*3NH3	NABH4*3NH3	NACS2CRCL6	NACS2CRCL6
NABH*4.5NH3	NABH4*4.5NH3	NAF	SODIUM-FLUORIDE
NABH4	NABH4	NAFECL4	NAFECL4
NABH4*2W	NABH4*2H2O	NAFEF3	NAFEF3
NABO2*2W	NABO2*2H2O	NAFEO2	NAFEO2

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
NAH2F3	NAH2F3	NAIO3*W	NAIO3*H2O
NAH2PO2	NAH2PO2	NAIO4	NAIO4
NAH2PO3	NAH2PO3	NAIO4*3W	NAIO4*3H2O
NAH2PO3*2.5W	NAH2PO3*2.5H2O	NAK(CNS)2	NACNS*KCNS
NAH2PO4	NAH2PO4	NAK3(CNS)4	NACNS*3KCNS
NAH2PO4*2W	NAH2PO4*2H2O	NALIB4O7	0.5NA2O*0.5LI2O*2B2O3
NAH2PO4*W	NAH2PO4*H2O	NALIB6O10	0.5NA2O*0.5LI2O*3B2O3
NAH3(SEO3)2	NAH3(SEO3)2	NALIB8O13	0.5NA2O*0.5LI2O*4B2O3
NAH3P2O7	NAH3P2O7	NALIICL	NALIICL
NAHC2	SODIUM	NAMGF3	NAMGF3
NAHC2O4	NAHC2O4	NAMNCL3	NAMNCL3
NAHC2O4*W	NAHC2O4*H2O	NAMNO4*3W	NAMNO4*3H2O
NAHCO3	SODIUM-BICARBONATE	NAMNO4*W	NAMNO4*H2O
NAHF2	NAHF2	NAMOF7	NAMOF7
NAHG	NAHG	NAN3	NAN3
NAHG2	NAHG2	NANBCL6	NANBCL6
NAHG4	NAHG4	NANBO3	NANBO3
NAHGC2N2I*2W	NAHG(CN)2I*2H2O	NANBO3*3.5W	NANBO3*3.5H2O
NAHPO3	NA2HPO3	NANBOCL4	NANBOCL4
NAHPO3*5W	NA2HPO3*5H2O	NANH2	NANH2
NAHS	NAHS	NANH3	NANH3
NAHS*2W	NAHS*2H2O	NANH4HPO4*4W	NANH4HPO4*4H2O
NAHSE	NAHSE	NANO2*NAOH	NANO2*NAOH
NAHSO4	NAHSO4	NANO3	SODIUM-NITRATE
NAHSO4*W	NAHSO4*H2O	NANO3*2NAOH	NANO3*2NAOH
NAI*2W	NAI*2H2O	NANO3*NAOH	NANO3*NAOH
NAI*3CH3OH	NAI*3CH3OH	NAOC2H5	NAOC2H5
NAI*4SO2	NAI*4SO2	NAOCH3	NAOCH3
NAI3	NAI3	NAOH	SODIUM-HYDROXIDE
NAIBR2	NAIBR2	NAOH*BF3	NAOH*BF3
NAICL2	NAICL2	NAOH*W	NAOH*H2O
NAICL4	NAICL4	NAPB	NAPB
NAIO2F2	NAIO2F2	NAPTBR6	NA2PTBR6
NAIO3	NAIO3	NAPTBR6*6W	NA2PTBR6*6H2O
NAIO3*5W	NAIO3*5H2O	NARB2CRCL6	NARB2CRCL6

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
NAREO4	NAREO4	NDCL2	NDCL2
NASB	NASB	NDCL3*6W	NDCL3*6H2O
NASN	NASN	NDF3*W	NDF3*H2O
NASO3F	NASO3F	NDI3O9	ND(IO3)3
NATACL6	NATACL6	NDN3O9	ND(NO3)3
NATEO4	NA2TEO4	NDN3O9*3W	ND(NO3)3*3H2O
NATHCL5*10W	NATHCL5*10H2O	NDN3O9*4W	ND(NO3)3*4H2O
NATICL3	NATICL3	NDN3O9*6W	ND(NO3)3*6H2O
NATL	NATL	NH28ALS2O20	NH4AL(SO4)2*12H2O
NAUCL6-A	NAUCL6-ALPHA	NH28CRS2O20	NH4CR(SO4)2*12H2O
NAUCL6-B	NAUCL6-BETA	NH2COONA	NH2COONA
NAUF6	NAUF6	NH2COONH4	AMMONIUM
NAUO3	NAUO3	NH3*B3H7	AMMONIATRIBORANE,TETRAGONAL-
NAWF6	NAWF6	NH3*BF3	NH3*BF3
NAWF7	NAWF7	NH3U2O6*3W	NH3(UO3)2*3H2O
NAZRF5	NAZRF5	NH3U3O9*5W	NH3(UO3)3*5H2O
NAZRSI2O7	NA2ZRSI2O7	NH4ALS2O8	AMMONIUM
NAZRSIO5	NA2ZRSIO5	NH4B5O8*4W	NH4B5O8*4H2O
NB1.136S2	NB1.136S2	NH4BO3*0.5W	NH4BO3*0.5H2O
NBB1.875	NBB1.875	NH4BR	AMMONIUM
NBB1.963	NBB1.963	NH4BR*1.5NH3	NH4BR*1.5NH3
NBCO2	NBCO2	NH4BR3	NH4BR3
NBCO3	NBCO3	NH4CL	AMMONIUM-CHLORIDE
NBCR2	NBCR2	NH4CN	AMMONIUM
NBGE0.15	NBGE0.15	NH4CNS*SO2	NH4CNS*SO2
NBGE0.54	NBGE0.54	NH4F	AMMONIUM
NBGE0.67	NBGE0.67	NH4H2ASO4	AMMONIUM
NBGE2	NBGE2	NH4H2PO2	NH4H2PO2
NBOBR3	NBOBR3	NH4H2PO4	AMMONIUM
ND2C3O9	ND2(CO3)3	NH4HCO3	AMMONIUM
ND2C6O12*10W	ND2(C2O4)3*10H2O	NH4HF2	AMMONIUM
ND2S3O12*8W	ND2(SO4)3*8H2O	NH4HS	AMMONIUM
ND2SE3O12*5W	ND2(SEO4)3*5H2O	NH4HSE	AMMONIUM
NDAL2	NDAL2	NH4HSO3	AMMONIUM
NDBR3O9*9W	ND(BRO3)3*9H2O	NH4HSO4	AMMONIUM-HYDROGEN-SULFATE

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
NH4HTE	AMMONIUM	NIAL	NIAL
NH4I*2NH3	NH4I*2NH3	NIB2O4	NI(BO2)2
NH4I*3SO2	NH4I*3SO2	NIBR2*3W	NIBR2*3H2O
NH4I*NH3	NH4I*NH3	NIBR2*6CH3OH	NIBR2*6CH3OH
NH4I3	NH4I3	NIBR2N2H6	NIBR2*2NH3
NH4IBR2	NH4IBR2	NIBR2NH3	NIBR2*NH3
NH4IBRCL	NH4IBRCL	NIC2N2	NI(CN)2-PRECIPITATED
NH4ICL2	NH4ICL2	NIC2N2O2	NI(CNO)2
NH4ICL4	NH4ICL4	NIC2N2S2	NI(CNS)2
NH4IO3	AMMONIUM	NIC2O4	NIC2O4
NH4N3	AMMONIUM	NIC4H6O4N4	NI(C2H3O2N2)2
NH4NO2	AMMONIUM	NICL2	NICKEL-CHLORIDE
NH4NO3	AMMONIUM-NITRATE	NICL2*2W	NICL2*2H2O
NH4OCN	AMMONIUM	NICL2*4W	NICL2*4H2O
NH4PF6	NH4PF6	NICL2*6W	NICL2*6H2O
NH4REO4	NH4REO4	NICL2N2H6	NICL2*2NH3
NH4SCN	AMMONIUM	NICL2NH3	NICL2*NH3
NH4TACL6	NH4TACL6	NICL2O8*6W	NI(CLO4)2*6H2O
NH4U2O4F5	NH4(UO2)2F5	NIF2*4W	NIF2*4H2O
NH4U2O4F5*3W	NH4(UO2)2F5*3H2O	NIFE2O4	NIFE2O4
NH4U2O4F5*4W	NH4(UO2)2F5*4H2O	NIH2C2O4	NI(HCO2)2
NH4VO3	NH4VO3	NII2N2H6	NII2*2NH3
NHG2BR	NHG2BR	NII2O6	NI(IO3)2
NI	NICKEL	NIN2H8C4O4	NI(NH2CH2COO)2
NI2I6PB	(NII2)2*PBI2	NIN2O6	NI(NO3)2
NI2I6PB*3W	(NII2)2*PBI2*3H2O	NIN2O6*3W	NI(NO3)2*3H2O
NI2P2O7	NI2P2O7	NIN2O6*6W	NI(NO3)2*6H2O
NI2SI	NI2SI	NIN6*W	NI(N3)2*H2O
NI2TE3	NI2TE3	NIN6H12SO4	NI(N2H4)3SO4
NI3N	NI3N	NIN6H18BR2	NI(NH3)6BR2
NI4SO10H6	NISO4*3NI(OH)2	NIN6H18CL2	NI(NH3)6CL2
NI4W	NI4W	NIN6H18I2	NI(NH3)6I2
NI6S5	NI6S5	NIN6H24C6CL2	NI(N2H8C2)3CL2
NI7S3O20H8	(NISO4)3*4NI(OH)2	NIN8H18O6	NI(NH3)6(NO3)2
NI7S6	NI7S6	NIO	NICKEL-OXIDE(BUNSENITE)

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
NIO2H2	NI(OH)2	PB2O2*PBCL2	(PBO)2*PBCL2
NIO8H8B2	NI(OH)2*2H3BO3	PB2SIO4	PB2SIO4
NIS-P	NIS-PRECIPITATED	PB2V2O7	PB2V2O7
NIS2O6*6W	NIS2O6*6H2O	PB3AM4I10*6W	(PBI2)3*4NH4I*6H2O
NISE	NISE	PB3ASI9*12W	(PBI2)3*ASI3*12H2O
NISEO3*2W	NISEO3*2H2O	PB3C2N2O3H2	PB(CN)2*2PBO*H2O
NISEO3*2W-P	NISEO3*2H2O-PRECIPITATED	PB3I6*4NH4I	(PBI2)3*4NH4I
NISO4*4W	NISO4*4H2O	PB3I6*ASI3	(PBI2)3*ASI3
NISO4*6W	NISO4*6H2O-ALPHA,GREEN	PB3I6*PI3	(PBI2)3*PI3
NISO4*7W	NISO4*7H2O	PB3I6*SBI3	(PBI2)3*SBI3
NITE	NITE	PB3I9P*12W	(PBI2)3*PI3*12H2O
NITE2	NITE2	PB3O2BR2	(PBO)2*PBBR2
NOVF6	NOVF6	PB3O3*PBCL2	(PBO)3*PBCL2
OSCL3	OSCL3	PB3P2O8	PB3(PO4)2
OSCL4	OSCL4	PB3SBI9*12W	(PBI2)3*SBI3*12H2O
P	PHOSPHORUS	PB3V2O8	PB3(VO4)2
P2H6*B2H6	(PH3)2*B2H6	PB4O3BR2	(PBO)3*PBBR2
P2O5	PHOSPHORUS-PENTOXIDE	PB4O6H6CL2	(PB(OH)2)3*PBCL2
P2S3	P2S3	PBBR2*2NH3	PBBR2*2NH3
P3N5	P3N5	PBBR2*3NH3	PBBR2*3NH3
PABR4	PABR4	PBBR2*5.5NH3	PBBR2*5.5NH3
PABR5	PABR5	PBBR2*8NH3	PBBR2*8NH3
PACL4	PACL4	PBBR2*NH3	PBBR2*NH3
PACL5	PACL5	PBBR2O6	PB(BRO3)2
PAI4	PAI4	PBBRF	PBBRF
PAOBR2	PAOBR2	PBC2O4	PBC2O4
PB	LEAD	PBC4H6O4	PB(CH3CO2)2
PB(N3)2-M	PB(N3)2-MONOCLINIC	PBC4H6O4*3W	PB(CH3CO2)2*3H2O
PB(N3)2-O	PB(N3)2-ORTHORHOMBIC	PBCL2	LEAD-CHLORIDE
PB(NO3)2	PB(NO3)2	PBCL2*1.5NH3	PBCL2*1.5NH3
PB(OH)2	PB(OH)2	PBCL2*2NH3	PBCL2*2NH3
PB(OH)2-P	PB(OH)2-PPTD	PBCL2*3.25NH	PBCL2*3.25NH3
PB2CL4*NH4CL	(PBCL2)2*NH4CL	PBCL2*8NH3	PBCL2*8NH3
PB2H	PD2H	PBCL2*NH3	PBCL2*NH3
PB2N6O	PB(N3)2*PBO	PBCL2*PBCO3	PBCL2*PBCO3

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
PBCLOH	PBCLOH	PBSO4	LEAD-SULFATE
PBFCL	PBFCL	PBSO4*2NH3	PBSO4*2NH3
PBH2C2O4	PB(HCO2)2	PBSO4*2PBO	PBSO4*2PBO
PBH2PO4	RBH2PO4	PBSO4*3PBO	PBSO4*3PBO
PBHPO3	PBHPO3	PBSO4*4NH3	PBSO4*4NH3
PBI2*0.5NH3	PBI2*0.5NH3	PBSO4*PBO	PBSO4*PBO
PBI2*2MGI2	PBI2*2MGI2	PBTEO4	PBTEO4
PBI2*2NH3	PBI2*2NH3	PD3SB	PD3SB
PBI2*2RBI	PBI2*2RBI	PDBR2	PDBR2
PBI2*2RBI*4W	PBI2*2RBI*4H2O	PDC2N2	PD(CN)2
PBI2*2ZNI2	PBI2*2ZNI2	PDC2N2S2	PD(CNS)2
PBI2*5NH3	PBI2*5NH3	PDCL2*2NH3	PDCL2*2NH3
PBI2*8NH3	PBI2*8NH3	PDCL2*4NH3	PDCL2*4NH3
PBI2*HI*5W	PBI2*HI*5H2O	PDI2*2NH3	PDI2*2NH3
PBI2*NH3	PBI2*NH3	PDI2*4NH3	PDI2*4NH3
PBI2*SNI2	PBI2*SNI2	PDO2H2	PD(OH)2-PRECIPITATED
PBI2*SNI2*8W	PBI2*SNI2*8H2O	PDO4H4	PD(OH)4-PRECIPITATED
PBI2O6	PB(IO3)2	PDSB	PDSB
PBI8CR2	PBI2*2CRI3	PDSB2	PDSB2
PBI8CR2H6O3	PBI2*2CRI3*3H2O	PDTE2	PDTE2
PBN2O6*3NH3	PB(NO3)2*3NH3	PH3*BCL3	PH3*BCL3
PBN2O6*6NH3	PB(NO3)2*6NH3	PH4BR	PH4BR
PBN2O6*NH3	PB(NO3)2*NH3	PH4CL	PH4CL
PBNA4S6O9	PBS2O3*2NA2S2O3	PH4I	PH4I
PBO*PBBR2	PBO*PBBR2	PO(OH)4	PO(OH)4
PBO*PBCL2	PBO*PBCL2	POCL3*BCL3	POCL3*BCL3
PBO*PBCO3	PBO*PBCO3	POS	POLONIUM
PBR5	PHOSPHORUS	PR2C3O9	PR2(CO3)3
PBRE2O8*2W	PB(REO4)2*2H2O	PR2C6O12*10W	PR2(C2O4)3*10H2O
PBS	LEAD-SULFIDE	PR2SE3O12*5W	PR2(SEO4)3*5H2O
PBS2C2N2	PB(SCN)2	PR2SE4O12H2	PR2(SEO3)3*H2SEO3
PBS2O3	PBS2O3	PR2SE4O17H12	PR2(SEO3)3*H2SEO3*5H2O
PBS2O6*4W	PBS2O6*4H2O	PRAL2	PRAL2
PBS3O6	PBS3O6	PRAL4	PRAL4
PBSO3	PBSO3	PRAS	PRAS

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
PRBI	PRBI	RASO4	RASO4
PRBR3O9*9W	PR(BRO3)3*9H2O	RB	RUBIDIUM
PRC	PRC	RB(UO2)2F5	RB(UO2)2F5
PRCL3*6W	PRCL3*6H2O	RB2BA(NO2)4	2RBNO2*BA(NO2)2
PRCL3*7W	PRCL3*7H2O	RB2CO3	RB2CO3
PRF3*W	PRF3*H2O	RB2CO3*1.5W	RB2CO3*1.5H2O
PRI3O9	PR(IO3)3	RB2CO3*3W	RB2CO3*3H2O
PRN3O9	PR(NO3)3	RB2CO3*W	RB2CO3*H2O
PRN3O9*6W	PR(NO3)3*6H2O	RB2COCL4	RB2COCL4
PRO3H3	PR(OH)3	RB2CRO4	RB2CRO4
PROCL	PROCL	RB2FECL4	RB2FECL4
PRSB	PRSB	RB2GECL6	RB2GECL6
PT	PLATINUM	RB2H2P2O7	RB2H2P2O7
PT3N6H18CL6	(PT(NH3)4)(PT(NH3)CL3)2	RB2IRCL6	RB2IRCL6
PTBR	PTBR	RB2NBOCL5	RB2NBOCL5
PTCL	PTCL	RB2PTCL4	RB2PTCL4
PTCL2*5NH3	PTCL2*5NH3	RB2PTCL6	RB2PTCL6
PTCL4*5W	PTCL4*5H2O	RB2S	RB2S
PTF6	PTF6	RB2SEO3	RB2SEO3
PTN2H6CL2-C	PT(NH3)2CL2-CIS	RB2SEO4	RB2SEO4
PTN2H6CL2-T	PT(NH3)2CL2-TRANS	RB2SIF6	RB2SIF6
PTN3H9CL2	(PT(NH3)3CL)CL	RB2SNBR6	RB2SNBR6
PTN3H9CL2O4	(PT(NH3)3CL)CLO4	RB2SNCL6	RB2SNCL6
PTN4H12CL2	(PT(NH3)4)CL2	RB2TEBR6	RB2TEBR6
PTN4H12CL2*W	(PT(NH3)4)CL2*H2O	RB2TEO3	RB2TEO3
PTN4H12I2	(PT(NH3)4)I2	RB2TEO3*3W	RB2TEO3*3H2O
PTN6H12O6	PT(NH3)4(NO3)2	RB2TEO3*W	RB2TEO3*H2O
PTO2H2	PT(OH)2	RB2THCL6	RB2THCL6
PTTE	PTTE	RB2THCL6*9W	RB2THCL6*9H2O
PTTE2	PTTE2	RB2TIBR6	RB2TIBR6
RA	RA	RB2TICL4	RB2TICL4
RA(IO3)2	RA(IO3)2	RB2TICL6	RB2TICL6
RA(NO3)2	RA(NO3)2	RB2UBR6	RB2UBR6
RACL2	RACL2	RB2UCL6	RB2UCL6
RACL2*2W	RACL2*2H2O	RB2ZNBR4	RB2ZNBR4

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
RB2ZNCL4	RB2ZNCL4	RBCACL3	RBCACL3
RB3AGI3	RB2AGI3	RBCEFEC6N6W2	RBCE(FE(CN)6)*2H2O
RB3COCL5	RB3COCL5	RBCL*ZNSO4	RBCL*ZNSO4
RB3CR2CL9	RB3CR2CL9	RBCLO3	RBCLO3
RB3CRCL6	RB3CRCL6	RBCLO4	RBCLO4
RB3CRO4F	RB3CRO4F	RBCN	RBCN
RB3SB	RB3SB	RBCOCL3	RBCOCL3
RB3SB7	RB3SB7	RBF*1.5W	RBF*1.5H2O
RB3TI2BR9	RB3TI2BR9	RBFECL3	RBFECL3
RB3TIBR6	RB3TIBR6	RBGDFEC6N6	RBGD(FE(CN)6)
RB3UO2F5	RB3UO2F5	RBH	RBH
RB3V2CL9	RB3V2CL9	RBHCO3	RBHCO3
RB3VCL6	RB3VCL6	RBHF2	RBHF2
RB4THCL8	RB4THCL8	RBHS	RBHS
RB4UCL8	RB4UCL8	RBHSE	RBHSE
RB5(UO2)2F9	RB5(UO2)2F9	RBHSO4	RBHSO4
RB5SB4	RB5SB4	RBI*3SO2	RBI*3SO2
RBAG4I5	RBAG4I5	RBI3	RBI3
RBB(CLO4)4	RBB(CLO4)4	RBIBR2	RBIBR2
RBBA2(NO2)5	RBNO2*2BA(NO2)2	RBIBRCL	RBIBRCL
RBBCL4	RBBCL4	RBICL2	RBICL2
RBBF4	RBBF4	RBICL4	RBICL4
RBBO2	RBBO2	RBIO3	RBIO3
RBBR2CL	RBBR2CL	RBKCL2	RBKCL2
RBBR3	RBBR3	RBMNCL3	RBMNCL3
RBBRCL2	RBBRCL2	RBMOF6	RBMOF6
RBBRO3	RBBRO3	RBN3	RBN3
RBC10	RBC10	RBNBCL6	RBNBCL6
RBC24	RBC24	RBNBO3	RBNBO3
RBC36	RBC36	RBNH2	RBNH2
RBC48	RBC48	RBNICL3	RBNICL3
RBC4H11O2	C2H5ORB*C2H5OH	RBNO2	RBNO2
RBC60	RBC60	RBNO3	RBNO3
RBC72	RBC72	RBOH	RBOH
RBC8	RBC8	RBOH*2W	RBOH*2H2O

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
RBOH*W	RBOH*H2O	SCAS	SCAS
RBPF6	RBPF6	SCCL3*6W	SCCL3*6H2O
RBPO3	RBPO3	SCH1.97	SCH1.97
RBPTNH3CL3	RBPTNH3CL3	SCH2	SCH2
RBREO4	RBREO4	SCH3C3O6	SC(HCO2)3
RBSB	RBSB	SCO2H2CL	SC(OH)2CL
RBSB2	RBSB2	SCO3H3	SC(OH)3
RBSO2F	RBSO2F	SE(OH)3CLO4	SE(OH)3CLO4
RBTACL6	RBTACL6	SEO2SO3	SEO2SO3
RBTICL3	RBTICL3	SI	SILICON
RBUCL5	RBUCL5	SIC-A	SILICON
RBUCL6	RBUCL6	SIC-B	SILICON
RBUF6	RBUF6	SIF4*2NC3H9	SIF4*2N(CH3)3
RBWF6	RBWF6	SIF4*2NH3	SIF4*2NH3
RE3SI	RE3SI	SIF4*NC3H9	SIF4*N(CH3)3
REAS2	REAS2	SIO2	SILICON-DIOXIDE
RECL5	RECL5	SISE2	SILICON
RHCL3C12H30S	RHCL3*3(C2H5)2S	SM2C2O3*10W	SM2(C2O3)*10H2O
RUBR3	RUBR3	SM2C3O9	SM2(CO3)3
RUCL3C12H30S	RUCL3*3(C2H5)2S	SM2S3O12	SM2(SO4)3
RUI3	RUI3	SM2S3O12*8W	SM2(SO4)3*8H2O
S	SULFUR	SM2S3O9	SM2(SO3)3
SB(OH)3	ANTIMONY	SM2SE3O12*8W	SM2(SEO4)3*8H2O
SB4O5CL2	SB4O5CL2	SMAS	SMAS
SBCL3*3RBCL	SBCL3*3RBCL	SMBR3O9*9W	SM(BRO3)3*9H2O
SBF3*2NH3	SBF3*2NH3	SMC2	SMC2
SBF3*3NH3	SBF3*3NH3	SMCL3*6W	SMCL3*6H2O
SBF3*4NH3	SBF3*4NH3	SMF3	SMF3
SBF3*6NH3	SBF3*6NH3	SMF3*W	SMF3*H2O
SBF3*NH3	SBF3*NH3	SMI3	SMI3
SBOCL	SBOCL	SMI3O9	SM(IO3)3
SC2C6O12	SC2(C2O4)3	SMN3O9	SM(NO3)3
SC2O5H5CL	SC2(OH)5CL	SMN3O9*6W	SM(NO3)3*6H2O
SC2S3O12	SC2(SO4)3	SMOCL	SMOCL
SC2SE3O9*10W	SC2(SEO3)3*10H2O	SN(OH)2-P	SN(OH)2-PPTD

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
SN(OH)4-P	SN(OH)4-PPTD	SR3P2	SR3P2
SNBR2	SNBR2	SR3P2O8	SR3(PO4)2
SNBR2*2NH3	SNBR2*2NH3	SR3SB2	SR3SB2
SNBR2*3NH3	SNBR2*3NH3	SR3UO6	SR3UO6
SNBR2*5NH3	SNBR2*5NH3	SR4AL2O7-A	(SRO)4*AL2O3-ALPHA
SNBR2*9NH3	SNBR2*9NH3	SR4AL2O7-B	(SRO)4*AL2O3-BETA
SNBR2*NH3	SNBR2*NH3	SR7FE10O22	(SRO)7*5FE2O3
SNBR4*8W	SNBR4*8H2O	SRB2F8	SR(BF4)2
SNC2H6CL2	SN(CH3)2CL2	SRBI	SRBI
SNCL2*2.5NH3	SNCL2*2.5NH3	SRBR2	STRONTIUM-BROMIDE
SNCL2*2W	SNCL2*2H2O	SRBR2*2NH3	SRBR2*2NH3
SNCL2*4NH3	SNCL2*4NH3	SRBR2*6W	SRBR2*6H2O
SNCL2*9NH3	SNCL2*9NH3	SRBR2*8NH3	SRBR2*8NH3
SNCL4*1.5PH3	SNCL4*1.5PH3	SRBR2*NH3	SRBR2*NH3
SNI2*2NH3	SNI2*2NH3	SRBR2*SRO*3W	SRBR2*SRO*3H2O
SNI2*3NH3	SNI2*3NH3	SRBR2*SRO*9W	SRBR2*SRO*9H2O
SNI2*5NH3	SNI2*5NH3	SRBR2*W	SRBR2*H2O
SNI2*9NH3	SNI2*9NH3	SRBR2CO0.5H3	SRBR2*0.5C2H5OH
SNI2*NH3	SNI2*NH3	SRBR2O6*W	SR(BRO3)2*H2O
SNOHCL*W	SNOHCL*H2O	SRBRH	SRBRH
SR2AL2SIO7	(SRO)2*AL2O3*SIO2	SRC2N2*4W	SR(CN)2*4H2O
SR2BI	SR2BI	SRC2O4	SRC2O4
SR2GE	SR2GE	SRC4H6O4	SR(CH3CO2)2
SR2O2*FE2O3	(SRO)2*FE2O3	SRC4H6O4.5H	SR(CH3CO2)2*0.5H2O
SR2PB	SR2PB	SRC4H6O6	SR(CH2OHCO2)2
SR2SB	SR2SB	SRCL2*2W	SRCL2*2H2O
SR2SIO4	SR2SIO4	SRCL2*6W	SRCL2*6H2O
SR2SN	SR2SN	SRCL2*SRO*9W	SRCL2*SRO*9H2O
SR2U3O11	SR2U3O11	SRCL2*W	SRCL2*H2O
SR2UO5	SR2UO5	SRCL2-A	SRCL2-ALPHA
SR3AL4CL18	(SRCL2)3*4ALCL3	SRCL2N8H24	SRCL2*8NH3
SR3AS2	SR3AS2	SRCL2NH3	SRCL2*NH3
SR3BI2	SR3BI2	SRCL2O8	SR(CLO4)2
SR3O3*AL2O3	(SRO)3*AL2O3	SRCL2O8*2W	SR(CLO4)2*2H2O
SR3O3*FE2O3	(SRO)3*FE2O3	SRCL2O8*4W	SR(CLO4)2*4H2O

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
SRCL2O8N2H6	SR(CLO4)2*2NH3	SRN6	SR(N3)2
SRCL2O8N6H18	SR(CLO4)2*6NH3	SRN6H18	SR(NH3)6
SRCL2O8N7H21	SR(CLO4)2*7NH3	SRO*AL2O3	SRO*AL2O3
SRCLH	SRCLH	SRO2H2*8W	SR(OH)2*8H2O
SRCN2	SRCN2	SRO2H2*W	SR(OH)2*H2O
SRCO3	SRCO3	SRS	SRS
SRF2	SRF2	SRS2I2O4	SRI2*2SO2
SRFCL	SRFCL	SRS2O6*4W	SRS2O6*4H2O
SRH2C2O4	SR(HCO2)2	SRS4I2O8	SRI2*4SO2
SRH2C2O4*2W	SR(HCO2)2*2H2O	SRSB	SRSB
SRH4P2O8	SR(H2PO4)2	SRSE	SRSE
SRHFO3	SRHFO3	SRSEO3	SRSEO3
SRHPO4	SRHPO4	SRSEO4	SRSEO4
SRI2*2NH3	SRI2*2NH3	SRSO3	SRSO3
SRI2*2PBI2	SRI2*2PBI2	SRUO4-A	SRUO4-ALPHA,RHOMBOHEDRAL
SRI2*2W	SRI2*2H2O	SRUO4-B	SRUO4-BETA,ORTHORHOMBIC
SRI2*6NH3	SRI2*6NH3	TA2H	TA2H
SRI2*6W	SRI2*6H2O	TA5SI3	TA5SI3
SRI2*8NH3	SRI2*8NH3	TASI2	TASI2
SRI2*NH3	SRI2*NH3	TB2C3O9	TB2(CO3)3
SRI2*W	SRI2*H2O	TB2C6O12*10W	TB2(C2O4)3*10H2O
SRI2O6	SR(IO3)2	TBAS	TBAS
SRI2O6*6W	SR(IO3)2*6H2O	TBBR3O9*9W	TB(BRO3)3*9H2O
SRI2O6*W	SR(IO3)2*H2O	TBCL3*6W	TBCL3*6H2O
SRI6PB2*7W	SRI2*2PBI2*7H2O	TBI3O9	TB(IO3)3
SRIH	SRIH	TBOCL	TBOCL
SRMG2-B	SRMG2-BETA	TH2CO17	TH2CO17
SRMOO3	SRMOO3	TH2CO7	TH2CO7
SRN2H4	SR(NH2)2	TH2FE17	TH2FE17
SRN2H8S2O8	SR(NH4)2(SO4)2	TH2FE7	TH2FE7
SRN2O2*5W	SRN2O2*5H2O	TH2N2O	TH2N2O
SRN2O4	SR(NO2)2	TH2NI17	TH2NI17
SRN2O4*W	SR(NO2)2*H2O	TH3GE	TH3GE
SRN2O6	SR(NO3)2	TH3GE2	TH3GE2
SRN2O6*4W	SR(NO3)2*4H2O	TH3GE5	TH3GE5

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
TH3S7	TH3S7	THNI5	THNI5
TH3SI2	TH3SI2	THOF2	THOF2
TH3SI5	TH3SI5	THOHI3*10W	TH(OH)I3*10H2O
TH7CO3	TH7CO3	THOI2*3.5W	THOI2*3.5H2O
TH7FE3	TH7FE3	THPB3	THPB3
TH7S12	TH7S12	THSI	THSI
THBR4*10W	THBR4*10H2O	THSI2	THSI2
THBR4*12W	THBR4*12H2O	THSN3	THSN3
THBR4*7W	THBR4*7H2O	THTL3	THTL3
THC	THC	TI	TITANIUM
THC4O8*6W	TH(C2O4)2*6H2O	TI3AL	TI3AL
THCL4*12NH3	THCL4*12NH3	TI5SI3-E	TI5SI3-EPSILON
THCL4*18NH3	THCL4*18NH3	TIAL	TIAL
THCL4*2W	THCL4*2H2O	TIAL3	TIAL3
THCL4*4NH3	THCL4*4NH3	TIAS	TIAS
THCL4*4W	THCL4*4H2O	TIBR4*2CH3CN	TIBR4*2CH3CN
THCL4*6NH3	THCL4*6NH3	TIBR4*2H2S	TIBR4*2H2S
THCL4*7NH3	THCL4*7NH3	TIBR4*2PH3	TIBR4*2PH3
THCL4*7W	THCL4*7H2O	TIBR4*H2S	TIBR4*H2S
THCL4*8W	THCL4*8H2O	TIBR4*PH3	TIBR4*PH3
THCL4*NH4CL	THCL4*NH4CL	TICL4*2CH3CN	TICL4*2CH3CN
THCO	THCO	TICL4*2H2S	TICL4*2H2S
THCO5	THCO5	TICL4*2PH3	TICL4*2PH3
THF4*2.5W	THF4*2.5H2O	TICL4*2POCL3	TICL4*2POCL3
THFE3	THFE3	TICL4*H2S	TICL4*H2S
THFE5	THFE5	TICL4*PH3	TICL4*PH3
THGE	THGE	TICL4*POCL3	TICL4*POCL3
THGE2	THGE2	TIF4*CH3CN	TIF4*CH3CN
THGE3	THGE3	TIO2	TITANIUM-OXIDE(RUTILE)
THH3.75	THH3.75	TIP	TIP
THIN3	THIN3	TISB	TISB
THN4O12	TH(NO3)4	TISI-G	TISI-GAMMA
THN4O12*4W	TH(NO3)4*4H2O	TISI2-B	TISI2-BETA
THN4O12*5W	TH(NO3)4*5H2O	TL2CO3	TL2CO3
THNI2	THNI2	TL2CRO4	TL2CRO4

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
TL2S	TL2S	U3O7-A	U3O7-ALPHA,TETRAGONAL
TL2SE	TL2SE	U3O7-B	U3O7-BETA,TETRAGONAL
TL2SE3O9	TL2(SEO3)3	U3O8-A	U3O8-ALPHA,ORTHORHOMBIC
TL2SEO4	TL2SEO4	U3P4	U3P4
TL2SO4	TL2SO4	U3SB4	U3SB4
TL2TE	TL2TE	U3SI	U3SI
TL2TICL6	TL2TICL6	U3SI2	U3SI2
TL4V2O7	TL4V2O7	U4O9	U4O9
TLBR*3NH3	TLBR*3NH3	UAL2	UAL2
TLBR3*4W	TLBR3*4H2O	UAL3	UAL3
TLBRO3	TLBRO3	UAL4	UAL4
TLCH3CO2	TLCH3CO2	UAS	UAS
TLCL*3NH3	TLCL*3NH3	UAS2	UAS2
TLCL2BR*4W	TLCL2BR*4H2O	UB1.98	UB1.98
TLCL3*3NH3	TLCL3*3NH3	UBI	UBI
TLCL3*4W	TLCL3*4H2O	UBI2	UBI2
TLCLBR2*4W	TLCLBR2*4H2O	UCL2BR	UCL2BR
TLHF2	TLHF2	UCL2BR2	UCL2BR2
TLI*3NH3	TLI*3NH3	UCL3BR	UCL3BR
TLIO3	TLIO3	UCLBR2	UCLBR2
TLN3	TLN3	UCLBR3	UCLBR3
TLNO3	TLNO3	UF2CL2	UF2CL2
TLO3H3	TL(OH)3	UF3CL	UF3CL
TLOCH3	TLOCH3	UF4*2.5W-O	UF4*2.5H2O-ORTHORHOMBIC
TLOH	TLOH	UF4-M	UF4-MONOCLINIC
TLONC	THALLOUS	UFCL3	UFCL3
TLSCN	TLCNS	UFE2	UFE2
TLVO3	TLVO3	UGA	UGA
TMC2	TMC2	UGA2	UGA2
TMI3O9	TM(IO3)3	UGA3	UGA3
TMOCL	TMOCL	UIN3	UIN3
U(OH)2SO4	U(OH)2SO4	UN0.997	UN0.997
U2O4CL3	(UO2)2CL3	UN1.466-B	UN1.466-BETA,SESQUINITRIDE
U3AS4	U3AS4	UN1.5	UN1.5
U3BI4	U3BI4	UN1.51-A	UN1.51-ALPHA,SESQUINITRIDE

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
UN1.59-A	UN1.59-ALPHA,SESQUINITRIDE	UO6C4H6	UO2(CH3CO2)2
UN1.606-A	UN1.606-ALPHA,SESQUINITRIDE	UO6C4H6*2W	UO2(CH3CO2)2*2H2O
UN1.674-A	UN1.674-ALPHA,SESQUINITRIDE	UO6CR*5.5W	UO2CRO4*5.5H2O
UN1.73-A	UN1.73-ALPHA,SESQUINITRIDE	UO8N2*2W	UO2(NO3)2*2H2O
UO2.86*0.5W	UO2.86*0.5H2O	UO8N2*3W	UO2(NO3)2*3H2O
UO2.86*1.5W	UO2.86*1.5H2O	UO8N2*6W	UO2(NO3)2*6H2O
UO2BR2*3W	UO2BR2*3H2O	UO8N2*W	UO2(NO3)2*H2O
UO2BR2*W	UO2BR2*H2O	UOF2	UOF2
UO2C2O4	UO2C2O4	UOF2*W	UOF2*H2O
UO2C2O4*3W	UO2C2O4*3H2O	UOFOH	UOF(OH)
UO2C2O4*W	UO2C2O4*H2O	UOFOH*0.5W	UOF(OH)*0.5H2O
UO2CL2*3W	UO2CL2*3H2O	UP	UP
UO2CL2*W	UO2CL2*H2O	UP2	UP2
UO2CO3	UO2CO3	UPB3	UPB3
UO2F2*3W	UO2F2*3H2O	US1.5	US1.5
UO2H2C2O4	UO2(HCO2)2	US1.9-A	US1.9-ALPHA,HYPOSTOICHIOMETRIC
UO2H2C2O4*W	UO2(HCO2)2*H2O	US2-B	US2-BETA
UO2KASO	UO2KASO4	US2O8*4W	U(SO4)2*4H2O
UO2KPO4	UO2KPO4	US2O8*8W	U(SO4)2*8H2O
UO2OHCL*2W	UO2(OH)CL*2H2O	US3	US3
UO2OHF*2W	UO2(OH)F*2H2O	USB	USB
UO2OHF*W	UO2(OH)F*H2O	USB2	USB2
UO2SEO3	UO2SEO3	USE1.33	USE1.33
UO2SEO4-A	UO2SEO4-ALPHA	USE1.5	USE1.5
UO2SO3	UO2SO3	USE2-A	USE2-ALPHA
UO2SO3*4.5W	UO2SO3*4.5H2O	USI	USI
UO2SO4*2.5W	UO2SO4*2.5H2O	USI2	USI2
UO2SO4*3.5W	UO2SO4*3.5H2O	USI3	USI3
UO2SO4*3W	UO2SO4*3H2O	USN3	USN3
UO2SO4*W	UO2SO4*H2O	USO6.2.5H2O	USO6.2.5H2O
UO2SO4-B	UO2SO4-BETA	USO6.3.5H2O	USO6.3.5H2O
UO2TEO3	UO2TEO3	UTE	UTE
UO3HBR*2W	UO2(OH)BR*2H2O	UTE1.33	UTE1.33
UO4*2W	UO4*2H2O	UTE3	UTE3
UO4*4W	UO4*4H2O	UTL3	UTL3

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
V2SI	V2SI	YCL3*3CH3NH2	YCL3*3CH3NH2
V3O11P2	(VO)3(PO4)2	YCL3*4CH3NH2	YCL3*4CH3NH2
V3SI	V3SI	YCL3*6W	YCL3*6H2O
V5AL8	V5AL8	YCL3*CH3NH2	YCL3*CH3NH2
V5SI3	V5SI3	YH2	YH2
VAL3	VAL3	YH2.6	YH2.6
VO2CL	VO2CL	YH3	YH3
VOCL	VOCL	YI3	YI3
VOCL2	VOCL2	YI3O9	Y(IO3)3
VOSO4	VOSO4	YNBO4	YNBO4
VSI2	VSI2	YO2H2CL	Y(OH)2CL
W	TUNGSTEN	YO3H3	Y(OH)3
WO2	TUNGSTEN-DIOXIDE	YRE3O12	Y(REO4)3
WO2BR2	WO2BR2	YZN	YZN
WO3	TUNGSTEN-TRIOXIDE	YZN11	YZN11
WOBR4	WOBR4	YZN2-A	YZN2-ALPHA
WSI2	WSI2	YZN3	YZN3
Y2C3O9	Y2(CO3)3	YZN4	YZN4
Y2C6O12*9W	Y2(C2O4)3*9H2O	YZN5	YZN5
Y2O5H5CL	Y2(OH)5CL	ZN	ZINC
Y2S3O12	Y2(SO4)3	ZN(OH)2	ZINC-HYDROXIDE
Y2S3O12*8W	Y2(SO4)3*8H2O	ZN(OH)2-B	ZINC-HYDROXIDE(BETA)
Y2SE3O9	Y2(SEO3)3	ZN(OH)2-E	ZINC-HYDROXIDE(EPSILON)
Y2ZN17	Y2ZN17	ZN2O3H3CL	ZN2(OH)3CL
YAS	YAS	ZN2P2O7	ZN2(P2O7)
YB2C6O12*5W	YB2(C2O4)3*5H2O	ZN3AS2O8	ZINC
YB2OC	YB2OC	ZN4C6N6O	(ZN(CN)2)3*ZNO
YBBR3O9*9W	YB(BRO3)3*9H2O	ZN4CL2O3*5W	ZNCL2*3ZNO*5H2O
YBC2	YBC2	ZN5BR2O4*13W	ZNBR2*4ZNO*13H2O
YBCL3*6W	YBCL3*6H2O	ZN5CL2O4*11W	ZNCL2*4ZNO*11H2O
YBH2	YBH2	ZN5N2O14H8	ZN(NO3)2*4ZN(OH)2
YBI3O9	YB(IO3)3	ZN6CL2O5*8W	ZNCL2*5ZNO*8H2O
YBOCL	YBOCL	ZN6I2O5*11W	ZNI2*5ZNO*11H2O
YC2	YC2	ZN9CL2O8*10W	ZNCL2*8ZNO*10H2O
YCL3*2CH3NH2	YCL3*2CH3NH2	ZNAL2O4	ZNAL2O4

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

Alias	Component Name	Alias	Component Name
ZNAS2	ZNAS2	ZNI2*2N2H4	ZNI2*2N2H4
ZNB2O4	ZN(BO2)2	ZNI2*2NH3	ZNI2*2NH3
ZNBR2*2N2H4	ZNBR2*2N2H4	ZNI2*4NH3	ZNI2*4NH3
ZNBR2*2NH3	ZNBR2*2NH3	ZNI2*6NH3	ZNI2*6NH3
ZNBR2*2W	ZNBR2*2H2O	ZNI2*NH3	ZNI2*NH3
ZNBR2*4NH3	ZNBR2*4NH3	ZNI2O6	ZINC
ZNBR2*6NH3	ZNBR2*6NH3	ZNN2H4	ZINC
ZNBR2*6NH3*W	ZNBR2*6NH3*H2O	ZNN2H6CS3	ZN(NH3)2CS3
ZNBR2*NH3	ZNBR2*NH3	ZNN2O6	ZINC
ZNC2H2O4	ZINC	ZNN2O6*2W	ZINC
ZNC2H6O6	ZINC	ZNN2O6*4W	ZINC
ZNC2N2	ZINC	ZNN2O6*6W	ZINC
ZNC2O4*2W	ZINC	ZNN2O6*W	ZINC
ZNC4H10O6	ZINC	ZNN6	ZINC
ZNC4H12O4N2	ZN(CH3CO2)2*2NH3	ZNO	ZINC-OXIDE
ZNC4H12O6N2	ZN(CH2OHCOO)2*2NH3	ZNO*2ZNSO4	ZNO*2ZNSO4
ZNC4H18O4N4	ZN(CH3CO2)2*4NH3	ZNO2H2-B	ZN(OH)2-BETA
ZNC4H18O6N4	ZN(CH2OHCOO)2*4NH3	ZNO2H2-E	ZN(OH)2-EPSILON
ZNC4H24O4N6	ZN(CH3CO2)2*6NH3	ZNO2H2-G	ZN(OH)2-GAMMA
ZNC4H24O6N6	ZN(CH2OHCOO)2*6NH3	ZNO2H2-P	ZN(OH)2-PPTD
ZNC4H30O4N8	ZN(CH3CO2)2*8NH3	ZNP2O6	ZN(PO3)2
ZNC4H6O4	ZINC	ZNS-1	ZINC-SULFIDE(SPHALENITE)
ZNC4H6O6	ZINC	ZNS-2	ZINC-SULFIDE(WURTZITE)
ZNC4H8O5	ZINC	ZNS2O6*6W	ZINC
ZNC4H8O7	ZINC	ZNSB	ZNSB
ZNC4H9O4N	ZN(CH3CO2)2*NH3	ZNSEO3*W	ZNSEO3*H2O
ZNCL2*2N2H4	ZNCL2*2N2H4	ZNSEO4	ZINC
ZNCL2*2NH3	ZNCL2*2NH3	ZNSEO4*6W	ZINC
ZNCL2*4NH3	ZNCL2*4NH3	ZNSEO4*W	ZINC
ZNCL2*5NH3*W	ZNCL2*5NH3*H2O	ZNSO4	ZINC-SULFATE
ZNCL2*6NH3	ZNCL2*6NH3	ZNSO4*ZNO2H2	ZNSO4*ZN(OH)2
ZNCL2*NH3	ZNCL2*NH3	ZNTIO3	ZNTIO3
ZNCL2AM4W0.5	ZNCL2*4NH3*0.5H2O	ZR2SI	ZR2SI
ZNCL2O8*6W	ZN(CLO4)2*6H2O	ZR3SI	ZR3SI
ZNCO3*W	ZINC	ZR3SI2	ZR3SI2

continued

Table 1.13 Components Available in SOLIDS Databank (continued)

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

Table 1.14 Parameters Available in the COMBUST Databank

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

† *Ideal gas at 25°C*

Table 1.15 Components Available in the COMBUST Databank

Alias	Component Name	Alias	Component Name
AR	ARGON	F2	FLUORINE
BR	BROMINE-ATOM	H	HYDROGEN-ATOM
BR2	BROMINE	H2	HYDROGEN
C	CARBON	H2N	AMIDOGEN
C2	CARBON-DIATOMIC	H2O	WATER
C2H2	ACETYLENE	H2S	HYDROGEN-SULFIDE
C2H4	ETHYLENE	H3N	AMMONIA
C2N2	CYANOGEN	HBR	HYDROGEN-BROMIDE
C3O2	CARBON-SUBOXIDE	HCL	HYDROGEN-CHLORIDE
CCL4	CARBON-TETRACHLORIDE	HE-4	HELIUM-4
CH	METHYLIDYNE	HF	HYDROGEN-FLUORIDE
CH2	METHYLENE	HI	HYDROGEN-IODIDE
CH2CL2	DICHLOROMETHANE	HN	IMIDOGEN
CH2O	FORMALDEHYDE	HNO	NITROXYL
CH3	METHYL	HO	HYDROXYL
CH3CL	METHYL-CHLORIDE	HO2	HYDROPEROXYL
CH4	METHANE	HS	SULFUR-MONOHYDRIDE
CHCL3	CHLOROFORM	I	IODINE-ATOM
CHN	HYDROGEN-CYANIDE	I2	IODINE
CHO	FORMYL	N	NITROGEN-ATOM
CL	CHLORINE-ATOM	N2	NITROGEN
CL2	CHLORINE	N2O	NITROUS-OXIDE
CN	CYANO	NO	NITRIC-OXIDE
CNO	NCO-RADICAL	NO2	NITROGEN-DIOXIDE
CO	CARBON-MONOXIDE	O	OXYGEN-ATOM
CO2	CARBON-DIOXIDE	O2	OXYGEN
COS	CARBONYL-SULFIDE	O2S	SULFUR-DIOXIDE
CS	CARBON-MONOSULFIDE	OS	SULFUR-MONOXIDE
CS2	CARBON-DISULFIDE	S2	SULFUR-DIATOMIC
F	FLUORINE-ATOM	S2	SULFUR-DIATOMIC

Binary Parameters for Activity Coefficient Models

Aspen Plus 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.
Aspen Plus 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.

Table 1.16 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 *Aspen Plus User Guide*, Chapter 31).

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

Aspen Plus contains built-in parameters for the Pitzer and electrolyte NRTL models.

The Pitzer Parameter

Many binary Pitzer model parameters are available in Aspen Plus. 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, Aspen Plus 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 Simulation Engine. They are not displayed on the Properties Parameters forms.

Table 1.17 lists the components and parameters available in the Pitzer databank. An X indicates that a parameter is in the databank; a dash (—) indicates that a parameter is not in the databank.

The Electrolyte NRTL Parameters

Electrolyte NRTL parameters are available in Aspen Plus. 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, Chapter 2, 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.

Table 1.17 The Pitzer Parameter Databank

Cation-cation and Anion-anion Parameters

CATION-CATION PAIRS	θ	$\frac{d\theta}{dT}$	ANION-ANION PAIRS	θ	$\frac{d\theta}{dT}$
CA+2, CO+2	X	—	BR-, OH-	X	—
CS+, BA+2	X	—	CL-,BR-	X	—
H+, LI+	X	—	CL-, OH-	X	—
H+, NA+	X	—	CL-,SO4-2	X	—
H+, K+	X	—	CL-,NO3-	X	—
H+, CS+	X	—	CL-, H2PO4-	X	—
H+, NH4+	X	—			
H+, SR+2	X	—			
H+, BA+2	X	—			
LI+, NA+	X	—			
LI+, K+	X	—			
LI+, CS+	X	—			
MG+2, CA+2	X	—			
NA+, K+	X	—			
NA+, CS+	X	—			
NA+, MG+2	X	—			
NA+, CA+2	X	—			
NA+, BA+2	X	—			
NA+, MN+2	X	—			
NA+, CO+2	X	—			
NA+, CU+2	X	—			
NA+, ZN+2	X	—			
K+, CS+	X	—			
K+, CA+2	X	—			
K+, BA+2	X	—			
NO+, CU+	X	—			

continued

Table 1.17 The Pitzer Parameter Databank (continued)

1-1 Electrolytes

ION1	ION2	$\beta(0)$	$\beta(1)$	C^{θ}	$\frac{d\beta(0)}{dT}$	$\frac{d\beta(1)}{dT}$	$\frac{dC^{\varphi}}{dT}$
H+	CL-	X	X	X	X	X	X
H+	BR-	X	X	X	X	X	X
H+	I-	X	X	X	X	X	X
H+	CLO4-	X	X	X	X	X	X
H+	NO3-	X	X	X	—	—	—
LI+	CL-	X	X	X	X	X	X
LI+	BR-	X	X	X	X	X	X
LI+	I-	X	X	—	—	—	—
LI+	OH-	X	X	—	—	—	—
LI+	CLO4-	X	X	X	X	X	X
LI+	NO2-	X	X	X	—	—	—
LI+	NO3-	X	X	X	—	—	—
NA+	CL-	X	X	X	X	X	X
NA	F-	X	X	—	—	—	—
NA	BR-	X	X	X	X	X	X
NA+	I-	X	X	X	X	X	X
NA+	OH-	X	X	X	X	X	X
NA+	CLO3-	X	X	X	X	X	X
NA+	CLO4-	X	X	X	X	X	X
NA+	BRO3-	X	X	X	X	X	—
NA+	CNS-	X	X	X	X	X	—
NA+	NO2-	X	X	X	—	—	—
NA+	NO3-	X	X	X	X	X	X
NA+	HCO3-	X	X	X	X	X	X
NA+	H2PO4-	X	X	X	—	—	—
NA+	H2ASO4-	X	X	—	—	—	—
NA+	BO2-	X	X	X	—	—	—
NA+	BF4-	X	X	X	—	—	—
K+	F-	X	X	X	X	X	X
K+	CL-	X	X	X	X	X	X
K+	BR-	X	X	X	X	X	X
K+	I-	X	X	X	X	X	X
K+	OH-	X	X	X	—	—	—
K+	CLO3-	X	X	—	X	X	—

continued

Table 1.17 The Pitzer Parameter Databank (continued)

1-1 Electrolytes (continued)

ION1	ION2	$\beta(0)$	$\beta(1)$	C^{θ}	$\frac{d\beta(0)}{dT}$	$\frac{d\beta(1)}{dT}$	$\frac{dC^{\varphi}}{dT}$
K+	BRO3-	X	X	—	—	—	—
K+	CNS-	X	X	X	X	X	X
K+	NO2-	X	X	X	—	—	—
K+	NO3-	X	X	X	X	X	X
K+	H2PO4-	X	X	—	X	X	X
K+	H2ASO4-	X	X	—	—	—	—
K+	PF6-	X	X	—	—	—	—
RB+	F-	X	X	X	X	X	—
RB+	CL-	X	X	X	X	X	—
RB+	BR-	X	X	X	X	X	—
RB+	I-	X	X	X	X	X	—
RB+	NO2-	X	X	X	—	—	—
RB+	NO3-	X	X	X	—	—	—
CS+	F-	X	X	X	X	X	—
CS+	CL-	X	X	X	X	X	X
CS+	BR-	X	X	X	X	X	—
CS+	I-	X	X	X	X	X	—
CS+	OH-	X	X	—	—	—	—
CS+	NO2-	X	X	X	—	—	—
CS+	NO3-	X	X	—	—	—	—
AG+	NO3-	X	X	X	—	—	—
TL+	CLO4-	X	X	—	—	—	—
TL+	NO3-	X	X	—	—	—	—
NH4+	CL-	X	X	X	X	X	X
NH4+	BR-	X	X	X	—	—	—
NH4+	CLO4-	X	X	—	—	—	—
NH4+	NO3-	X	X	X	—	—	—
LI+	CH3COO-	X	X	X	—	—	—
NA+	CHO2-	X	X	X	—	—	—
NA+	CH3COO-	X	X	X	—	—	—
NA+	CH3CH2CHO-	X	X	X	—	—	—
K+	CH3COO-	X	X	X	—	—	—
RB+	CH3COO-	X	X	X	—	—	—
CS+	CH3COO-	X	X	X	—	—	—
TL+	CH3COO-	X	X	X	—	—	—

continued

Table 1.17 The Pitzer Parameter Databank (continued)

2-1 and 1-2 Electrolytes

ION1	ION2	$\beta(0)$	$\beta(1)$	C^{θ}	$\frac{d\beta(0)}{dT}$	$\frac{d\beta(1)}{dT}$	$\frac{dC^{\varphi}}{dT}$
MG+2	BR-	X	X	X	X	X	—
MG+2	I-	X	X	X	—	—	—
MG+2	CLO4-	X	X	X	X	X	—
MG+2	NO3-	X	X	X	X	X	—
CA+2	CL-	X	X	X	X	X	—
CA+2	BR-	X	X	X	X	X	—
CA+2	I-	X	X	X	—	—	—
CA+2	CLO4-	X	X	X	X	X	X
CA+2	NO3-	X	X	X	X	X	—
SR+2	CL-	X	X	X	X	X	—
SR+2	BR-	X	X	X	X	X	—
SR+2	I-	X	X	X	—	—	—
SR+2	CLO4-	X	X	X	X	—	X
SR+2	NO3-	X	X	X	X	X	—
BA+2	CL-	X	X	X	X	X	X
BA+2	BR-	X	X	X	X	X	—
BA+2	I-	X	X	X	—	—	—
BA+2	OH-	X	X	—	—	—	—
BA+2	CLO4-	X	X	X	—	—	—
BA+2	NOs3-	X	X	—	X	X	—
MN+2	CL-	X	X	X	—	—	—
CO+2	CL-	X	X	X	—	—	—
CO+2	BR-	X	X	X	—	—	—
CO+2	I-	X	X	X	—	—	—
CO+2	NO3-	X	X	X	—	—	—
NI+2	CL-	X	X	X	—	—	—
CU+2	CL-	X	X	X	—	—	—
CU+2	NO3-	X	X	X	—	—	—
ZN+2	CL-	X	X	X	—	—	—
ZN+2	BR-	X	X	X	—	—	—
ZN+2	I-	X	X	X	—	—	—

continued

Table 1.17 The Pitzer Parameter Databank (continued)

2-1 and 1-2 Electrolytes (continued)

ION1	ION2	$\beta(0)$	$\beta(1)$	C^{θ}	$\frac{d\beta(0)}{dT}$	$\frac{d\beta(1)}{dT}$	$\frac{dC^{\varphi}}{dT}$
ZN+2	CLO4-	X	X	X	X	X	X
ZN+2	NO3-	X	X	X	—	—	—
CD+2	NO3-	X	X	X	—	—	—
PB+2	CLO4-	X	X	X	—	—	—
PB+2	NO3-	X	X	X	—	—	—
UO2+2	CL-	X	X	X	—	—	—
UO2+2	CLO4-	X	X	X	—	—	—
UO2+2	NO3-	X	X	X	—	—	—
LI+	SO4-2	X	X	X	X	X	X
NA+	SO4-2	X	X	X	X	X	X
NA+	S2O3-2	X	X	X	—	—	—
NA+	CRO4-2	X	X	X	—	—	—
NA+	CO3-2	X	X	X	X	X	X
NA+	HPO4-2	X	X	X	—	—	—
NA+	HASO4-2	X	X	X	—	—	—
K+	SO4-2	X	X	—	X	X	—
K+	CRO4-2	X	X	X	—	—	—
K+	PT(CN)4-2	X	X	X	—	—	—
K+	HPO4-2	X	X	X	—	—	—
K+	HASO4-2	X	X	X	—	—	—
RB+	SO4-2	X	X	—	X	X	—
CS+	SO4-2	X	X	X	X	X	—
NH4+	SO4-2	X	X	X	—	—	—
NA+	FUMARATE-2	X	X	X	—	—	—
NA+	MALEATE-2	X	X	X	—	—	—

continued

Table 1.17 The Pitzer Parameter Databank (continued)

3-1 and 1-3 Electrolytes

ION1	ION2						
AL+3	CL-	X	X	X	—	—	—
SR+3	CL-	X	X	X	—	—	—
Y+3	CL-	X	X	X	—	—	—
LA+3	CL-	X	X	X	X	X	X
CE+3	CL-	X	X	X	—	—	—
PR+3	CL-	X	X	X	—	—	—
ND+3	CL-	X	X	X	—	—	—
SM+3	CL-	X	X	X	—	—	—
EU+3	CL-	X	X	X	—	—	—
GD+3	CL-	X	X	X	—	—	—
TB+3	CL-	X	X	X	—	—	—
DY+3	CL-	X	X	X	—	—	—
HO+3	CL-	X	X	X	—	—	—
ER+3	CL-	X	X	X	—	—	—
TM+3	CL-	X	X	X	—	—	—
YB+3	CL-	X	X	X	—	—	—
LU+3	CL-	X	X	X	—	—	—
CR+3	CL-	X	X	X	—	—	—
CR+3	NO3-	X	X	X	—	—	—
GA+3	CLO4-	X	X	X	—	—	—
IN+3	CL-	X	X	—	—	—	—
LA+3	NO3-	X	X	X	X	X	X
PR+3	NO3-	X	X	X	—	—	—
SM+3	NO3-	X	X	X	—	—	—
GD+3	NO3-	X	X	X	—	—	—
TB+3	NO3-	X	X	X	—	—	—
ER+3	NO3-	X	X	X	—	—	—
TR+3	NO3-	X	X	X	—	—	—
YB+3	NO3-	X	X	X	—	—	—
LA+3	CLO4-	X	X	X	X	X	X
PR+3	CLO4-	X	X	X	—	—	—
ND+3	CLO4-	X	X	X	—	—	—
SM+3	CLO4-	X	X	X	—	—	—
GD+3	CLO4-	X	X	X	—	—	—

continued

Table 1.17 The Pitzer Parameter Databank (continued)

3-1 and 1-3 Electrolytes (continued)

ION1	ION2						
TB+3	CLO4-	X	X	X	—		—
DY+3	CLO4-	X	X	X	—	—	—
HO+3	CLO4-	X	X	X	—	—	—
ER+3	CLO4-	X	X	X	—	—	—
TM+3	CLO4-	X	X	X	—	—	—
YB+3	CLO4-	X	X	X	—	—	—
LU+3	CLO4-	X	X	X	—	—	—
NA+	PO4-3	X	X	X	—	—	—
NA+	ASO4-3	X	X	X	—	—	—
K+	PO4-3	X	X	X	—	—	—
K+	P3O9-3	X	X	X	—	—	—
K+	ASO4-3	X	X	X	—	—	—
K+	FE(CN)6-3	X	X	X	X	X	—
K+	CO(CN)6-3	X	X	X	—	—	—

4-1 and 5-1 Electrolytes

ION1	ION2						
TH+4	CL-	X	X	X	—	—	—
TH+4	NO3-	X	X	X	—	—	—
NA+	P2O7-4	X	X	—	—	—	—
K+	P2O7-4	X	X	X	—	—	—
K+	FE(CN)6-4	X	X	X	X	X	—
K+	MO(CN)8-4	X	X	X	—	—	—
K+	W(CN)8-4	X	X	X	—	—	—
K+	P3O10-5	X	X	X	—	—	—
NA+	P3O10-5	X	X	X	—	—	—

continued

Table 1.17 The Pitzer Parameter Databank (continued)

2-2 Electrolytes

ION1	ION2	$\beta(0)$	$\beta(2)$	$\beta(3)$	C^{φ}	$\frac{D\beta(0)}{DT}$	$\frac{d\beta(2)}{DT}$	$\frac{d\beta(3)}{DT}$	$\frac{DC^{\varphi}}{DT}$
MG+2	SO4-2	X	X	X	X	X	X	X	X
NI+2	SO4-2	X	X	X	X	—	—	—	—
CU+2	SO4-2	X	X	X	X	X	X	X	X
ZN+2	SO4-2	X	X	X	X	X	X	X	X
CD+2	SO4-2	X	X	X	X	X	X	X	X
CO+2	SO4-2	X	X	X	—	—	—	—	—
CA+2	SO4-2	X	X	X	—	—	X	X	—
BE+2	SO4-2	X	X	X	X	—	—	—	—
MN+2	SO4-2	X	X	X	X	—	—	—	—
UO2+2	SO4-2	X	X	X	X	—	—	—	—

References

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

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2 Electrolytes Data

Aspen Plus provides extensive built-in parameters for the electrolyte NRTL model. These parameters were developed using data for over 30 industrially important electrolytic systems. This chapter 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 (<—>)
- Complete dissociation reaction indicated by an arrow (—>)
- Salt precipitation reaction indicated by a two way arrow (<—>). 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 Aspen Plus

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
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

continued

Table 2.1 Electrolytes Data Available in Aspen Plus (continued)

System	Apparent Components
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, HBr, 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:

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$H_2S + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HS^-$$

$$HS^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + S^{-2}$$

$$CO_2 + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + CO_3^{-2}$$

$$AMP^+ + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + AMP$$

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:

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$CO_2 + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + CO_3^{-2}$$

$$NH_3 + H_2O \quad <\!\!-\!\!> \quad NH_4^+ + OH^-$$

$$NH_3 + HCO_3^- \quad <\!\!-\!\!> \quad NH_2CO_2^- + H_2O$$

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:

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$H_2O + NH_3 \quad <\!\!-\!\!> \quad NH_4^+ + OH^-$$

$$HCN + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + CN^-$$

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:

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$NH_3 + H_2O \quad <\!\!-\!\!> \quad NH_4^+ + OH^-$$

$$H_2S + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HS^-$$

$$HS^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + S^{-2}$$

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:

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$H_2O + NH_3 \quad <\!\!-\!\!> \quad NH_4^+ + OH^-$$

$$H_2S + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HS^-$$

$$HS^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + S^{-2}$$

$$H_3PO_4 + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + H_2PO_4^-$$

$$H_2PO_4^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HPO_4^{-2}$$

$$HPO_4^{-2} + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + PO_4^{-3}$$

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:

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$H_2O + NH_3 \quad <\!\!-\!\!> \quad NH_4^+ + OH^-$$

$$SO_2 + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HSO_3^-$$

$$HSO_3^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + SO_3^{-2}$$

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:

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$H_2O + NH_3 \quad <\!\!-\!\!> \quad NH_4^+ + OH^-$$

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:

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$H_2S + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HS^-$$

$HS^- + H_2O$	<—>	$H_3O^+ + S^{-2}$
$2H_2O + CO_2$	<—>	$H_3O^+ + HCO_3^-$
$HCO_3^- + H_2O$	<—>	$H_3O^+ + CO_3^{-2}$
$NaCL$	<—>	$Na^+ + Cl^-$
$NaCL(s)$	<—>	$Na^+ + Cl^-$

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:

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

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:

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$2H_2O + Cl_2 \quad <\!\!-\!\!> \quad H_3O^+ + Cl^- + HClO$$

$$HClO + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + ClO^-$$

$$HCl + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + Cl^-$$

Range of Applicability

Temperature 0 – 100ºC

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:

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

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:

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$H_2S + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HS^-$$

$HS^- + H_2O$ <—> $H_3O^+ + S^{-2}$

$2H_2O + CO_2$ <—> $H_3O^+ + HCO_3^-$

$HCO_3^- + H_2O$ <—> $H_3O^+ + CO_3^{-2}$

$DEA^+ + H_2O$ <—> $DEA + H_3O^+$

$DEACOO^- + H_2O$ <—> $DEA + HCO_3^-$

Range of Applicability

Temperatures	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:

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$DGA + 2H_2O \quad <\!\!-\!\!> \quad DGA^+ + OH^-$$

$$H_2S + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HS^-$$

$$HS^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + S^{-2}$$

$$CO_2 + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + CO_3^{-2}$$

$$HCO_3^- + DGA \quad <\!\!-\!\!> \quad H_2O + DGACOO^-$$

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, SO_2, SO_3, CO, CO_2, NO, NO_2, 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 and $Ca(OH)_2$. Henry's law is used for SO_2, CO, CO_2, NO, N_2, O_2, 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:

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$CO_2 + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + CO_3^{-2}$$

$$SO_3 + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HSO_4^-$$

$$H_2O + H_2SO_4 \quad <\!\!-\!\!> \quad H_3O^+ + HSO_4^-$$

$$H_2O + HSO_4^- \quad <\!\!-\!\!> \quad H_3O^+ + SO_4^{-2}$$

$$HCl + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + Cl^-$$

$$H_2O + HF \quad <\!\!-\!\!> \quad H_3O^+ + F^-$$

$$H_2O + HNO_3 \quad <\!\!-\!\!> \quad H_3O^+ + NO_3^-$$

$$H_2O + HNO_2 \quad <\!\!-\!\!> \quad H_3O^+ + NO_2^-$$

$$SO_2 + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HSO_3^-$$

$$HSO_3^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + SO_3^{-2}$$

$$SeO_2 + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HSeO_3^-$$

$$HSeO_3^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + SeO_3^{-2}$$

$$H_2SeO_3 + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HSeO_3^-$$

$$Hg^{+2} + Hg \quad <\!\!-\!\!> \quad Hg_2^{+2}$$

$Hg^{+2} + 2H_2O$ <—> $H_3O^+ + Hg(OH)^+$

$Hg(OH)^+ + 2H_2O$ <—> $H_3O^+ + Hg(OH)_2$

$Hg^{+2} + Cl^-$ <—> $HgCl^+$

$HgCl^+ + Cl^-$ <—> $HgCl_2$

$HgCl_2 + Cl^-$ <—> $HgCl_3^-$

$NO + NO_2 + H_2O$ <—> $2HNO_2$

$HgCl_2 + 3H_2O + 0.5C$ <—> $Hg + 2Cl^- + 2H_3O^+ + 0.5CO_2$

$SO_2 + 2H_2O + 0.5SeO_2$ <—> $HSO_4^- + H_3O^+ + 0.5Se$

$SO_2 + NO_2$ <—> $SO_3 + NO$

$SO_2 + 0.5O_2$ <—> SO_3

$SO_2 + NO_2$ <—> $SO_3 + NO$

$Ca(OH)^+$ <—> $Ca^{+2} + OH^-$

$2NO_2 + 0.5O_2 + H_2O$ <—> $2HNO_3$

$CaO + H_2O$ <—> $Ca(OH)^+ + OH^-$

$HgCl_2 + 5H_2O + SO_2$ <—> $Hg + 2Cl^- + 3H_3O^+ + HSO_4^-$

Hg_2Cl_2 <—> $Hg_2^{+2} + 2Cl^-$

$HgCl_2(s)$ <—> $HgCl^+ + Cl^-$

$CaSO_4*2H_2O(s)$ <—> $Ca^{+2} + SO_4^{-2} + 2H_2O$

$CaF_2(s)$ <—> $Ca^{+2} + 2F^-$

$Ca(OH)_2(s)$ <—> $Ca(OH)^+ + OH^-$

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 CO_2 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:

$$K_2CO_3 \quad <\!\!-\!\!> \quad 2K^+ + CO_3^{-2}$$

$$KHCO_3 \quad <\!\!-\!\!> \quad K^+ + HCO_3^-$$

$$CO_2 + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + CO_3^{-2}$$

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$K_2CO_3(s) \quad <\!\!-\!\!> \quad 2K^+ + HCO_3^-$$

$$KHCO_3(s) \quad <\!\!-\!\!> \quad K^+ + HCO_3^-$$

Range of Applicability

Temperature	70 – 140ºC
Pressure	up to approximately 150 psia
K_2CO_3 concentration	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:

$2H_2O$	<—>	$H_3O^+ + OH^-$
$CO_2 + H_2O$	<—>	$H_3O^+ + HCO_3^-$
$HCO_3^- + H_2O$	<—>	$H_3O^+ + CO_3^{-2}$
$DEA^+ + H_2O$	<—>	$DEA + H_3O^+$
$DEACOO^- + H_2O$	<—>	$DEA + HCO_3^-$
K_2CO_3	<—>	$2K^+ + CO_3^{-2}$
$KHCO_3$	<—>	$K^+ + HCO_3^-$

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:

$$HBr + H_2O \quad <\!\!-\!\!> \quad HBr + H_2O$$

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:

$$HCl + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + Cl^-$$

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:

$$H_2O + HCl \quad <\!\!-\!\!> \quad H_3O^+ + Cl^-$$

$$MgCl_2 \quad <\!\!-\!\!> \quad Mg^{+2} + 2Cl^-$$

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.

A. 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:

$$H_2O + HF \quad <\!\!-\!\!> \quad H_3O^+ + F^-$$

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:

$$HI + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + I^-$$

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:

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$H_2S + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HS^-$$

$$HS^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + S^{-2}$$

$$CO_2 + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + CO_3^{-2}$$

$$MDEA^+ + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + MDEA$$

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:

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$H_2S + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HS^-$$

$$HS^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + S^{-2}$$

$$CO_2 + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + CO_3^{-2}$$

$$MEA^+ + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + MEA$$

$$MEACOO^- + H_2O \quad <\!\!-\!\!> \quad HCO_3^- + MEA$$

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:

$$H_2O + HNO_3 \quad <\!\!-\!\!> \quad H_3O^+ + NO_3^-$$

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_3 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).

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:

$KOH \quad <\!\!-\!\!> \quad K^+ + OH^-$

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:

$$NaOH \quad <\!\!-\!\!> \quad Na^{+} + OH^{-}$$

Range of Applicability

Temperature	0 – 200ºC
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 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:

$2H_2O$	<—>	$H_3O^+ + OH^-$
$2H_2O + SO_2$	<—>	$H_3O^+ + HSO_3^-$
$HSO_3^- + H_2O$	<—>	$H_3O^+ + SO_3^{-2}$
$NaOH$	<—>	$Na^+ + OH^-$

Range of Applicability

Temperature	35 – 90ºC
NaOH concentration	up to 8 molal
SO_2 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 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 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 shown below.

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$H_2S + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HS^-$$

$$HS^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + S^{-2}$$

$$CO_2 + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + CO_3^{-2}$$

$$NH_3 + H_2O \quad <\!\!-\!\!> \quad NH_4^+ + OH^-$$

$$NH_3 + HCO_3^- \quad <\!\!-\!\!> \quad NH_2CO_2^- + H_2O$$

Range of Applicability

Temperature	0 – 120°C
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:

$$2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + OH^-$$

$$H_2S + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HS^-$$

$$HS^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + S^{-2}$$

$$CO_2 + 2H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HCO_3^-$$

$$HCO_3^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + CO_3^{-2}$$

$$NH_3 + H_2O \quad <\!\!-\!\!> \quad NH_4^+ + OH^-$$

$$NH_3 + HCO_3^- \quad <\!\!-\!\!> \quad NH_2CO_2^- + H_2O$$

$$NaOH \quad <\!\!-\!\!> \quad NA^+ + OH^-$$

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 H_2O-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:

$$H_2O + H_2SO_4 \quad <\!\!-\!\!> \quad H_3O^+ + HSO_4^-$$

$$H_2O + HSO_4^- \quad <\!\!-\!\!> \quad H_3O^+ + SO_4^{-2}$$

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 + H_2SO_4

Solution Chemistry

The aqueous phase reactions considered in this system are:

$$H_2SO_4 + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + HSO_4^-$$

$$HSO_4^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + SO_4^{-2}$$

$$HBr + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + Br^-$$

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:

$$H_2O + H_2SO_4 \quad <\!\!-\!\!> \quad H_3O^+ + HSO_4^-$$

$$HSO_4^- + H_2O \quad <\!\!-\!\!> \quad H_3O^+ + SO_4^{-2}$$

$$H_2O + HCl \quad <\!\!-\!\!> \quad H_3O^+ + Cl^-$$

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.

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3 Group Contribution Method Functional Groups

The tables in this chapter list the groups for each of the group contribution methods available in Aspen Plus.

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.

UNIFAC Functional Groups

Tables 3.12 and 3.13 list the UNIFAC groups built into Aspen Plus. 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.

Tables 3.14 through 3.19 indicate the main groups for which group interaction parameters are available for the various UNIFAC models.

Groups within a main group have the same interaction parameter values. An X is used to indicate that the parameter is available. A dash (–) indicates that the parameter is not available.

For compatibility with earlier releases of Aspen Plus, the UNIFAC group interaction parameters, revisions 3 and 4, have been retained. They are listed in Tables 3.18 and 3.19. To use these parameters, you must modify the UNIFAC option set. Select the GMUFR3 or GMUFR4 model on the properties Option-Sets.Model form.

Table 3.1 Ambrose Method Functional Groups

Functional Group †	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 ††	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, -OH3 †††	127

† *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.*

†† *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.*

††† *Includes naphthenic alcohols and glycols, but not aromatic alcohols, such as xylenol.*

continued

Table 3.1 Ambrose Method Functional Groups (continued)

Functional Group †	Group Number
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

† *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.*

†† *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.*

††† *Includes naphthenic alcohols and glycols, but not aromatic alcohols, such as xylenol.*

Table 3.1 Ambrose Method Functional Groups (continued)

Functional Group †	Group Number
Silicon	
>Sl<	153
>SlH-	154
-Sl-O-	155
-Sl-O-(ring)	156

† *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.*

†† *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.*

††† *Includes naphthenic alcohols and glycols, but not aromatic alcohols, such as xylenol.*

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 †	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) ††	132

† *CD represents a carbon atom joined to another carbon atom by a double bond.*

†† *CT represents a carbon atom joined to another carbon atom by a triple bond.*

continued

Table 3.2 Benson Method Functional Groups (continued)

Functional Group	Group Number
Hydrocarbon Groups	
CT-(C)	133
CT-(CD)	134
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
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

††† *CB represents a carbon atom in an aromatic ring.*

‡ *CA represents the central carbon atom of an allene group, >C=C=C<. The end carbons are treated as normal CD atoms.*

‡‡ *CBF represents a carbon atom at the border of two or three fused aromatic rings.*

continued

Table 3.2 Benson Method Functional Groups (continued)

Functional Group	Group Number
Oxygen-Containing Compounds	
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

continued

Table 3.2 Benson Method Functional Groups (continued)

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
Nitrogen-Containing Compounds	
C-(N)(H)3	229

continued

Table 3.2 Benson Method Functional Groups (continued)

Functional Group	Group Number
Nitrogen-Containing Compounds	
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) ‡‡‡	240
NI-(C)	241
NI-(CB)	242
NA-(H) §	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

‡‡‡ *NI represents a double-bonded nitrogen in imines; NI-(CB) represents a pyridine nitrogen.*

§ *NA represents a double-bonded nitrogen in azo compounds.*

continued

Table 3.2 Benson Method Functional Groups (continued)

Functional Group	Group Number
Nitrogen-Containing Compounds	
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
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
Halogen Groups	
C-(CL)(H)(C)2	292
C-(CL)(C)3	293
C-(BR)3(C)	294
C-(BR)(H)2(C)	295

continued

Table 3.2 Benson Method Functional Groups (continued)

Functional Group	Group Number
Halogen Groups	
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
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

continued

Table 3.2 Benson Method Functional Groups (continued)

Functional Group	Group Number
Halogen Groups	
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) §§	337
Cis (halogen)(halogen) §§	338
Cis (alkane)(halogen) §§	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

§§ *Halogen refers to CL, BR, and I.*

continued

Table 3.2 Benson Method Functional Groups (continued)

Functional Group	Group Number
Organosulfur Groups	
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
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

continued

Table 3.2 Benson Method Functional Groups (continued)

Functional Group	Group Number
Ring Corrections for Sulfur-Containing Compounds	
Thiophene	399
Symmetry and Optical Isomers Corrections §§§	
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
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

§§§ *Required to estimate absolute entropy, which is used to estimate standard Gibbs free energy of formation.*

continued

Table 3.2 Benson Method Functional Groups (continued)

Functional Group	Group Number
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
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

Table 3.2 Benson Method Functional Groups (continued)

Functional Group	Group Number
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
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 †	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) ††	132

† *CD represents a carbon atom joined to another carbon atom by a double bond.*

†† *CT represents a carbon atom joined to another carbon atom by a triple bond.*

continued

Table 3.2A BensonR8 Method Functional Groups (continued)

Functional Group	Group Number
Hydrocarbon Groups	
CT-(C)	133
CT-(CD)	134
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
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

††† *CB represents a carbon atom in an aromatic ring.*

‡ *CA represents the central carbon atom of an allene group, >C=C=C<. The end carbons are treated as normal CD atoms.*

‡‡ *CBF represents a carbon atom at the border of two or three fused aromatic rings.*

continued

Table 3.2A BensonR8 Method Functional Groups (continued)

Functional Group	Group Number
Oxygen-Containing Compounds	
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

continued

Table 3.2A BensonR8 Method Functional Groups (continued)

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
Nitrogen-Containing Compounds	
C-(N)(H)3	229

continued

Table 3.2A BensonR8 Method Functional Groups (continued)

Functional Group	Group Number
Nitrogen-Containing Compounds	
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) ‡‡‡	240
NI-(C)	241
NI-(CB)	242
NA-(H) §	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

‡‡‡ *NI represents a double-bonded nitrogen in imines; NI-(CB) represents a pyridine nitrogen.*

§ *NA represents a double-bonded nitrogen in azo compounds.*

continued

Table 3.2A BensonR8 Method Functional Groups (continued)

Functional Group	Group Number
Nitrogen-Containing Compounds	
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
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
Halogen Groups	
C-(CL)(H)(C)2	292
C-(CL)(C)3	293
C-(BR)3(C)	294
C-(BR)(H)2(C)	295

continued

Table 3.2A BensonR8 Method Functional Groups (continued)

Functional Group	Group Number
Halogen Groups	
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
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

continued

Table 3.2A BensonR8 Method Functional Groups (continued)

Functional Group	Group Number
Halogen Groups	
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) §§	337
Cis (halogen)(halogen) §§	338
Cis (alkane)(halogen) §§	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

§§ *Halogen refers to CL, BR, and I.*

continued

Table 3.2A BensonR8 Method Functional Groups (continued)

Functional Group	Group Number
Organosulfur Groups	
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
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

continued

Table 3.2A BensonR8 Method Functional Groups (continued)

Functional Group	Group Number
Ring Corrections for Sulfur-Containing Compounds	
Thiophene	399
Symmetry and Optical Isomers Corrections §§§	
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
SYMMETRY	405
OPTICAL-ISOMER	406

§§§ *Required to estimate absolute entropy, which is used to estimate standard Gibbs free energy of formation.*

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
O=CH- (aldehyde)	125
-COO- (ester)	126
Sulfur Increments	
-S- (aliphatic)	127
Sulfur Increments	
-S- (hetero, aromatic)	128
2-Thiophenyl	129
3-Thiophenyl	130
-S-S- (aliphatic)	131
-SH	132

continued

Table 3.3 Bondi Method Functional Groups (continued)

Functional Group	Group Number
Sulfur Increments	
>S=O (aliphatic)	133
>SO2 (aliphatic)	134
-O-SO2-O- (aliphatic)	135
Halogen Increments	
-F (aliphatic) †	136
-F (aromatic)	137
-F (other)	138
-CL (aliphatic) †	139
-CL (aromatic, per)	140
-CL (aromatic, mono, di, tri)	141
-CL (other)	142
-BR (aliphatic) †	143
-BR (aromatic)	144
-BR (other)	145
-I (aliphatic) †	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

† *Substitution on 1, normal-aliphatic.*

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

continued

Table 3.3A Ducros Method Functional Groups (continued)

Functional Group	Group Number
Cyclopentadiene	149
Cyclohexane	150
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
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

continued

Table 3.3A Ducros Method Functional Groups (continued)

Functional Group	Group Number
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
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

Table 3.3A Ducros Method Functional Groups (continued)

Functional Group	Group Number
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
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

Table 3.3A Ducros Method Functional Groups (continued)

Functional Group	Group Number
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
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

Table 3.3A Ducros Method Functional Groups (continued)

Functional Group	Group Number
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
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

Table 3.3A Ducros Method Functional Groups (continued)

Functional Group	Group Number
C-(C)(H)2(HG)	705
C-(C)2(H)(HG)	706
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
Phosphorus Groups	
P-(C)3	739

Table 3.3A Ducros Method Functional Groups (continued)

Functional Group	Group Number
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 †	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
-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

† *For adjacent pairs of >CH-, use group 152.*

continued

Table 3.4 Fedors Method Functional Groups (continued)

Functional Group	Group Number
Halogen Increments	
-F ††	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
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

† *For adjacent pairs of >CH-, use group 152.*

†† *For -F substitution on nonaromatic C=C, use group 153.*

Table 3.4A Gani Method Functional Groups

Functional Group	Group Number
The First-Order Groups	
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
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

continued

Table 3.4A Gani Method Functional Groups (continued)

Functional Group	Group Number
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
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

continued

Table 3.4A Gani Method Functional Groups (continued)

Functional Group	Group Number
-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	
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
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

continued

Table 3.4A Gani Method Functional Groups (continued)

Functional Group	Group Number
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
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

continued

Table 3.4A Gani Method Functional Groups (continued)

Functional Group	Group Number
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
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

continued

Table 3.4A Gani Method Functional Groups (continued)

Functional Group	Group Number
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
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

continued

Table 3.4A Gani Method Functional Groups (continued)

Functional Group	Group Number
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
=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

continued

Table 3.5 Joback Method Functional Groups (continued)

Functional Group	Group Number
>NH (nonring	130
>NH (ring)	131
>N- (nonring)	132
-CN	133
-NO2	134
-N= (nonring) †	135
-N= (ring)	136
=NH	137
Sulfur Increments	
-SH	138
-S- (nonring)	139
-S- (ring)	140

† *The contributions for VC, DGFORM, and CPIG are missing.*

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
-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

continued

Table 3.6A Li-Ma Method Functional Groups (continued)

Functional Group	Group Number
-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
>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

continued

Table 3.6A Li-Ma Method Functional Groups (continued)

Functional Group	Group Number
=CHCL	180
=CHBR	181
-CF2- (ring)	188
>CF- (ring)	189
-CFH- (ring)	190
-CHCL- (ring)	191
-CHBR- (ring)	192
-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

continued

Table 3.6A Li-Ma Method Functional Groups (continued)

Functional Group	Group Number
=CH- (connect benzene ring)	182
=CH- (connect ring)	183
=C=	184
=CH2	185
=CH-	186
=C<	187
-CH3 (connect naphthalene ring)	201
-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
Ring Increments	
>CH2	110
>CH-	111
>CH †	112
Ring Increments	
>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

† *This >CH- group represents a carbon atom common to two condensed saturated rings.*

continued

Table 3.7 Lydersen Method Functional Groups (continued)

Functional Group	Group Number
Oxygen Increments	
-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
Sulfur Increments	
-S- (ring)	140
=S	141
Other Increments	
>SI<[††]	142
>B-[†† †††]	143
>SIH-	144
>SIH3	145
-SI-O-	146
-SI-O- (ring)	147

†† *The contribution for VC is missing for groups 142, >Si< and 143, >B-.*

††† *The contribution for PC is missing for group 143, >B-.*

Table 3.7A Mostafa Method Functional Groups

Functional Group	Group Number
Cations	
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
Cs+1	1055
Cu+1	1056

continued

Table 3.7A Mostafa Method Functional Groups (continued)

Functional Group	Group Number
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

continued

Table 3.7A Mostafa Method Functional Groups (continued)

Functional Group	Group Number
Mg+2	1108
Mn+2	1110
Mn+3	1111
Mn+4	1112
Mn+5	1113
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

continued

Table 3.7A Mostafa Method Functional Groups (continued)

Functional Group	Group Number
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
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

continued

Table 3.7A Mostafa Method Functional Groups (continued)

Functional Group	Group Number
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
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

continued

Table 3.7A Mostafa Method Functional Groups (continued)

Functional Group	Group Number
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
Th+2	1286
Er+2	1287
CH2+2	1727
Anions	
As-3	1301
Br-1	1303
C-4	1304

continued

Table 3.7A Mostafa Method Functional Groups (continued)

Functional Group	Group Number
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
H2PO2-1	1619

continued

Table 3.7A Mostafa Method Functional Groups (continued)

Functional Group	Group Number
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 †	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
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	

† *R represents radicals, such as Methyl. Groups 140 through 159 are valid radical types.*

continued

Table 3.8 Ogata-Tsuchida Method Functional Groups (continued)

Functional Group	Group Number	Radical, R, showing deviations >5K
RCOOH	129	
RCOOMe	130	
RCOOEt	131	
RCOOPr	132	
RCOOPh	133	
(RCO)20	134	Hep
CLCH2COOR †	135	
CL2CHCOOR	136	
BRCH2COOR	137	
NCCH2COOR	138	
CH2=CHCOOR	139	
Radical Type		
METHYL	140	
ETHYL	141	
N-PROPYL	142	
ISOPROPYL	143	
N-BUTYL	144	
SEC-BUTYL	145	
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	

† *R represents radicals, such as Methyl. Groups 140 through 159 are valid radical types.*

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

continued

Table 3.10 Parachor Method Functional Groups (continued)

Functional Group	Group Number
Alkyl Groups	
CH3-CH2-CH(C2H5)-	130
CH3-C(CH3)2-	131
CH3-CH2-C(CH3)2-	132
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
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
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

continued

Table 3.11A Ruzicka Method Functional Groups (continued)

Functional Group	Group Number
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
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

continued

Table 3.11A Ruzicka Method Functional Groups (continued)

Functional Group	Group Number
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
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

continued

Table 3.11A Ruzicka Method Functional Groups (continued)

Functional Group	Group Number
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
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

continued

Table 3.11A Ruzicka Method Functional Groups (continued)

Functional Group	Group Number
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
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

continued

Table 3.11A Ruzicka Method Functional Groups (continued)

Functional Group	Group Number
Thiacyclohexane	395
Thiophene	399

Table 3.12 UNIFAC Method Functional Groups

Main Group	Group	V-L	L-L	LBY †	DMD< ††	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 †††	—	—	—	X	1025	1,1 -	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 ‡	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) ‡‡	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

† *Lyngby modified UNIFAC model.*

†† *Dortmund modified UNIFAC model.*

continued

Table 3.12 UNIFAC Method Functional Groups (continued)

Main Group	Group	V-L	L-L	LBY †	DMD ††	Group Number	Example Component	Example Component Constituent Groups
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
	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 ‡‡‡	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-CH_2O CH_2 †††	—	—	—	X	1620	Tetrahydrofuran	2 c-CH_2, 1 c-CH_2OCH_2
	c-CH_2O $(CH2)^1/_2$	—	—	—	X	1625	1,3 - dioxane	1 c-CH2, 2 c-$CH2O(CH2)^1/_2$
	c-$(CH_2)^1/_2O(CH2)^1/_2$	—	—	—	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
NH_2	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

† *Lyngby modified UNIFAC model.*

†† *Dortmund modified UNIFAC model.*

††† *c denotes cyclic functional group.*

‡‡‡ *FCH2O denotes CH2-O group in a furan ring.*

continued

Table 3.12 UNIFAC Method Functional Groups (continued)

Main Group	Group	V-L	L-L	LBY †	DMD ††	Group Number	Example Component	Example Component Constituent Groups
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
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

† *Lyngby modified UNIFAC model.*

†† *Dortmund modified UNIFAC model.*

continued

Table 3.12 UNIFAC Method Functional Groups (continued)

Main Group	Group	V-L	L-L	LBY †	DMD ††	Group Number	Example Component	Example Component Constituent Groups
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

† *Lyngby modified UNIFAC model.*

†† *Dortmund modified UNIFAC model.*

continued

Table 3.12 UNIFAC Method Functional Groups (continued)

Main Group	Group	V-L	L-L	LBY †	DMD ††	Group Number	Example Component	Example Component Constituent Groups
COO	COO	X	—	—	X	3300	Dimethyl oxalate	2 CH3, 2 COO
SiH2	Si	X	—	—	—	3350	Hexamethyldisiloxane	6 CH3, 1 SiO, 1 Si
	SiH	X	—	—	—	3355	Heptamethyltrisiloxane	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	Octamethylcyclotetrasiloxane	8 CH3, 4 SiO
	SiHO	X	—	—	—	3405	1,1,3,3-Tetramethyl-	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	Trichlorofluoromethane	1 CCl3F
	CCl2F	X	—	—	—	3505	Tetrachloro-1,2-	2 CCl2F
	HCCl2F	X	—	—	—	3510	Dichlorofluoromethane	1 HCCl2F
	HCClF	X	—	—	—	3515	1-Chloro-1,2,2,2,-	1 CF3, 1HCClF
	CClF2	X	—	—	—	3520	1,2 Dichlorotetrafluoroethane	2 HCClF2
	HCClF2	X	—	—	—	3525	Chlorodifluoromethane	1 HCCl2F
	CClF3	X	—	—	—	3530	Chlorotrifluoromethane	1 CClF3
	CCl2F2	X	—	—	—	3535	Dichlorodifluoromethane	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-Methylethylacetamid	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
	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

† *Lyngby modified UNIFAC model.*

†† *Dortmund modified UNIFAC model.*

continued

Table 3.12 UNIFAC Method Functional Groups (continued)

Main Group	Group	V-L	L-L	LBY †	DMD ††	Group Number	Example Component	Example Component Constituent Groups
	CHS	X	—	—	—	3660	Diisopropylsulfide	4 CH3, 1 CH, 1 CHS
Morpholine	MORPH	X	—	—	—	3700	Morpholine	1 MORPH
Thiophene	C_4H_4S	X	—	—	—	3750	Thiophene	1 C4H4S
	C_4H_3S	X	—	—	—	3755	2 - Methylthiophene	1 CH3, 1 C4H3S
	C_4H_2S	X	—	—	—	3760	2,3 - Dimethylthiophene	2 CH3, 1 C4H2S
NH3 §	NH3	—	—	X	X	3800	Ammonia	1 NH3
H2 §	H2	—	—	X	X	3810	Hydrogen	1 H2
N2 §	N2	—	—	X	X	3820	Nitrogen	1 N2
O2 §	O2	—	—	X	X	3830	Oxygen	1 O2
CO §	CO	—	—	X	X	3840	Carbon monoxide	1 CO
CO2 §	CO2	—	—	X	X	3850	Carbon dioxide	1 CO2
H2S §	H2S	—	—	X	X	3860	Hydrogen sulfide	1 H2S
AR §	AR	—	—	X	X	3870	Argon	1 AR
C2H6 §§	C2H6	—	—	X	—	3880	Ethane	1 C2H6
C3H6 §§	C3H6	—	—	X	—	3890	Propylene	1 C3H6
C3H8 §§	C3H8	—	—	X	—	3900	Propane	1 C3H8
C4H10 §§	C4H10	—	—	X	—	3910	n-Butane	1 C4H10

† *Lyngby modified UNIFAC model.*

†† *Dortmund modified UNIFAC model.*

§ *Functional groups used in Henry's Law application and in PSRK and RKSMHV2 equations of state.*

§§ *Functional groups used in the Lyngby modified UNIFAC model used in the RKSMHV2 equation of state option set.*

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 †

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	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	X																																										
CHO	X	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	-	-	-	-	-	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	-	-																																		
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	-	-	-	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																										
CH2NO2	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	-	-	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	-	X	-	-	-	-	-	-	-																						
FURFURAL	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	-	-	-	-																				
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	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	-	X	-																

continued

† *H. K. Hansen, P. Rasmussen, Aa. Fredenslund, M. Schiller, and J. Gmehling, Ind. Eng. Chem. Res.30 (10), (1991), p. 2352.*

Table 3.14 Vapor-Liquid Systems UNIFAC Group Interaction Parameters † (continued)

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
ACRYLONI	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	-
CF2	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
SIH2	X	-	X	-	X	-	X	-	X	-	-	-	X	X	X	-	-	-	-	-	-	-	-	-	-
SIO	X	-	X	-	-	-	-	-	-	-	-	-	-	X	X	-	-	-	-	-	-	-	-	X	-
NMP	X	X	X	X	X	-	X	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	-	X
CCLF	X	-	X	-	X	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
CON	X	X	-	-	X	-	X	-	-	-	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-
OCCOH	X	X	X	X	X	-	X	-	X	-	X	-	-	-	-	-	-	-	X	-	-	X	-	X	X
CH4S	X	X	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	X	-
MORPHOLI	X	X	X	X	X	X	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
THIOPHEN	X	-	X	X	X	X	-	X	X	-	-	-	-	-	-	-	-	X	-	-	-	-	-	X	-

MAIN GROUP	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
ACRYLONI	-	-	-	-	-	-	-	-	-	-															
CL(C=C)	X	-	X	-	-	-	-	-	X	-	X														
ACF	-	-	-	-	-	-	-	-	-	-	-	-													
DMF	X	-	-	X	-	X	-	-	X	X	X	X	-												
CF2	-	-	-	-	-	-	-	-	-	-	-	-	X	X											
COO	X	-	X	-	X	X	X	X	-	X	X	X	-	X	-										
SIH2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-									
SIO	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X								
NMP	-	-	-	X	-	X	-	-	-	-	-	X	-	-	-	-	-	-							
CCLF	X	-	-	-	-	-	-	-	-	-	-	-	-	-	X	-	-	-	-						
CON	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-					
OCCOH	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-				
CH4S	-	-	-	X	-	-	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-			
MORPHOLI	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-		
THIOPHEN	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	

† *H. K. Hansen, P. Rasmussen, Aa. Fredenslund, M. Schiller, and J. Gmehling, Ind. Eng. Chem. Res.30 (10), (1991), p. 2352.*

Table 3.15 Liquid-Liquid Systems UNIFAC Group Interaction Parameters[†]

MAIN GROUP	CH*	CH*=CH*	ACH*	ACCH*	OH	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																	
CH*CL2	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													
CH*NO2	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	-	-	-										
(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	-	-	-						
P2	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	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	

[†] *T. Magnussen, P. Rasmussen, and Aa. Fredenslund, Ind. Eng. Chem.Process Des. Dev. 20, (1980), pp. 331–339.*

Table 3.16 Group Interaction Parameters for Lyngby Modified UNIFAC †

MAIN GROUP	CH2	C=C	ACH	ACCH2	OH	CH3OH	H2O	ACOH	CH2CO	CHO	CH2COO	HCOO	CH2O	CH2NH2	NH2	CH2NH	CH2N	ACNH2	C5H4N	CH2CN	COOH	CCL	CCL2	CCL3	CCL4
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	X	X														
CH2O	X	X	X	X	X	X	X	X	X	X	X	X													
CH2NH2	X	X	X	X	X	X	X	X	X	X	X	X	X												
NH2	X	X	X	X	X	X	X	X	-	-	-	X	-	X											
CH2NH	X	X	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	-	-	-								
C5H4N	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						
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	X		
CCL4	X	X	X	X	X	X	X	X	X	-	X	X	X	X	X	X	X	X	X	X	X	X	X	X	

† *B. L. Larsen, P. Rasmussen, and Aa. Fredenslund, Ind. Eng. Chem. Res. 26, (1987), p. 2274.*

Table 3.17 Group Interaction Parameters for Dortmund Modified UNIFAC Model [†]

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	C#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	-																																	
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	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																									
CCL2	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																							
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	-	-	X	X	X	X	-	X																					
CH2NO2	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	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	-	X	-	-	-	-	-	-	-	-	-	-	-															
I	X	-	X	X	X	X	-	-	X	X	X	-	X	-	-	-	-	-	-	X	-	X	-	X	-	X	-	X	-	-	-														

continued

† *J. Gmehling, J. Li, and M. Schiller, Ind. Eng. Chem. Res. 32, (1993), pp. 178-193.*

Table 3.17 Group Interaction Parameters for Dortmund Modified UNIFAC Model † (continued)

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
BR	X	X	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	-	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	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	X	-	-	-	-						
CF2	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	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	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	-	-	-	-	X	-	-	-	X	X	X	-	-	X			
HCOOH	X	-	X	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	X	-	-	X	-	-	-	X	-	-	X	-	X	-	-	-	-	X	X	-	-

† J. Gmehling, J. Li, and M. Schiller, Ind. Eng. Chem. Res. 32, (1993), pp. 178-193.

Table 3.18 Group Interaction Parameters for UNIFAC Model Revision 3 †

MAIN GROUP	CH2	C=C	ACH	ACCH2	OH	CH3OH	H2O	ACOH	CH2CO	CHO	CH2COO	HCOO	CH2O	CH2NH2	CH2NH	CH2N	ACNH2	C5H4N	CH2CN	COOH
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
CCL3	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
ACCL	X	X	X	X	X	X	X	-	X	-	X	-	-	X	X	X	X	-	X	-
CH2NO2	X	X	X	X	X	X	X	-	X	-	-	-	X	-	-	-	-	-	-	-
ACNO2	X	-	X	X	X	-	X	-	-	-	-	-	-	-	-	-	X	-	-	-
CS2	X	X	X	X	X	X	X	-	X	-	X	-	X	-	-	-	-	-	X	-
CH2SH	X	-	X	-	X	X	-	-	X	-	-	X	X	X	-	-	-	-	X	-
FURFURAL	X	-	X	X	X	-	X	-	X	-	X	-	-	-	-	-	-	-	-	-
(CH2OH)2	X	-	X	X	X	-	X	X	-	-	X	-	X	-	-	-	X	-	-	-
I	X	-	X	-	X	-	-	-	X	-	X	-	X	-	-	-	-	-	-	-
BR	X	-	X	X	X	-	-	-	X	-	-	-	X	-	-	-	-	-	-	-
CH#C	X	X	-	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	X	-
DMSO	X	X	X	X	X	X	X	-	X	-	X	-	X	-	-	-	-	-	-	-

MAIN GROUP	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
CCL2	X																				
CCL3	X	X																			
CCL4	X	X	X																		
ACCL	X	-	-	X																	
CH2NO2	-	-	-	X	X																
ACNO2	-	-	-	X	-	X															
CS2	X	-	X	X	-	-	-														
CH2SH	X	-	-	-	-	-	-	-													
FURFURAL	-	-	X	X	-	-	-	-	-												
(CH2OH)2	-	-	-	-	-	X	-	-	-	-											
I	-	X	X	X	-	X	-	-	-	-	-										
BR	X	-	-	X	X	X	-	-	-	-	-	-									
CH#C	-	-	-	-	-	X	-	-	-	-	-	-	X								
DMSO	-	X	X	X	-	-	-	-	X	-	X	-	-	-	X						

continued

		Group Contribution Method Functional Groups								

† E. A. Macedo, U. Weidlich, J. Gmehling, and P. Rasmussen, *Ind. Eng. Chem. Process Des. Dev.*, 22, (1983), p. 676.

Table 3.18 Group Interaction Parameters for UNIFAC Model Revision 3 † (continued)

```
                                                         F (       A
                                                         U C       CC
                      C   C                        C     R H       RL
          A   C    C  H   HC  ACC                  HA CF 2         Y(
          C   H  AH   2HC2H CC5HC  CCCA 2C  HU O    CD LC
      CCAC   3HC2C CCHN2 HNH2O CCCCC NNC2R H    HM O=ADC C
MAIN  H=CHO O2OCH OO2HN 2H4CO CLLLC OOSSA )  B#S NCCMF O
GROUP 2CH2H HOHOO OOO2H N2NNH L234L 222HL 2IRCO I)FF2 O

ACRYLONI X---- -X--- ----- ---X- ----- ----- -----
CL(C=C)  XXX-X X--X- X-X-- ---XX X-XX- X-X-- ----- -
ACF      X-XXX X---- ----- ----- ---X- ----- ----- --
DMF      XXXXX XX-X- --X-- -X--- ---X- ---X- X--XX ---
CF2      X---- ----- ----- ----- ----- ----- ----- ----

COO      XXXXX XXXX- XXX-X ---XX -XXXX --X-- -X--X XX---
```

† E. A. Macedo, U. Weidlich, J. Gmehling, and P. Rasmussen, *Ind. Eng. Chem. Process Des. Dev.*, 22, (1983), p. 676.

Table 3.19 Group Interaction Parameter for UNIFAC Model Revision 4 †

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	X
C=C	X	X
ACH	X	X	X
ACCH2	X	X	X	X
OH	X	X	X	X	X
CH3OH	X	X	X	X	X	X
H2O	X	X	X	X	X	X	X
ACOH	X	X	X	X	X	X	X	X
CH2CO	X	X	X	X	X	X	X	X	X
CHO	X	X	X	X	X	X	X	-	X	X
CH2COO	X	X	X	X	X	X	X	X	X	X	X
HCOO	X	X	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
CH2NH	X	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	-	-	X	-	-	X
C5H4N	X	-	X	X	X	X	X	X	X	-	-	-	-	-	-	-	-	X
CH2CN	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
CCL3	X	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	X
ACCL	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
ACNO2	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
CH2SH	X	-	X	-	X	X	-	-	X	-	-	X	X	X	-	-	-	-	X	-	X	-	-	-	-	-	-	-	X
FURFURAL	X	-	X	X	X	-	X	-	X	-	X	-	-	-	-	-	-	-	-	-	-	-	X	X	-	-	-	-	-	X
(CH2OH)2	X	-	X	X	X	-	X	X	-	-	X	-	X	-	-	-	X	-	-	-	-	-	-	-	-	X	-	-	-	-	X
I	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
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	-	-	-	X

continued

† D. Tiegs, P. Rasmussen, J. Gmehling, and Aa. Fredenslund, Ind. Eng. Chem. Res. 26, (1987), p. 159.

Table 3.19 Group Interaction Parameter for UNIFAC Model Revision 4 † (continued)

																													F	(					A								
																													U	C					C	C							
											C			C												C				R	H					R	L							
				A		C			C		H			H	C		A	C	C							H	A		C	F	2					Y	(							
				C		H		A	H		2	H	C	2	H	C	C	5	H	C		C	C	C	A	2	C		H	U	O			C	D	L	C					S		
	C	C	A	C		3	H	C	2	C	C	C	H	N	2	H	N	H	2	O	C	C	C	C	C	N	N	C	2	R	H			H	M	O	=	A	D	C	C	I	S	N
MAIN	H	=	C	H	O	O	2	O	C	H	O	O	2	H	N	2	H	4	C	O	C	L	L	L	C	O	O	S	S	A	)		B	#	S	N	C	C	M	F	O	H	I	M
GROUP	2	C	H	2	H	H	O	H	O	O	O	O	O	2	H	N	2	N	N	H	L	2	3	4	L	2	2	2	H	L	2	I	R	C	O	I	)	F	F	2	O	2	O	P
ACRYLONI	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							
ACF	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	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	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	X	X	-	-	-	X			
SIH2	X	-	X	-	X	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X		
SIO	X	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X	X	
NMP	X	-	X	X	X	-	X	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	X

† D. Tiegs, P. Rasmussen, J. Gmehling, and Aa. Fredenslund, Ind. Eng. Chem. Res. 26, (1987), p. 159.

❖ ❖ ❖ ❖

4 Property Sets

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 Aspen Plus. 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	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 CVMX	Specific heat at saturation Constant volume heat capacity	V L L1 L2V L L1 L2 S T	•	•	•	MOLE-HEAT-CAPACITY or MOLE-HEAT-CAPACITY or MASS-HEAT-CAPACITY
DGMIX	Gibbs free energy of mixing	L L1 L2 T	•	•	•	MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
DGMX	Free energy departure	V L L1 L2 S T	•	•	•	MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW

continued

Table 4.1 Mixture Thermodynamic Properties (continued)

Enthalpy, Entropy, Gibbs Energy, Heat Capacity (continued)

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
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-ENTHALPY or MASS-ENTHALPY
GIGMX	Ideal gas free energy	V 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 †	Excess free energy	L L1 L2 S	•	•	•	MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
HIGMX	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 †	Excess enthalpy	L L1 L2 S	•	•	•	MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
SIGMX	Ideal gas entropy	V	•		•	MOLE-ENTROPY or MASS-ENTROPY
SMX	Entropy	V L L1 L2 S T	•	•	•	MOLE-ENTROPY or MASS-ENTROPY MASS-HEAT-CAPACITY

Other Properties

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
MWMX	Molecular weight	V L L1 L2 S T			•	—
PBUB	Bubble point pressure	V L L1 L2 T	•		•	PRESSURE
PCMX ††	Critical pressure	V L L1 L2 S T			•	PRESSURE
PDEW	Dew point pressure	V L L1 L2 T	•		•	PRESSURE
PRES	Pressure					PRESSURE
PRMX †††	Reduced pressure	V L L1 L2 S T			•	—
SONVELMX	Sonic velocity	V L L1 L2 T	•	•	•	
TBUB	Bubble point temperature	V L L1 L2 T		•	•	TEMPERATURE
TCMX ††	Critical temperature	V L L1 L2 S T			•	TEMPERATURE

† *PHASE = L is not allowed if two liquid phases are present.*

†† *Pseudocritical property; mole-fraction average of the pure component critical properties*

††† *Based on pseudocritical property*

continued

Table 4.1 Mixture Thermodynamic Properties (continued)

Other properties (continued)

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
TDEW	Dew point temperature	V L L1 L2 T		•	•	TEMPERATURE
TEMP	Temperature					TEMPERATURE
TRMX †††	Reduced temperature	V L L1 L2 S T			•	—
VCMX ††	Critical volume	V L L1 L2 S T			•	MOLE-VOLUME
ZCMX ††	Critical compressibility factor	V L L1 L2 S T			•	—
ZMX	Compressibility factor	V L L1 L2 S	•	•	•	—
ABSHUMID	Absolute humidity	V				—
RELHUMID	Percent relative humidity	V				—
COMB-O2	Amount of O2 needed to completely combust a given material	V L L1 L2 S				MOLES or MASS

† *PHASE = L is not allowed if two liquid phases are present.*

†† *Pseudocritical property; mole-fraction average of the pure component critical properties*

††† *Based on pseudocritical property*

Table 4.2 Thermodynamic Properties of Components in Mixtures

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
GAMMA †	Activity coefficient	L L1 L2 S	•	•	•	—
GAMPC †	Activity coefficient pressure correction	L L1 L2 S	•	•	•	—
GAMUS †	Unsymmetrically normalized activity coefficient	L L1 L2	•	•	•	—
KLL2	Liquid-liquid K-value		•	•	•	—
KVL ††	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
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 †	Fugacity coefficient	V L L1 L2 S	•	•	•	—
PPMX	Partial pressure	V			•	PRESSURE
SSOLFACT	Solubility safety factor †††	V L L1 L2	•	•	•	—
SSOLUB	Equilibrium solubility of a freeze-out component	V L L1 L2	•	•	•	—
TFREEZ	Freeze-out temperature of a component ‡	V L L1 L2	•	•	•	TEMPERATURE
TFRZMARG	Temperature safety margin ‡‡	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			•	—

† *PHASE=L is not allowed if two liquid phases are present.*

†† *Vapor-liquid K-value for PHASE=L1 is returned if two liquid phases are present.*

††† *Ratio of equilibrium solubility of the freeze-out component and its mole-fraction*

‡ *Temperature at which a component at its given concentration just begins to freeze out*

‡‡ *Temperature safety margin is defined as stream temperature — freeze-out temperature (TFREEZ)*

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	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	•	•		—
DH	Enthalpy departure	V L L1 L2 S	•	•		MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
DHVL †	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	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	Ideal gas enthalpy	V	•			MOLE-ENTHALPY, MASS-ENTHALPY or ENTHALPY-FLOW
PHI	Fugacity coefficient	V L L1 L2 S	•	•		PRESSURE
PHIPC	Fugacity coefficient pressure correction	L L1 L2 S	•	•		—
PL ††	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	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

† *Should be obtained using FLASHCURVE with VFRAC=0.*

†† *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.*

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	•	•		—
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

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 ††	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

PROPNAME †	Description	PHASE	TEMP	PRES	BASIS	Units
DMX	Diffusion coefficient	V L L1 L2	•	•	•	DIFFUSIVITY

Pure Components

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

† *PHASE=L is not allowed if two liquid phases are present.*

†† $RE = \frac{(mass\ flow)}{\frac{\pi}{4} viscosity}$ *Dimensionless Reynolds Number can be computed from RE by dividing by pipe diameter (Reynolds Number* $\frac{RE}{D}$ *).*

Table 4.6 Petroleum-Related Properties for Mixtures

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
ANILPT	Aniline point	V L L1 L2 T			•	TEMPERATURE
API	API gravity	V L L1 L2 T	•	•	•	—
CETANENO	Cetane number	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
MABP	Mean average boiling point	V L L1 L2 T			•	TEMPERATURE
PHYDRATE ††	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	V L L1 L2 T				PRESSURE
SG	Specific gravity	V L L1 L2 T			•	—
SGAIR	Specific gravity (ref.AIR at	V	•	•	•	—
THYDRATE ††	Hydrate formation temperature	V			•	TEMPERATURE
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	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 †††	ASTM D86 curve	V L L1 L2 T			•	TEMPERATURE

† *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.)*

†† *The effect of inhibitors on hydrate formation temperature and pressure is not observed.*

††† *Temperature calculated for LVPCT=0, 5, 10, 30, 50, 70, 90, 95, 100*

continued

Table 4.6 Petroleum-Related Properties for Mixtures † (continued)

Distillation Curves (continued)

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
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 †††	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 †††	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	TEMP	PRES	BASIS	Units
D2887T	ASTM D2887 temperature	V L L1 L2 T			•	TEMPERATURE
D86T ‡	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 ‡	ASTM D1160 temperature	V L L1 L2 T		•	•	TEMPERATURE

† *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.)*

††† *Temperature calculated for LVPCT=0, 5, 10, 30, 50, 70, 90, 95, 100*

‡ *LVPCT required*

continued

Table 4.6 Petroleum-Related Properties for Mixtures † (continued)

Distillation Temperature (continued)

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
D1160TWT	ASTM D1160 temperature at a given weight percent	V L L1 L2 T		•	•	TEMPERATURE
TBPT ‡	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 ‡	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	TEMP	PRES	BASIS	Units
D2887WT	ASTM D2887 weight percent	V L L1 L2 T	•		•	—
D86LV ‡‡	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 ‡‡	ASTM D1160 liquid volume percent	V L L1 L2 T	•	•	•	—
D1160WT	ASTM D1160 weight percent	V L L1 L2 T	•	•	•	—
TBPLV ‡‡	True boiling point liquid volume percent	V L L1 L2 T	•		•	—
TBPWT	True boiling point weight percent	V L L1 L2 T	•		•	—
VACLV ‡‡	Vacuum liquid volume percent	V L L1 L2 T	•		•	—
VACWT	Vacuum weight percent	V L L1 L2 T		•	•	—

† *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.)*

‡ *LVPCT required*

‡‡ *TEMP required*

‡‡‡ *Reports flow rates in 100 deg F or 50 deg C increments.*

continued

Table 4.6 Petroleum-Related Properties for Mixtures † (continued)

Flow Rates for Petroleum Cuts

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
CUTS-E ‡‡‡	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 ‡‡‡	Flow rates for petroleum cuts and light ends in Deg. C	V L L1 L2 T	•		•	MOLE-FLOW, MASS-FLOW, VOLUME-FLOW

Petroleum Property from ASSAY Analysis

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
ANILPT	Aniline point	V L L1 L2 T			•	TEMPERATURE
AROMATIC	Aromatic content	V L L1 L2 T			•	—
CARBON	Carbon content	V L L1 L2 T			•	TEMPERATURE
CLOUDPT	Cloud point	V L L1 L2 T			•	TEMPERATURE
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			•	—
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			•	—
NITROGEN	Nitrogen 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

† *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.)*

‡‡‡ *Reports flow rates in 100°F or 50°C increments.*

continued

Table 4.6 Petroleum-Related Properties for Mixtures † (continued)

Petroleum Property from ASSAY Analysis (continued)

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
REFINDEX	Refractive index	V L LI L2 T			•	—
ROC-NO	Research octane number	V L LI L2 T			•	—
SMOKEPT	Smoke point	V L LI L2 T			•	LENGTH
SULFUR	Sulfur content	V L LI L2 T			•	—
VANADIUM	Vanadium content	V L LI L2 T			•	—
VISC	Viscosity	V L LI L2 T	•		•	VISCOSITY
VLOCKIDX	Vapor knock index	V L LI L2 T			•	—
WARMIDX	Warm-up index	V L LI L2 T			•	—

Petroleum Property Curves

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
ANILCRV	Aniline point curve	V L LI L2 T			•	TEMPERA
AROMCRV	Aromatic content curve	V L LI L2 T			•	—
BAS-NCRV	Basic Nitrogen content curve	V L LI L2 T			•	—
CARBCRV	Carbon content curve	V L LI L2 T			•	—
FLASHCRV	Flash point curve	V L LI L2 T			•	TEMPERA
FREEZCRV	Freeze point curve	L LI L2 T			•	TEMPERA
HYDROCRV	Hydrogen content curve	V L LI L2 T			•	—
IRONCRV	Iron content curve	V L LI L2 T			•	—
KNOCKCRV	Antiknock index curve	V L LI L2 T			•	—
KVISCCRV	Kinematic viscosity curve	V L LI L2 T			•	DIFFUSIVI
LUM-NCRV	Luminometer number curve	V L LI L2 T			•	—
MERCCRV	Mercaptan content curve	V L LI L2 T			•	—
METALCRV	Metal content curve	V L LI L2 T			•	—
MOCNCRV	Motor octane number curve	V L LI L2 T			•	—
NAPHCRV	Naphthene content curve	V L LI L2 T			•	—
NICKCRV	Nickel content curve	V L LI L2 T			•	—
OLEFCRV	Olefin content curve	V L LI L2 T			•	—
OXYGEN	Oxygen content curve	V L LI L2 T			•	—
PARACRV	Paraffin content curve	V L LI L2 T			•	—

† *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.)*

continued

Table 4.6 Petroleum-Related Properties for Mixtures † (continued)

Petroleum Property Curves (continued)

PROPNAME	Description	PHASE	TEMP	PRES	BASIS	Units
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 LI L2 T	•		•	—
RVPCRV	Reid vapor pressure curve	V L LI L2 T			•	PRESSURE
SMOKCRV	Smoke point curve	V L LI L2 T			•	LENGTH
SULFCRV	Sulfur content curve	V L LI L2 T			•	—
TOT-NCRV	Total nitrogen content curve	V L LI L2 T			•	—
UOPKCRV	Watson UOP K curve	V L L1 L2 T			•	—
VANACRV	Vanadium content curve	V L LI L2 T			•	—
VISCCRV	Viscosity curve	V L LI L2 TV	•		•	DIFFUSIVITY
VLOCKCRV	Vapor knock index curve	V L LI L2 T			•	—
WARMICRV	Warm-up index curve	V L L1 L2 T			•	—

† *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.)*

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	—
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	S	•	MASS-DENSITY
ENTHALPY	Enthalpy	S	•	MASS-ENTHALPY
HEAT-CAPACITY	Heat capacity	S	•	MASS-HEAT-CAPACITY

† *All properties are component properties. Nonconventional component mixture properties cannot be computed using PROP-SET.*

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
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 MASS-HEAT-CAPACITY
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

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