

Component Management

Adding/Modifying Components

DDBSP – Dortmund Data Bank Software Package



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1. Introduction

The Dortmund Databank (DDB) contains two major parts, a pure component properties database and several databanks for mixture properties. Both parts have one thing in common – the underlying component list.

The component list contains actually four component lists. One large list for “normal” mostly organic components, a shorter list for electrolytes and salts, and a very short list for adsorptives, plus a list for polymers.

A. Content

The main component list contains not only strictly component defining information but also some additional data. The complete list is

- One English name
- One alternative name
- Molecular formula
- CAS registry number (code)
- Two Antoine vapor pressure equation parameter sets
- Critical temperature, pressure, and volume
- Acentric factor
- Heat of fusion
- Melting temperature
- Dipole moment
- Molecular weight
- One liquid(!) density at one temperature (preferably at 25 °C). This density is used for the Wilson g^E model.
- Original UNIFAC and modified UNIFAC (Dortmund) group assignment information
- UNIQUAC r and q values

The electrolyte list data file contains

- Name
- Formula
- Molecular weight
- CAS registry number (code)
- Dielectric constant with temperature
- Frequency
- One density
- Groups (ions)
- Gibbs energy of formation parameters
- Heat of formation parameters
- Heat capacity parameters
- Melting temperature
- Heat of fusion
- Two heat capacity values for liquid and crystal
- DDB basic number (if the electrolyte or salt is also available in the main component list)
- Volatility flag (yes if electrolyte is volatile, HCl for example)
- Information on associates

The adsorbent list contains

- Name

The polymer list contains

- Name
- List of monomers

- List of polymers (if polymer is a copolymer)

B. Usage

The normal component list is used in every database. The salts list has been introduced for the VLE database containing electrolytes and the salt solubilities database. The adsorptives are used in the adsorbent-adsorptive equilibrium database.

The list have been separated because of using special component- resp. electrolyte-specific parameters for calculation models. This is also the reason for not using a short list of components restricted to names, formula, and maybe CAS registry numbers but to include a multitude of further data. The selection of data is also completely arbitrary since parameters only for a few models are included whereas other models find their parameters in different files.

2. Editing the Main Component List

Components Salts Adsorbents Ions Groups Polymers Flash Points

More Save Find New Clear App.Priv. Export Artist Print Stat. Web

Specification

Component number: 1 < > 51395 components

Main name: Acetaldehyde

Alternative name: Ethanal

Formula: C2H4O CAS-No.: 75-07-0

Antoine constants T [°C] P [mmHg]

| | | | | | | | | |
|----------------|---------|---------|---------|--------|-----|-----|----|-------------|
| Low pressure: | 7.05640 | 1070.60 | 236.000 | Range: | -63 | 47 | °C | Tb=293.55 K |
| High pressure: | 7.16094 | 1154.01 | 248.700 | | 20 | 109 | °C | Tb=294.07 K |

Values

| | | | | | |
|--------------------|----------|----------------------|-------------------|---------|-------|
| Crit. pressure: | 5573.875 | kPa | Heat of fusion: | 3217.0 | J/mol |
| Crit. temperature: | 461.00 | K | Melting point: | 150.20 | K |
| Crit. volume: | 154.0 | cm ³ /mol | Dipole moment: | 2.69000 | Debye |
| Acentric factor: | 0.30300 | | Molecular weight: | 44.053 | g/mol |

Density: 778.00 kg/m³ at 298.15 K Volume=56.62 cm³/mol

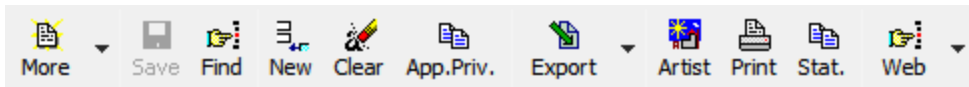
UNIFAC groups and UNIQUAC parameters

| | | | | | | | | | | | | | | | | | |
|---------------------|---|------|------|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| UNIFAC groups: | 2 | 1001 | 1020 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| mod. UNIFAC groups: | 2 | 1001 | 1020 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

UNIQUAC r-value: 1.89910 UNIQUAC q-value: 1.79600

Overwrite values by PRIVATE.PCP entries

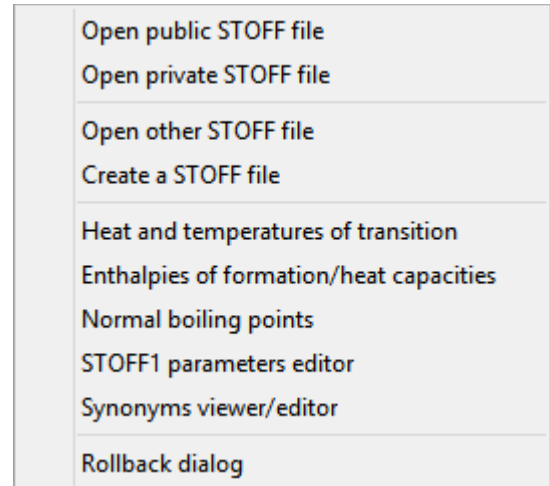
A. The Tool Bar





This button opens a context menu which allows to open the public and private component basic file and also to open another file (neither public nor private) or to create a new file.

The other commands open special subdialogs for special data files or to call other programs (“Condensed Data Sheet”) if available. These dialogs are explained later.



The “Save” button is only enabled if changes have been made and allows to store the changes.



The “Find” button calls the *ComponentSelection* program which allows searching for components by different criteria.

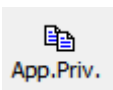


The “New” button opens a dialog for entering a new component. The dialog displays the current number of components in the private and the public list and allows to enter two names, the CAS registry code, the molecular weight and a formula. Only the specification of a primary name obligatory.

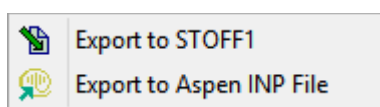
The new component can be appended either to the public list or the private list. All additional entries are initialized and empty.



The Clear button erases all entries. It is not possible to completely remove an existing component.



This button allows to copy a public (DDBST) component to the private component list. This can be used to add a private component which is the same as a public component but with different additional data like modified T_c , P_c , etc.



The button *Export to STOFF1* allows updating an (almost) twin file called STOFF1. This file contains some additional data (parameters) but has to be kept synchronous for some calculations. Usually this synchronization is done automatically.

The “Export to Aspen INP File” writes critical temperature, pressure, and volume, melting point, molecular weight, acentric factor, Antoine constants (low pressure), and UNIQUAC constants to an INP file.



The button calls the structure editor Artist – if available. Artist will show the structure of the component – if available.



The Print button allows printing a component sheet but it displays it in a dialog beforehand.

```

Data set no. 1
=====
German Name:      Ethanal
English Name:    Acetaldehyde
Empirical Formula: C2H4O
CAS-No.:        75-07-0

Antoine Constants (low):  P [mmHg]  T [°C]
      7.05640    1070.60    236.000
Limits:    -63    47 °C
      Resulting Normal Boiling Point: 293.55 K

Antoine Constants (High): P [mmHg]  T [°C]
      7.16094    1154.01    248.700
Limits:    20    109 °C
      Resulting Normal Boiling Point: 294.07 K

Groups for UNIFAC:
      2 1001 1020    0    0    0    0    0
Groups for mod. UNIFAC (Do):
      2 1001 1020    0    0    0    0    0

r-Value:        1.8991
q-Value:        1.7960

Dipole Moment:   2.6900      Debye
Molecular Weight: 44.053

Density:         778.0000 kg/m3 at T = 298.15 K

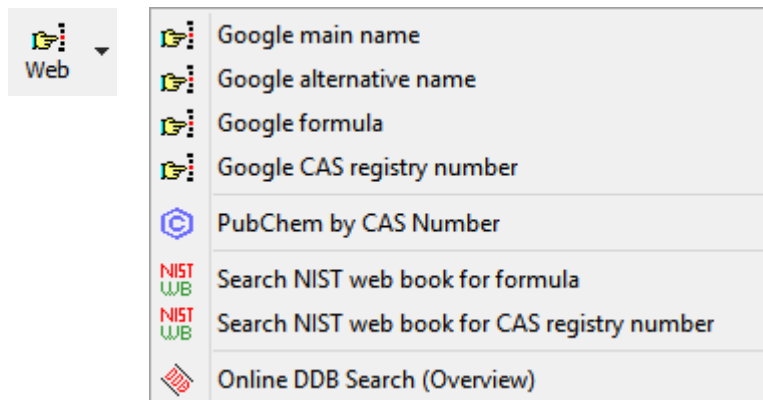
Critical Temperature: 461.00 K
Critical Pressure:    5572.875 kPa
Critical Volume:     154.00 cm3/mol
Acentric Factor:     0.3030
Melting Enthalpy:    3217.50 J/mol
Melting Temperature: 150.20 K
    
```



This button displays statistics on the component file.

```

Number of Components:      51092
1591 are PLEASE USE references and 0 empty places
      (-> 49501 normal entries)
CAS-Numbers:              29815
Molecular Weights:        49141
Melting Points:           4701
Heats of Fusion:          1789
Densities:                2128
Antoine-Constants (High Pr.): 466
Antoine-Constants (Low Pr.): 5725
Artificial Antoine-Constants (Low Pr.): 965
UNIFAC-Group Definitions: 21974
UNIFAC (DO)-Group Definitions: 20940
Critical Temperatures:    1568
Critical Pressures:       1233
Critical Volumes:         1113
Acentric Factors:         1086
r-Values for UNIQUAC:     11437
q-Values for UNIQUAC:     11437
Dipole Moments:            666
    
```




The first four submenu entries allow searching by the google.com search engine for

- main and alternative name
- the formula and
- the CAS registry number

The search is done by sending an URL to the system's standard web browser. Typical URL for names and CAS-RN search look like

- <http://www.google.com/search?q=Ethanal>
- <http://www.google.com/search?q=71-43-2>

The  menu items call the installed web browser and try to find information in the NIST web book (<http://webbook.nist.gov>) by the formula or CAS registry number.

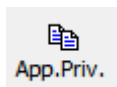
B. Private and Public Compound Files

The Dortmund Data Bank software supports two distinct data bank systems. The first system contains the delivered data banks from DDBST GmbH. The other system contains data banks created by our customers.

The data banks are organized by their location. There's a folder for the public (delivered) data banks and there's a folder for the private (customer's) data banks. Both data banks are integrated seamlessly in the retrieval, plot, prediction, and fit software. The display makes no significant difference between public and private databanks and components. In most cases the numbers changes only the sign. The public components and the data sets from a public data bank have positive numbers and the private components and sets are identified by negative numbers.

Private data banks can be build up with data sets containing information for private and public components. The public data bank contains only public components.

a. Copy Public Components to the Private Component List



This function has been created for a quick update or modification of values stored in the public compound file.

The public component list should be modified by users for two reasons.

1. The first reason is that this file is changed by DDBST GmbH and will be overwritten if an update is distributed. Every change a customer has made to any fields will be lost.

2. The other reason is that errors introduced by changing delivered values is due to problems when reenacting old calculations. Be aware that other people would have other parameters for the same component. This will lead to confusion.

One solution is to copy the public component into the private component list and add or modify the values there.

Another possibility is implemented by storing different values in a separate file named 'PRIVATE.PCP'. This file is a pure text file containing the same information (and some more) as the compound definition file but it allows to overwrite entries. A detailed description follows later.


C. The Data Fields

a. Component Specification

The “Component Number” is mostly called “DDB number” of the component. The compound list contains two fields, one main name (English) and one alternative name.

Both names have a maximum length of 127 characters. The nomenclature of the components have been following the nomenclature of the authors of the experimental papers. This explains why many names don't follow CAS or IUPAC naming rules.

The formula can have up to 31 characters and digits and the CAS registry number can contain up to ten digits (excluding hyphens). The CAS registry number is written with hyphens.

The  button changes the capitalization of the names.

The program automatically checks the validity of formula and CAS registry number. If a formula contains wrong symbols it is displayed in red. If the CAS registry number check sum is wrong it is displayed in red and the correct check sum is displayed.

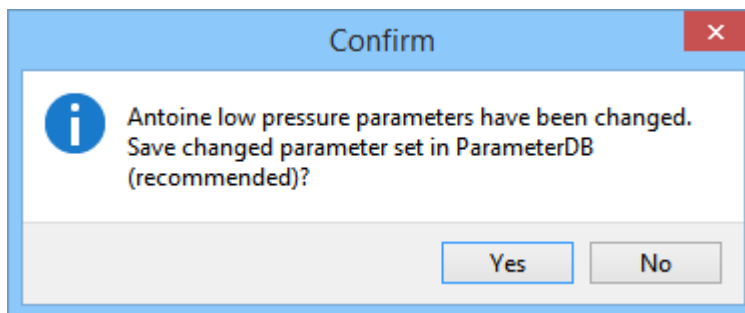
Components with wrong formulas or CAS registry numbers can be stored anyway.

b. Antoine Constants

| Antoine constants | | T [°C] | P [mmHg] | Range: | | Tb |
|-------------------|---------|---------|----------|--------|-----|----------------|
| Low pressure: | 8.20417 | 1642.89 | 230.300 | -57 | 80 | °C Tb=351.47 K |
| High pressure: | 7.68117 | 1332.04 | 199.200 | 77 | 243 | °C Tb=351.44 K |

Antoine parameters are given in [°C] as temperature unit and [mmHg] as pressure unit. The component file contains two Antoine parameter sets. One (“Low Pressure”) is normally used for vapor pressure below the normal boiling point and the other (“High Pressure”) is used above the normal boiling point. The “Range” field contain the validity range of both sets. If a parameter set is available the program displays the normal boiling points calculated from the parameters.

Antoine constants are normally stored in the ParameterDDB, the parameter data bank. To ensure consistency between the ParameterDDB and this entry in the component file the program asks to



store changed data also in the ParameterDDB. This is not a compulsory step but it is highly recommended and should only be omitted if the new parameters are stored only for a temporary reason.

c. Values

| Values | | | |
|--------------------|--------------------------------------|-------------------|----------------------------|
| Crit. pressure: | 6383.475 kPa | Heat of fusion: | 5017.5 J/mol |
| Crit. temperature: | 516.20 K | Melting point: | 158.65 K |
| Crit. volume: | 167.0 cm ³ /mol | Dipole moment: | 1.69000 Debye |
| Acentric factor: | 0.63500 | Molecular weight: | 46.069 g/mol |
| Density: | 785.00 kg/m ³ at 298.15 K | Volume= | 58.69 cm ³ /mol |

Most of these values are used for calculations, either fits or predictions. The density entry is used only for the Wilson g^E model and can be hypothetical for components which are solid at approx. 25 °C (= ambient temperature).

Stored and Displayed Units

| Value | Shown Unit | Internal Unit |
|----------------------|----------------------|----------------------|
| Critical Pressure | kPa | atm |
| Critical Temperature | K | K |
| Critical Volume | cm ³ /mol | cm ³ /mol |
| Acentric Factor | - | - |
| Density | kg/m ³ | g/cm ³ |
| Density Temperature | K | °C |
| Heat of Fusion | J/mol | cal/mol |
| Melting Point | K | °C |
| Dipole Moment | Debye | Debye |
| Molecular Weight | g/mol | g/mol |

The program displays some of the values in units which are different from the units the values are stored. These units have been selected for being compatible with units used in the pure component properties database.

This was mainly done for being able to compare the component's values with the experimental values.

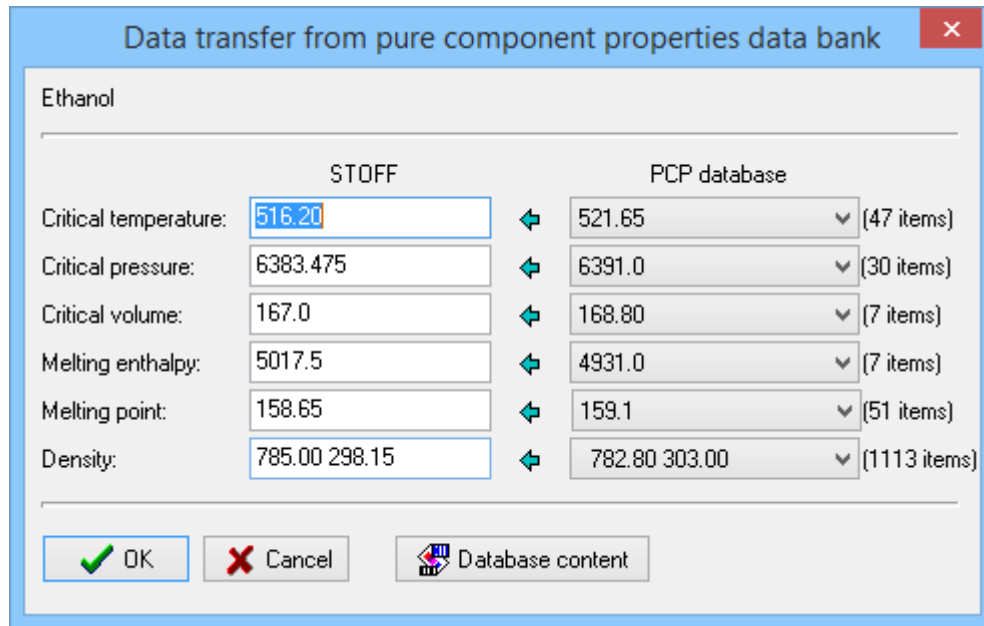
Data Transfer from Pure Component Properties Data Bank


It is possible to retrieve data from the pure component properties database and update the values in the component file from experimental data. This function can be called by the button.

| |
|--------|
| 168.80 |
| 166.30 |
| 167.20 |
| 167.20 |
| 161.00 |
| 165.00 |
| 167.00 |

Values from the PCP database can be obtained for six properties shown in the dialog. The drop-down combo boxes below the “PCP Database” title contain all found data points from the PCP database.

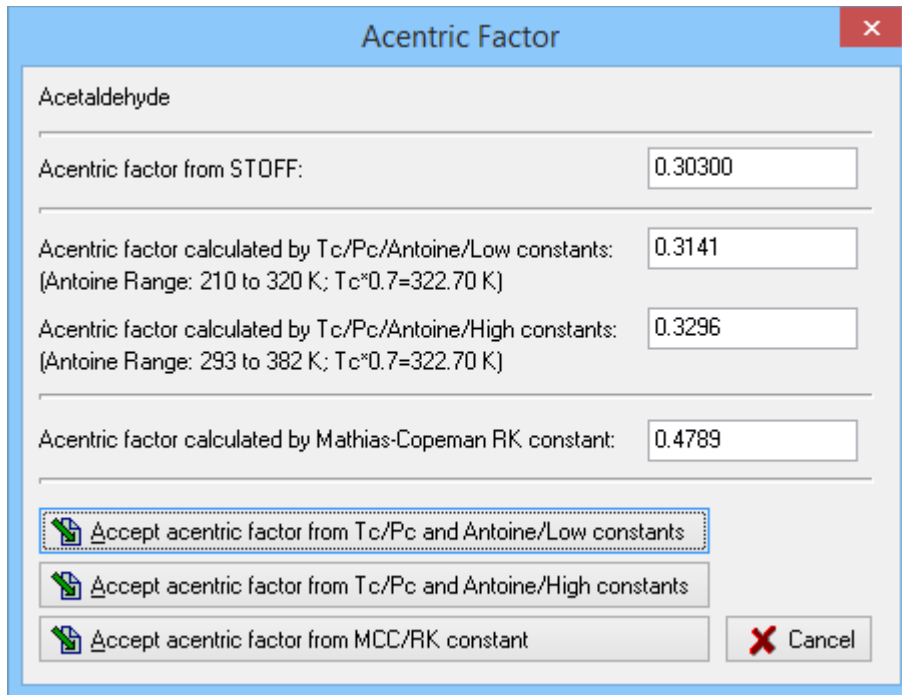
The density must be a liquid density near 25 °C because this density is used for the Wilson g^E model.



The button  Database content invokes the Dortmund Data Bank program and will display all available pure component properties in the DDB.

Obtain the Acentric Factor from Antoine Constants and Critical Data





The dialog displays the old value and two new values from both Antoine parameter sets – if available.

$$\omega = -\log P_r^S - 1.000$$

$$\text{with } P_{Sr} = \frac{P^S}{P_c} \text{ at } T_r = 0.7$$

with

The equation is

ω : Acentric Factor

P^S : Saturated Vapor Pressure

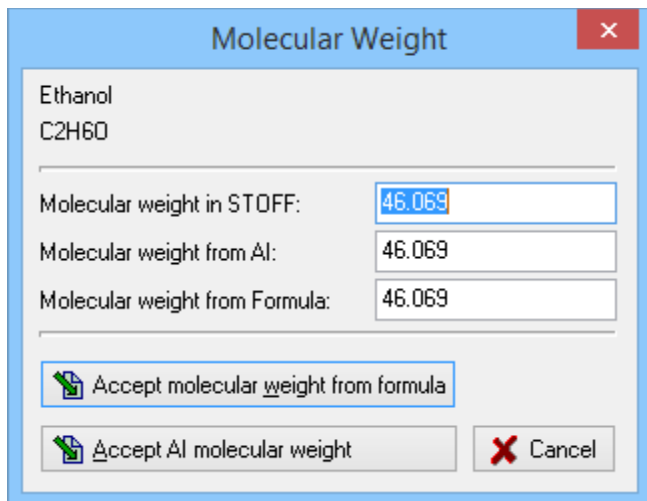
T_c : Critical Temperature

P_c : Critical Pressure

Index r : Reduced Value

Calculate the Molecular Weight from Formula and Structure

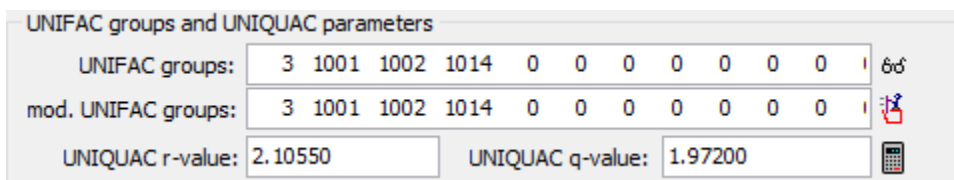




The dialog displays the original value and two calculated values. The second molecular weight has been obtained from molecular structure (by an Automatic Incrementation function). The structure is only available if the Artist program package is present.


The third field shows the molecular weight calculated from the empirical formula stored in the component file (C₂H₄O in the example).

d. UNIFAC Groups and UNIQUAC Parameters

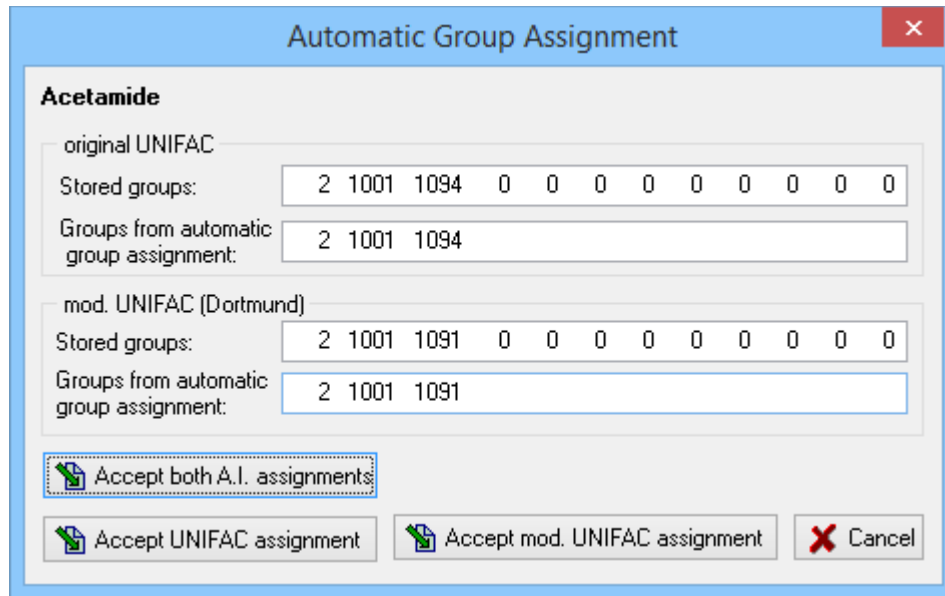


The groups for both UNIFAC models are encoded. The first number is the amount of different groups (subgroups) in the molecule. The following numbers list the single group as 'count times thousand plus subgroup number'. "1020" means one time subgroup 20. The maximum number of different subgroups is seven (eight numbers including the group count).

Obtain UNIFAC Groups from Molecular Structure

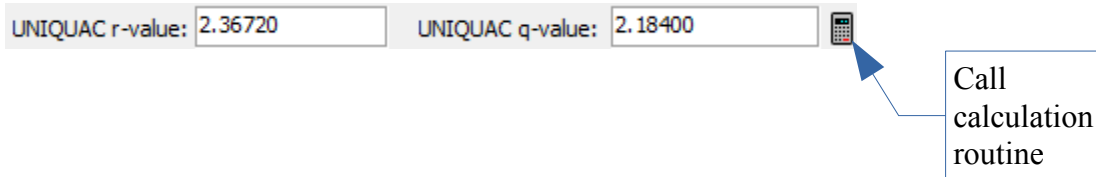
The button  displays the dialog.

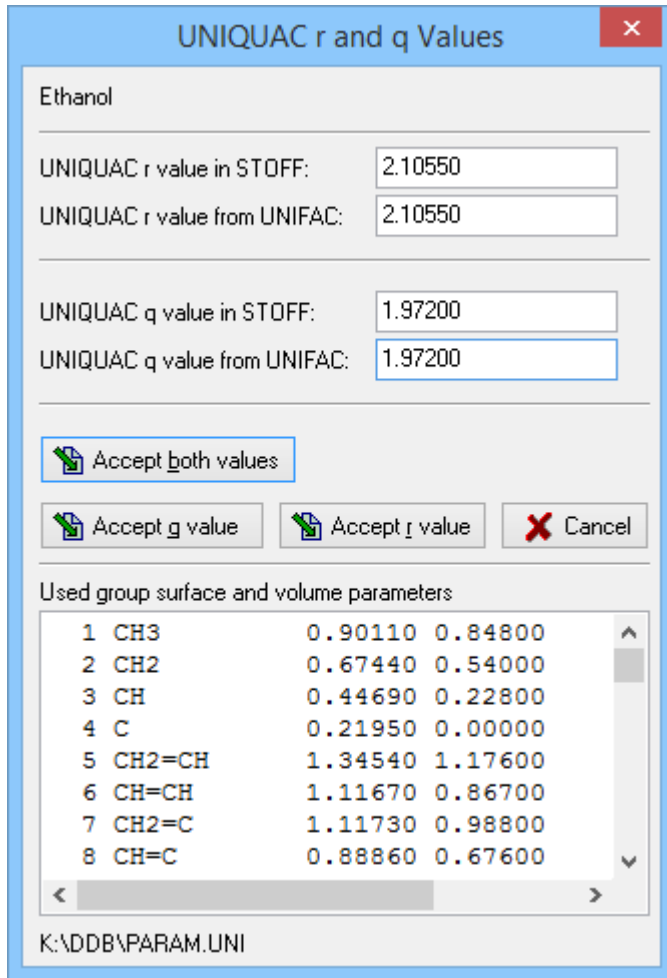
This function uses the automatic fragmentation (also called *automatic incrementation* – A.I.) algorithms. Therefore the Artist program package – including the structure database – has to be available.



The fragmentation schemes only contains published group definitions – not any additional groups from the UNIFAC consortium. Pending zeros don't have any significance.


Calculate UNIQUAC r and q Values from UNIFAC Group Surfaces and Volumes






The dialog displays the originally stored values and the recalculated values obtained by summing up the surfaces and volumes of the original UNIFAC subgroups. The used group values are listed below.

Details Display

Selecting the button  opens a dialog with a detailed display of the groups. The upper part display the complete list of main and subgroup of both the original UNIFAC and the modified UNIFAC (Dortmund) models. The lower grid show the current group assignment.

This dialog allows to edit the list of group by dragging **subgroups** from the complete list above to the component's list below.

The 'Count' column in the component's UNIFAC or mod. UNIFAC list is editable.

The  Use button allows to copy the modified list of groups to main editing window.

This dialog is non-modal, therefore it is possible to have both the main and this dialog displayed together.

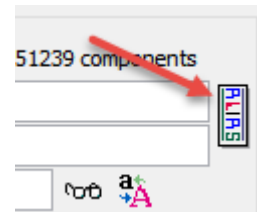
| Main Group Number | Main Group Name |
|-------------------|-----------------|
| 1 | CH2 |
| 2 | C=C |
| 3 | ACH |
| 4 | ACCH2 |
| 5 | OH |
| 6 | CH3OH |

| Count | Subgroup | Maingroup |
|-------|----------|-------------|
| 1 | 1 CH3 | 1 CH2 |
| 1 | 94 AMH2 | 46 CON (AM) |

| Count | Subgroup | Maingroup |
|-------|----------|-----------|
| 1 | 1 CH3 | 1 CH2 |
| 1 | 91 CONH2 | 47 CONR |

D. Synonyms Management

The main DDB component file only contains two names for every component. The synonyms database allows to store any amount of additional names, numbers, trademarks, etc. for a component.

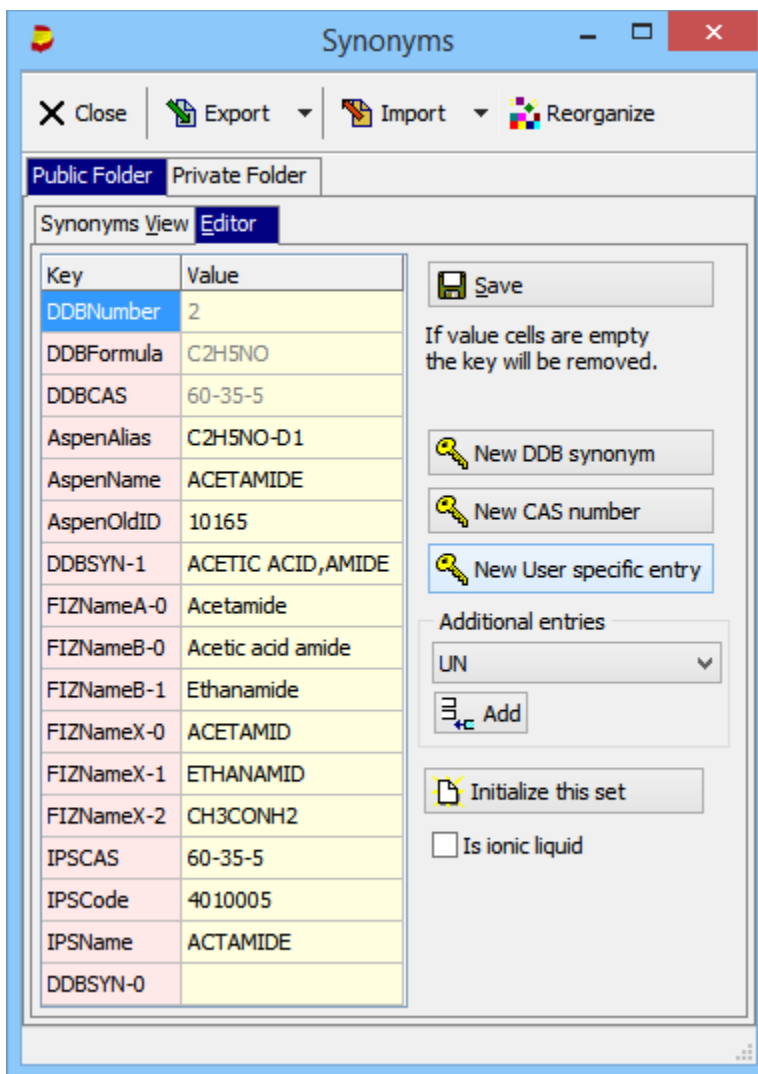


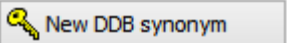
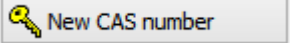

The screenshot shows the 'Synonyms' application window. At the top, there are menu options: Close, Export, Import, and Reorganize. Below the menu is a toolbar with 'Public Folder' and 'Private Folder' tabs. The main area has 'Synonyms View' and 'Editor' tabs. A 'Dataset number' field contains '174' and a 'Search names' field is empty. A 'Clear Search List' button is on the right. The main data area is a table with the following content:

| DDB# | FIZ Synonyms | Aspen Names | DDB Synonyms | Other Synonyms |
|--------------------------|---|----------------------------------|-------------------------------|---|
| 174 H2O 7732-18-5 | Water Eau R 718 Ice H2O[16]1 WASSER H2O HYDROGEN OXIDE H2O1 | Alias: H2O Name: WATER | WATER | AspenOldID: 11450 IPSCAS: 7732-18-5 IPSCCode: 16020200 IPName: H2O |
| 175 C8H10 108-38-3 | 1,3-Dimethylbenze 1,3-Xylene 3-XYLLOL 1,3-DIMETHYLBEN; 1,3-DIMETHYLBEN; 3-METHYLTOLUENE 3-XYLENE M-DIMETHYLBENZE M-XYLENE | Alias: C8H10-2 Name: M-XYLENE | M-XYLENE BENZENE, 1,3-DIME | 1307 : AspenOldID: 10881 IPSCAS: 108-38-3 IPSCCode: 12010110 IPName: MXYLENE UN: 1307 |

Three types of synonyms are displayed separately from 'other' synonyms. These are old DDB synonyms, synonyms entered by the FIZ CHEMIE, and Aspen names resp. aliases.

A synonyms data set is a list of key/value pairs. The keys specify the type of synonym or data and the value specifies the name.



The synonyms editor displays these key/ value pairs in a grid. The light red column contains the key and the light yellow column contains the values. Only the values can be edited directly in the grid (AspenAlias C2H4O-1). New keys have to be added by the buttons ,  or . The box 'Additional Entries' contains a list of predefined keys which are read from an “ini” file (STOFFEditor.ini). The file contains four blocks.

```
[StandardPredefinedKeysUnique]
1=AspenAlias
[StandardPredefinedKeysNumbered]
1=DDBSYN-
[AdditionalPredefinedKeysUnique]
1=UN
[AdditionalPredefinedKeysNumbered]
1=DDBSYN-
```

The [StandardPredefinedKeys...] are always inserted in the editing grid if none of these entries are available. The value cell is empty.

The [AdditionalPredefinedKeys...] are only displayed in the drop-down-selection control.

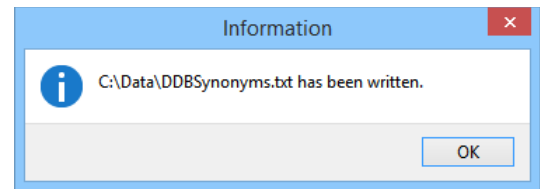
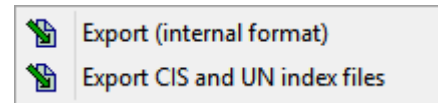
The [...Numbered] entries can occur multiple times – numbers are appended - whereas the [...Unique] entries can occur only one time.

Single keys cannot be deleted directly but the program removes keys with an empty value cell when saving and the entire data can be removed by the  button.

a. Export

The DDB synonyms can be exported completely to a text file by *Export (internal format)*. This file can be used to modify synonyms outside the component editor.

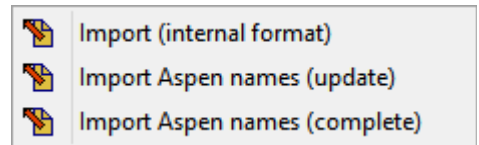
Export CIS and UN index files are mainly a DDB internally used exports to write CIS and UN number to smaller files than the DDB synonyms file to accelerate the search for these numbers in the component selection program.



b. Import

“Import (Internal Format) van read the exported data in the same format.

“Import Aspen Names” can read Aspen name information from the “purecompstruct.mdb” file provided by Aspen. This import might be out-dated because Aspen changed the names management.



c. Reorganize

The DDB synonyms grows over time because of changes and additions. Reorganizing can increase the search performance. Reorganizing the public DDB synonyms file is never necessary but larger private files can profit.

E. Additional Files

Some of the pure component data are not stored in the main component file. For some of these files additional dialogs have been added. These dialogs can be opened by the drop-down-menu entries.

1. DHT.DAT Editor
Heats of transitions and transition temperatures in the solid phase, used for SLE calculations. Up to three temperature/heat pairs can be added.
2. HGCP.DAT Editor
Heat and Gibbs Energy of Formation, and parameters for a heat capacity equation.
3. NBP.DAT Editor
Normal boiling points
4. STOFF1 Parameters
Editor for a variety of equations for vapor pressures, liquid densities, second virial coefficient and heat of vaporization. The equation numbers are “DIPPR numbers – 99”, e. g. equation DIPPR no. 100 is no. 1 in the STOFF1 file.

3. Replace Component Definition File Entries for Calculations

As stated in chapter “Private and Public Compound Files” the data entries in the public compound definition files are not allowed.

One possibility to modify the data nevertheless has been mentioned already. Public components can be copied into the private component list. This doesn't solve the problem entirely because the data bank contains public components and a user would have to alter the component list in public data banks in order to use the private component duplicate.

There's another solution: All calculation programs (and the `StoffEditor`) are looking for a file named `PRIVATE.PCP` in the `DDB` folder for private data banks. This file contains selected data for specified components.

This file has to be edited currently by hand. Its format is pure text and the single values are identified by tags.

The possible tags are

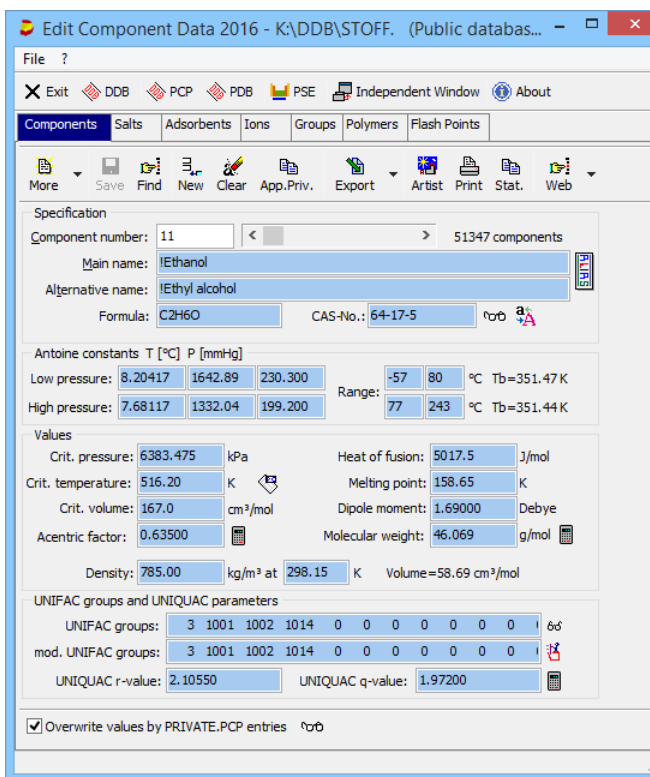
| Tag | Description |
|-------------------|---|
| DDB# | DDB component number |
| COM | Comment |
| INIT | Initialize all value for a component (see description of the ‘Clear’ button) |
| GNAM | German name (up to 48 characters) |
| EMPF | Empirical formula (up to 12 characters) |
| ENAM | English name (up to 48 characters) |
| CASN | CAS registry number |
| ANTN | Low pressure Antoine constants (P [mm Hg], T [°C]), Line entries: A, B, C, lower temperature limit, upper temperature limit |
| ANTH | High pressure Antoine constants (P [mm Hg], T [°C]), Line entries: A, B, C, lower temperature limit, upper temperature limit |
| CRID | critical properties and dipole moment Line entries: T_c [K], P_c [atm], V_c [cm ³ /mol], acentric factor, and dipole moment Values can be separated by commas. |
| MPT | Melting temperature in [°C] |
| HFSN | heat of fusion [cal/mol] |
| UNRQ | UNIQUAC r and q values |
| INKU | Structural information of original UNIFAC. Groups are encoded |
| INKM | Structural information of mod. UNIFAC (Dortmund variant). |
| MWGH | molecular weight [g/mol] |
| LDEN | Liquid density [g/cm ³] and temperature [°C] |
| INK# ¹ | Structural information of ASOG, mod. UNIFAC (Lyngby) and both PSRK models. Structural information is preceded by model numbers: 1: mod. UNIFAC (Lyngby) 2: ASOG 3: PSRK and PSRK2 13: PSRK extended (32 Groups) |
| TRAN ¹ | Transition temperature and heat Line Entries: T_{Tr} [K], H_{Tr} [J/mol] |
| MCRK ¹ | Mathias-Copeman constants for Soave-Redlich-Kwong equation of state used in PSRK. Line entries: $c_1, c_2, c_3, T_{min}, T_{max}$ [K] |

¹ This information is not available in the compound definition file.

The following frame shows the content of a PRIVATE.PCP file. In this special case every entry is written. This is not necessary. If some tags are not given, the calculation programs always use the entries from the compound definition file.

```

DDB# 11
INIT
GNAM ETHANOL
ENAM ETHANOL
EMPF C2H6O
CASN 64-17-5
ANTN      8.20417    1642.89    230.341   -57    80
ANTH      7.68117    1332.04    199.177    77   243
CRID      516.2000   63.0000    167.0000    0.6350   1.6900
MPT      -114.500
HFSN      1199.200
UNRQ      2.10550    1.97200
INKU          3      1001      1002      1014
INKM          3      1001      1002      1014
MWGH          46.069
LDEN          0.785000      25.00
;
INK# 1          3      1001      1002      1012
INK# 2          2      2001      1006
INK# 3          3      1001      1002      1014
TRAN 0.00      0.0    0.00      0.0    0.00      0.0
MCRK 1.3327    0.9695    -3.1879    206      490
    
```



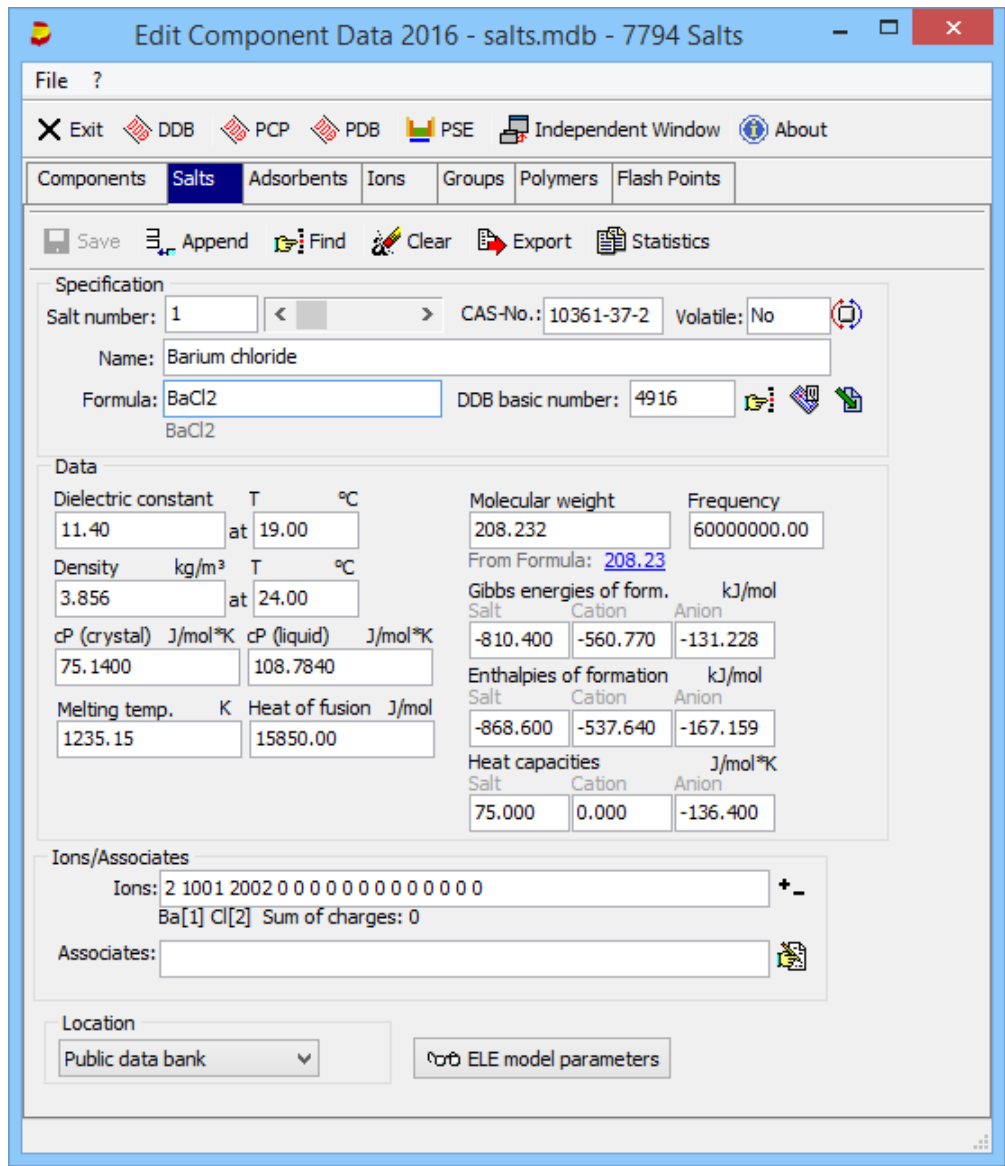
If entries have been replaced by entries from the “Private.PCP” file the component editor shows blue background on the affected data fields.

Additionally, both names are prefixed by an exclamation mark if at least one entry has been modified.


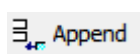
4. Editing the Salt/Electrolyte List



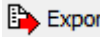
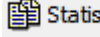
The list of electrolytes has been introduced mainly for being able to stored some kind of recommended electrolyte specific values. The selection of properties has been arbitrary and senseless from the current point of view.

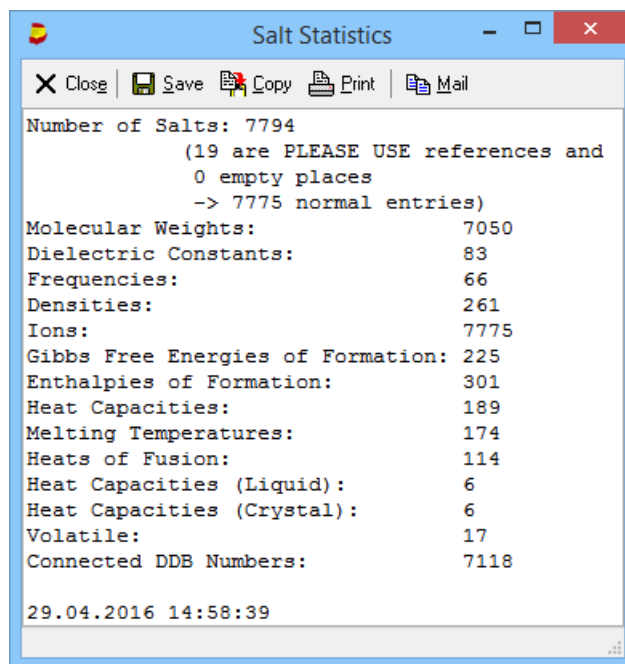
The electrolyte numbers are used in the ELE (vapor-liquid equilibria) and ESLE (salt solubilities) databases.



A. The Tool Bar



-  Save Saves changes
-  Append Appends an empty salt/electrolyte data set

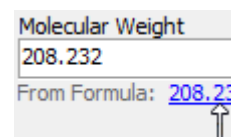
-  **Find** The Find button calls the ComponentSelection program which allows to search electrolytes by different criteria.
-  **Clear** Initializes data fields
-  **Export** Export all data sets to old-style salt files (needed in other programs).
-  **Statistics** Shows an overview over the number of salts and stored properties.



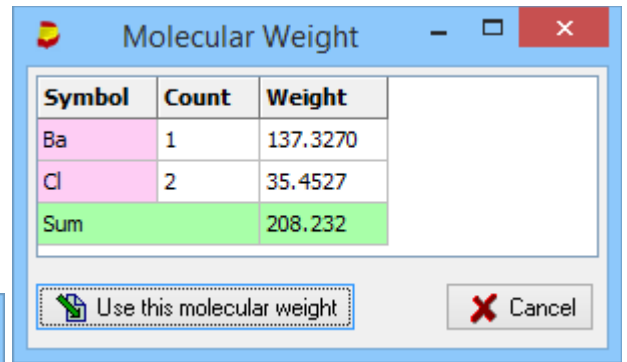
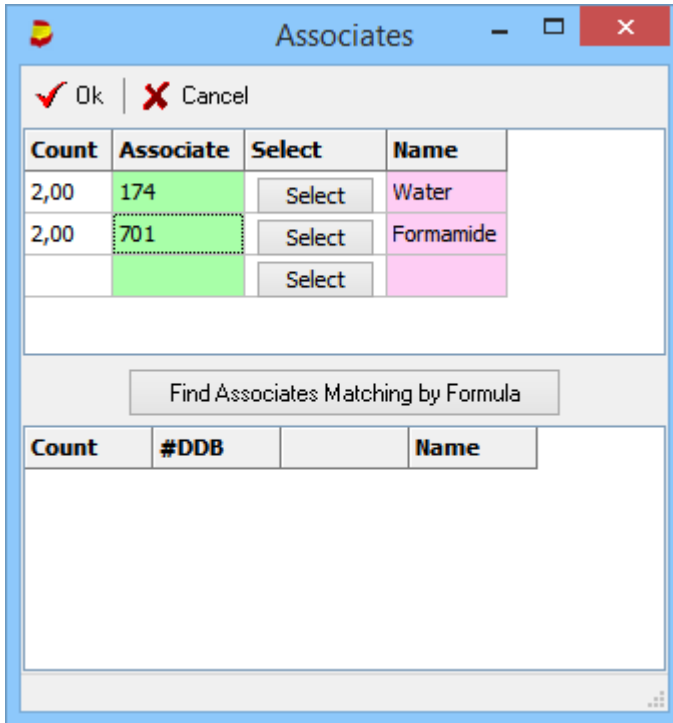
B. Basic Entries


The electrolyte list contains

- a single name entry
- a formula
- a CAS registry number
- a DDB basic number. Many electrolytes are also part of the main component list (for the EGLE - gas solubilities - and PCP - pure component properties - databanks). The button  opens a component selection dialog and the button  displays the connected entry of the main component list.
- a molecular weight. The molecular weight can be calculated from the formula.
The program displays the molecular weight calculated from the formula and a click on the blue label open a details dialog.
- a dielectric constant (with temperature)



- a single density value (with temperature)
- a frequency (Hz)
- heat capacities
- energies and enthalpies of formation
- a melting temperature
- a heat of fusion



- a list of ions in encoded form. The first number gives the number of different ions and the following specify the ions count (thousands) plus ions number (“2012” means 2 times ion no. 12 – CO₃).
- a list of associates. This is a list of number pairs. The first is the count and the second is the main component number (“2.5 174” means two and half water molecules). The button  opens a small editing dialog for the associates. The associates can either be entered directly if the DDB number is known or by the “Select” button and the standard component selection dialog. The count is a floating point number to allow entering, for example, one-half or a one-third of a molecule like 0.5 Water molecules. The “Find Associates Matching By Formula” helps searching the DDB numbers of associates.

This does only work if the associates in the empirical formula are separated by stars (e.g. “Zn(NO3)2*2HCONH2*2H2O”)

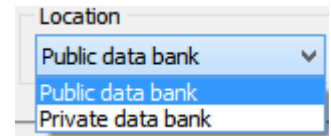
- a flag if the electrolyte is volatile (true for HCl, false for NaCl).

C. Private and Public Salts and Electrolytes Lists

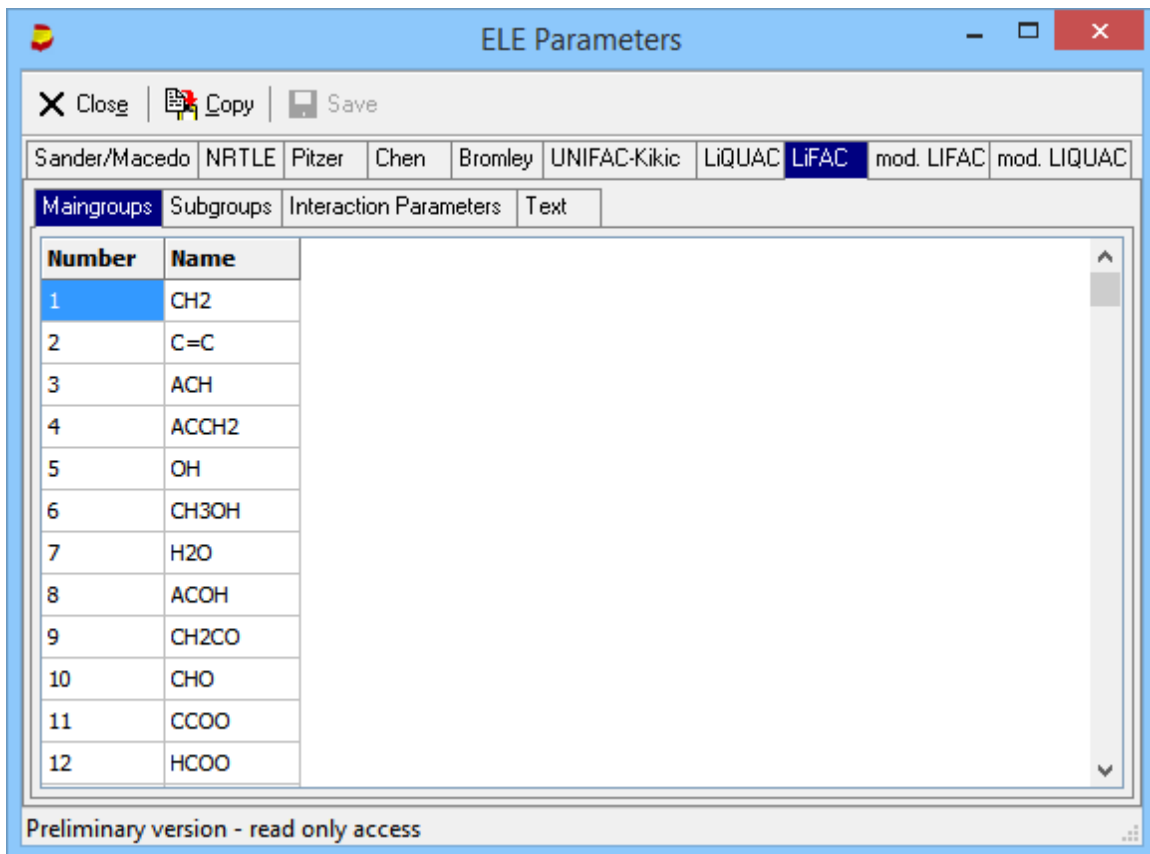
Like the normal component's list the salt editor supports two distinct electrolytes lists. One public list delivered from DDBST GmbH, and a private list created by customers.

The two buttons allow to switch between both lists. If a private file does not yet exist it will be created on the fly.

Private ESLE and ELE databanks can be build from private and public components and electrolytes whereas the public databases only contain public components and electrolytes.



D. ELE Parameters



The ELE parameters dialog only allows to view the parameters for several models for the estimation of vapor-liquid equilibria of electrolyte containing systems., editing is not supported.

5. Ions

The component editor provides an editor for an ions list. These ions are the “groups” of a salt and are widely used for different models.

| Number | Ion | Formula | Charge (Z) | Mol. Weight [g/mol] | Radius of Ion [Ångström] | Delta-Hf 298.15 K [KJ/mol] | Delta-Gf 298.15 K [KJ/mol] | Delta-cP 298.15 K [J/(mol K)] | D _i |
|--------|-----|---------|------------|---------------------|--------------------------|----------------------------|----------------------------|-------------------------------|----------------|
| 1 | Ba | Ba | 2 | 137.327 | 1.98 | -537.64 | -560.77 | 0 | |
| 2 | Cl | Cl | -1 | 35.453 | 0.99 | -167.159 | -131.228 | -136.4 | |
| 3 | F | F | -1 | 18.998 | 0.72 | -332.63 | -278.79 | -106.7 | |
| 4 | I | I | -1 | 126.904 | 0 | -55.19 | -51.57 | -142.3 | |
| 5 | NO3 | NO3 | -1 | 62.005 | 0 | -207.4 | -111.3 | -86.6 | |
| 6 | SO3 | SO3 | -2 | 80.064 | 0 | -635.5 | -486.5 | 0 | |
| 7 | Be | Be | 2 | 9.012 | 0.9 | -382.8 | -379.73 | 0 | |
| 8 | Br | Br | -1 | 79.904 | 1.14 | -119.57 | -104.16 | -72.3 | |
| 9 | SO4 | SO4 | -2 | 96.064 | 0 | -909.27 | -744.53 | -293 | |
| 10 | S | S | -2 | 32.066 | 1.84 | 33.1 | 85.8 | 0 | |

Show ions containing

The list contains the formula (without charges), the charge, the molecular weight, the radius of the ions, and some thermodynamic properties. The grid is editable.



The context menu of the grid

- Display all salts containing "Ba"
- Copy Hf, Gf, cP values in salt file for "Ba"
- Calculate molecular weight of Ba
- Add "Ba" to salt's ion list

- 1
- 2
- 3
- 4
- 5
- 6
- 7
- 8
- 9
- Other

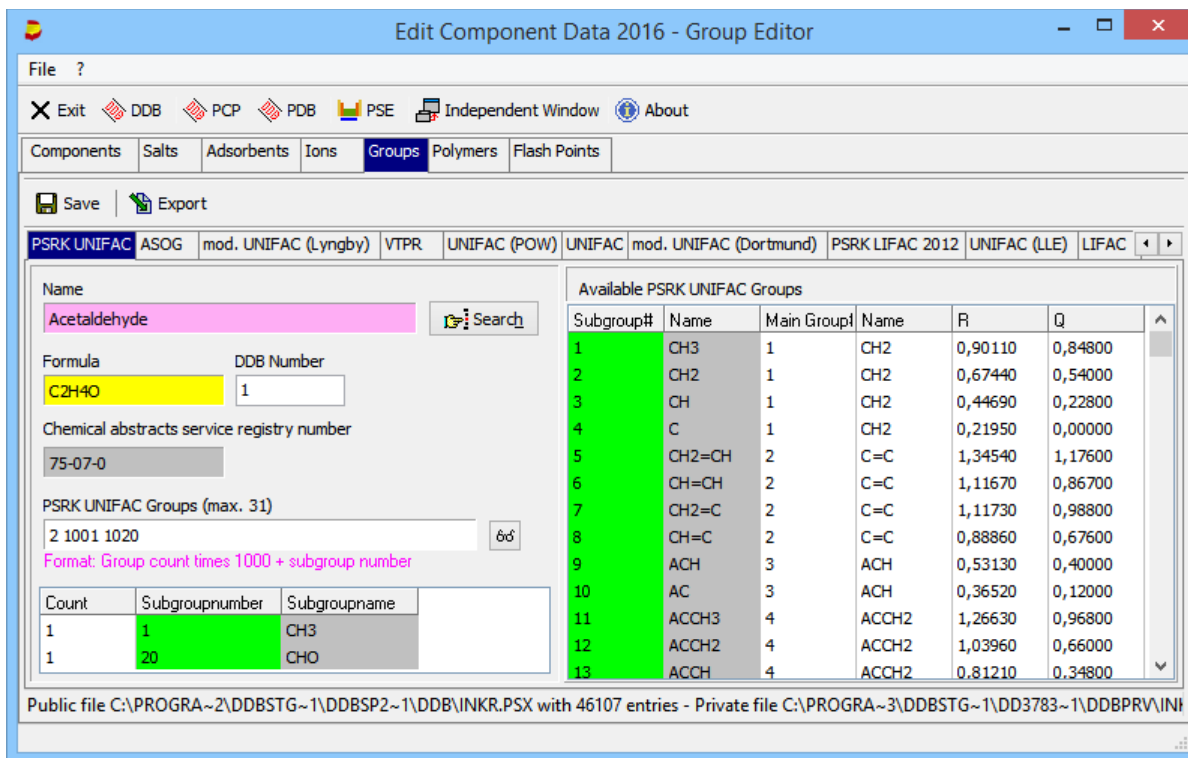
allows

1. searching for all salts containing the ion of the selected line. The salts found will be displayed in the standard component selection program.
2. updating the salts basic file with the H_f, G_f, and c_p values.
3. Calculating the molecular weight of an ion
4. Add the selected ion to the list of ions in the current salt data set.

| Gibbs Energies of Form. kJ/mol | | |
|--------------------------------|----------|----------|
| Salt | Cation | Anion |
| -810.400 | -560.770 | -131.228 |
| Enthalpies of Formation kJ/mol | | |
| Salt | Cation | Anion |
| -868.600 | -537.640 | -167.159 |
| Heat Capacities J/mol*K | | |
| Salt | Cation | Anion |
| 75.000 | 0.000 | -136.400 |

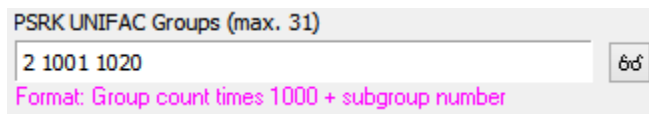
6. Groups

The “Groups” page allows editing group list for the implemented mixture group contribution methods.



This dialog displays the name, formula, CAS-RN and the DDB number of the currently edited component.

The group assignment is displayed in a read-only field because editing the list of groups is performed in the grid below that display field.



The grid allows to enter the group count directly in the left column. Adding subgroups is done by dragging a line from the list of groups to editing grid. Lines are removed by double-clicking.

| Count | Subgroupnumber | Subgroupname |
|-------|----------------|--------------|
| 5 | 9 | ACH |
| 1 | 10 | AC |
| 1 | 24 | CH3O |

This group can also be used for the original UNIFAC and modified UNIFAC (Dortmund) group assignments.

7. Polymers

A. List of Polymers

| # | Names | Monomer | Copolymer Parts |
|---|--|----------------------|-------------------------------|
| 5 | poly(n-butyl methacrylate) | (C8H14O2)n | |
| 6 | poly(vinyl acetate) poly(1-acetyloxyethylene) PVA, PVAc | (C4H6O2)n | |
| 7 | ethylene/vinyl acetate copolymer poly[ethylene-co-(vinyl acetate)] EVA | (C2H4)n(C4H6O2) m | 1 Ethylene 2 Vinyl acetate |
| 8 | poly(methyl methacrylate) poly(methyl-2-methylpropenoate) PMMA | (C5H8O2)n | |
| 9 | polypropylene polypropene Polv(1-methylethylene). PP | (C3H6)n | |

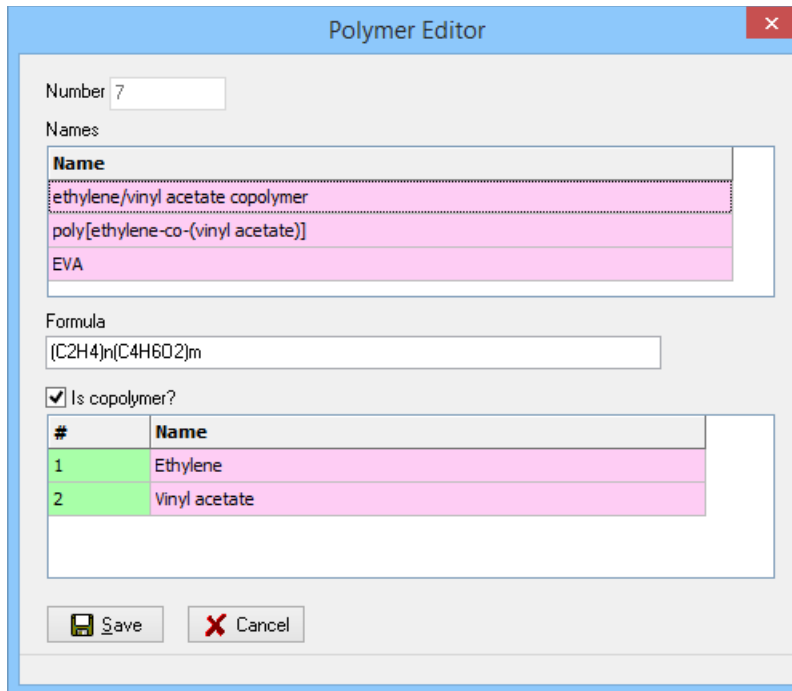
The list of polymers contains names for the polymer, a description of its monomers, and, in case of copolymers, the polymer's monomers. Details like mean molecular weights, mean chain length, supplier, and other details are stored within the single polymer data sets only.

B. Editing Polymers

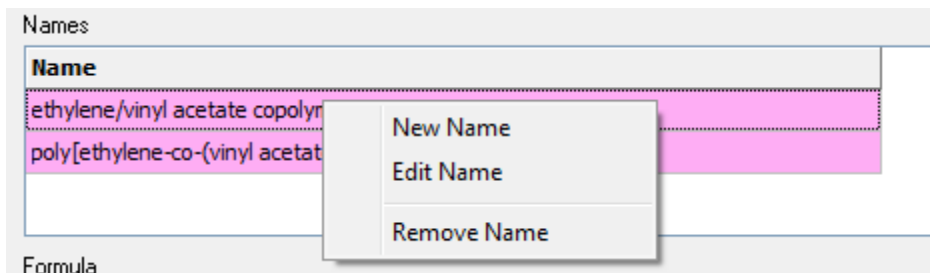
The editor for a single polymer can be opened by a double-click on the grid line or by a context menu.

| | | | |
|---|---|--|-----------------------------|
| 6 | poly(vinyl acetate) | | |
| 7 | ethylene/vinyl acetate copolymer poly[ethylene-co-(vinyl acetate)] | | 1 Ethylene vinyl acetate |
| 8 | poly(methyl methacrylate) | | |

The editor allows to enter several names (one main name and an unlimited number of synonyms). The formula is intended for the description of the monomer's formula. If the polymer described is actually a copolymer the list of building monomers can be added.

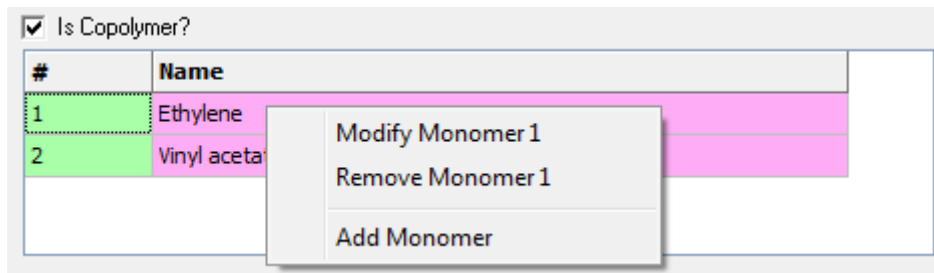


The editing function are all in context menus. The names can be in the grid, whereas the monomers in the copolymer



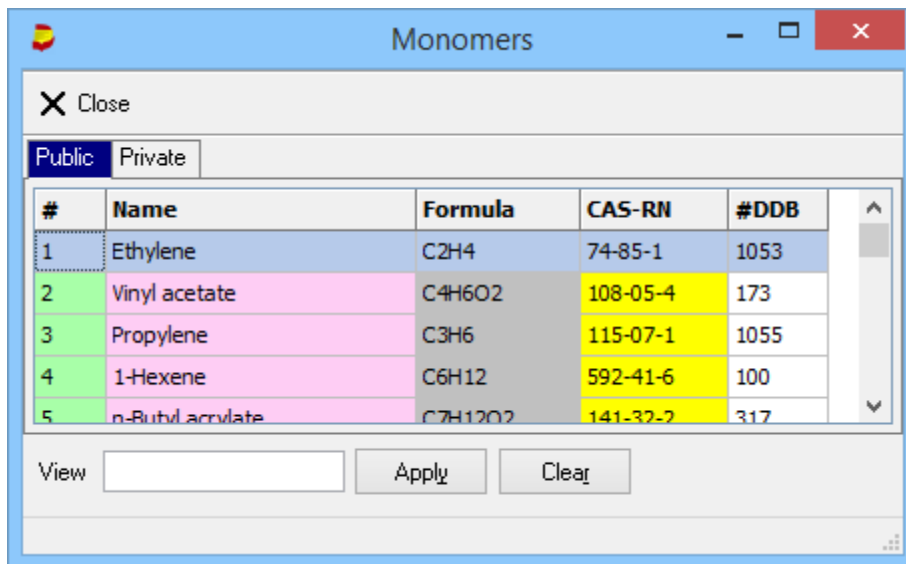
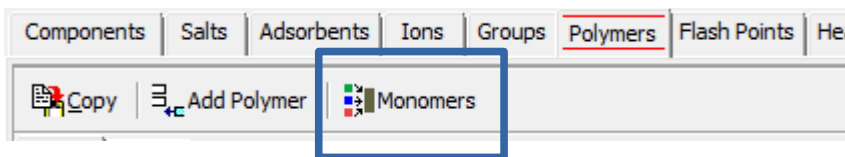
block must be edited by a sub dialog.

C. Editing Monomers

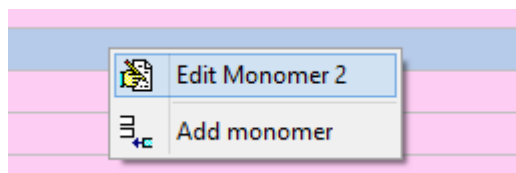


Monomers are managed in a separate list. This list is used in the copolymer editor (part of the polymer editor dialog) but can also be displayed by the button

Monomers in the tool bar if the polymer list display. The editor for single monomers can be call through the context menu of the monomer's

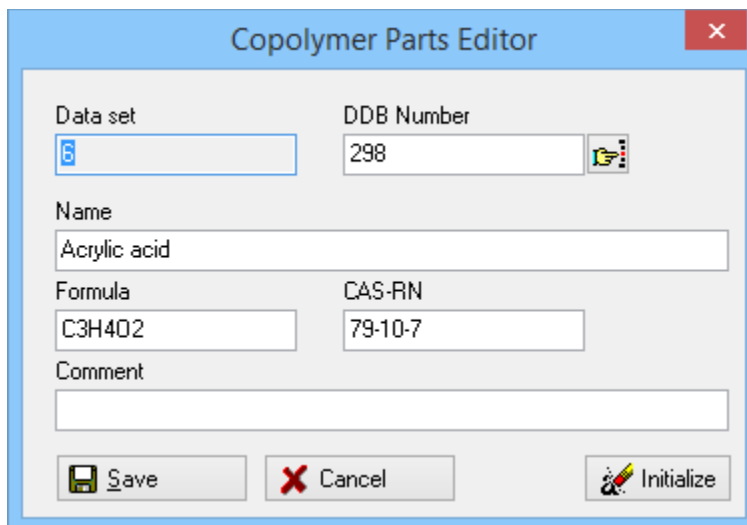


grid.

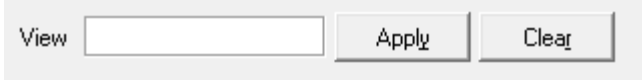



The editor allows to edit a single name, a formula, a CAS registry numbers and a comment.

If the monomer is part of the normal DDB component list its DDB number can and should be specified. If a DDB



number has been selected it is possible to use the entries from the component basic file to fill the entries of this dialog.

The  part of the Monomers dialog allows to shorten the list of monomers by filtering the names by the text entered. For example, if the filter is set to “Acrylat” only monomers with the name's part “Acrylat” are displayed. Capitalization is ignored.

 removes the filter and display the entire list again.

8. Flash Points

File ?

Exit DDB PCP PDB

PSE Independent Window About

Components Salts Adsorbents Ions Groups Polymers **Flash Points**

Save Copy Export

Name
Ethanol Search

Formula DDB Number
C2H6O 11

| Property | Value |
|---|-------|
| Flash Point [°C] | 12 |
| Fully Miscible with Water at 15°C | yes |
| Lower Explosion Limit [g/m ³] | 59 |
| Lower Explosion Limit [Vol-%] | 3.10 |
| Upper Explosion Limit [g/m ³] | 532 |
| Upper Explosion Limit [Vol-%] | 27.70 |
| O ₂ Limiting Concentration [Vol-%] | 8.50 |
| Max. Explosion Pressure [bar] | 8.40 |
| Ignition Temperature [°C] | 400 |
| Max. Experimental Safe Gap [mm] | 0.89 |
| Temperature Class | T2 |
| Explosion Group | IIB |

Brandes E., Möller W.,
Sicherheitstechnische Kenngrößen, Band 1: Brennbare Flüssigkeiten und Gase,
Wirtschaftsverlag NW, Verlag für neue Wissenschaft GmbH, Bremerhaven

Almost all the entries are from

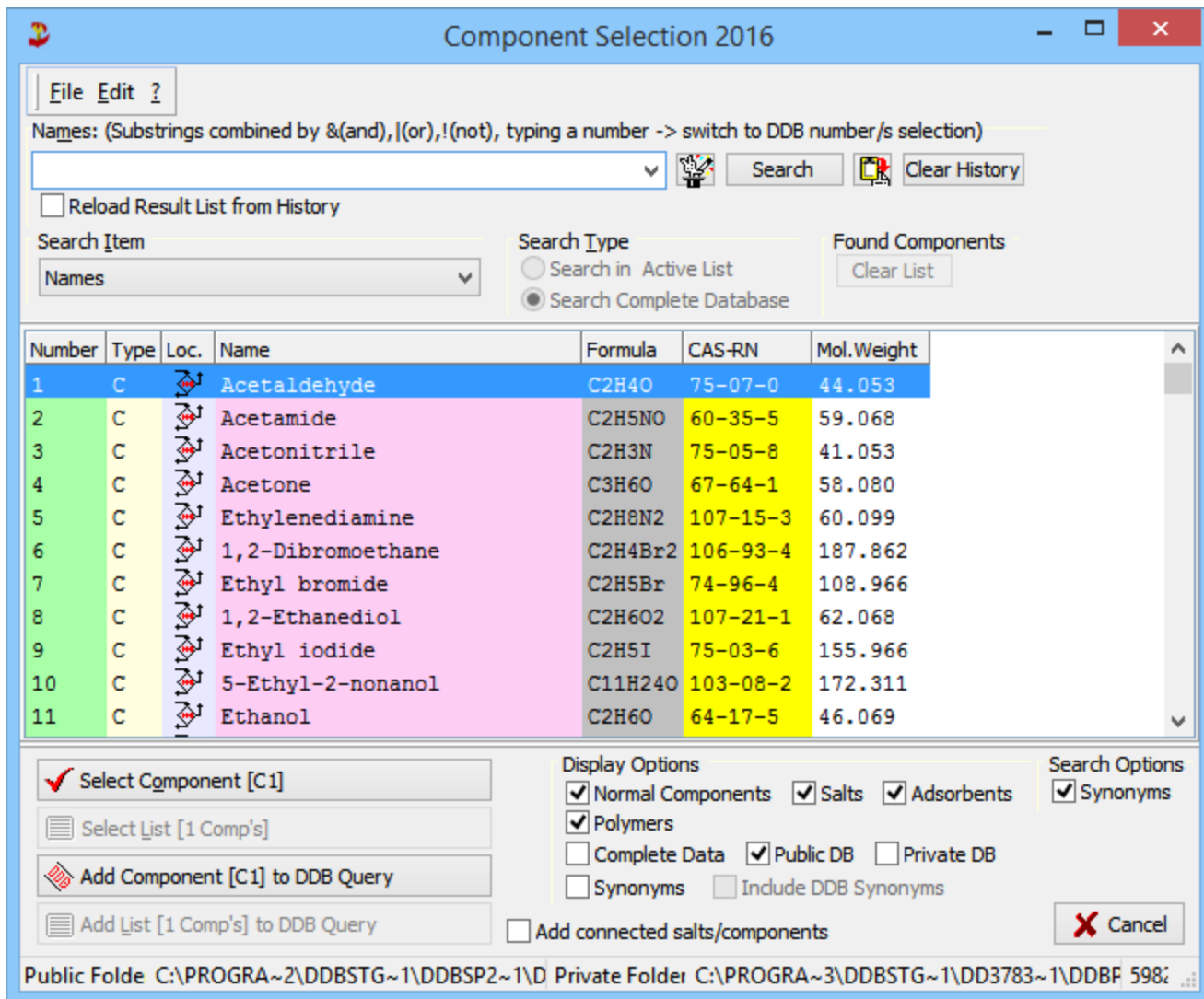
Brandes E., Möller W., “Sicherheitstechnische Kenngrößen”, Band 1: Brennbare Flüssigkeiten und Gase”,
Wirtschaftsverlag NW, Verlag für neue Wissenschaft GmbH, Bremerhaven

(“Safety-related characteristics”, Volume 1: “Inflammable Liquids and Gases”)

Data are available for almost 1900 components – but the data sets are rarely complete.

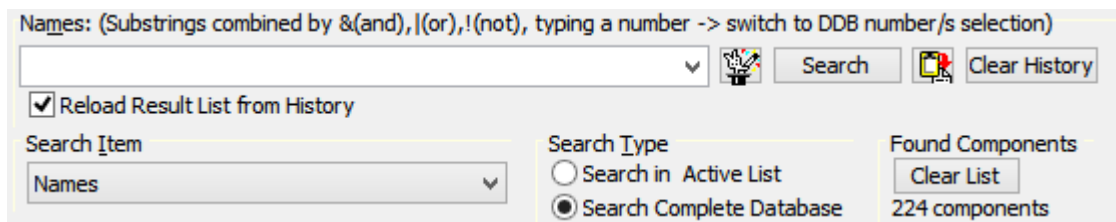
9. Searching Components

The DDB software uses a single dialog to search for components by a variety of criteria.



A. Dialog Parts

a. Search Queries



This part allows to specify a search by different criteria.

b. Component List

This part displays the list of components – either the complete list or a search result

| Number | Type | Loc. | Name | Formula | CAS-RN | Mol.Weight |
|--------|------|------|-------------------|---------|----------|------------|
| 1 | C | | Acetaldehyde | C2H4O | 75-07-0 | 44.053 |
| 2 | C | | Acetamide | C2H5NO | 60-35-5 | 59.068 |
| 3 | C | | Acetonitrile | C2H3N | 75-05-8 | 41.053 |
| 4 | C | | Acetone | C3H6O | 67-64-1 | 58.080 |
| 5 | C | | Ethylenediamine | C2H8N2 | 107-15-3 | 60.099 |
| 6 | C | | 1,2-Dibromoethane | C2H4Br2 | 106-93-4 | 187.862 |
| 7 | C | | Ethyl bromide | C2H5Br | 74-96-4 | 108.966 |
| 8 | C | | 1,2-Ethanediol | C2H6O2 | 107-21-1 | 62.068 |
| 9 | C | | Ethyl iodide | C2H5I | 75-03-6 | 155.966 |
| 10 | C | | 5-Ethyl-2-nonanol | C11H24O | 103-08-2 | 172.311 |

c. Display Options

The display options change the component display:

- Component types. The DDB know four types of components:
 - Normal components
 - Salts
 - Adsorbents
 - Polymers
- Complete Data. This option extends the display of normal components by several properties like T_c , P_c , V_c , etc.
- DDB Location. Two locations are supported. The public list is the data bank distributed by DDBST and the private list is from the user.
- Synonyms. This option allows to display synonyms directly in the component list. The DDB synonyms are normally not very useful and can be showed or hidden separately.

Display Options

 Normal Components
 Salts
 Adsorbents
 Polymers
 Complete Data
 Public DB
 Private DB
 Synonyms
 Include DDB Synonyms

Search Options

 Synonyms

| Number | Type | Loc. | Name | Formula | C |
|--------|------|------|---|---------|---|
| 1 | C | | ACETALDEHYD Acetaldehyde AspenAlias: C2H4O-1 AspenID: 10151 AspenName: ACETALDE Ethanal OXOETHANE UN: 1089 | C2H4O | 7 |

The search option “Synonyms” allows switching the synonyms search on or off. The synonyms search is rather slow and if the names are simple a search in the main names might be sufficient.

d. Commands

Select Component [C1]

Select List [5 Comp's]

Add Component [C1] to DDB Query

Add List [5 Comp's] to DDB Query
 Add connected salts/components

These buttons allow to

- select a single component (the currently selected component, the components's code is appended to the button's caption)
- select a list of components (the list's size is appended to the button's caption)

- add a single component to the Dortmund Data Bank query
- add a list com components to the Dortmund Data Bank query.

The first two buttons will close the dialog but the latter two will keep the search result window open.

The option “Add connected salts/components” is necessary for components that are both in the normal component list and in the salt list. The reason is that salts are treated as normal components in most data banks. Salts are treated as separate components only in the salt solubilities (ESLE) data bank and in the vapor-liquid equilibria data bank containing salts (ELE). The reason is that only for these kind of data salt-specific parameters are needed.

B. Search Criteria

The different search types can be set by the drop-down menu in the “Search Item” area of the dialog. This control has a context menu where the single entries are repeated.

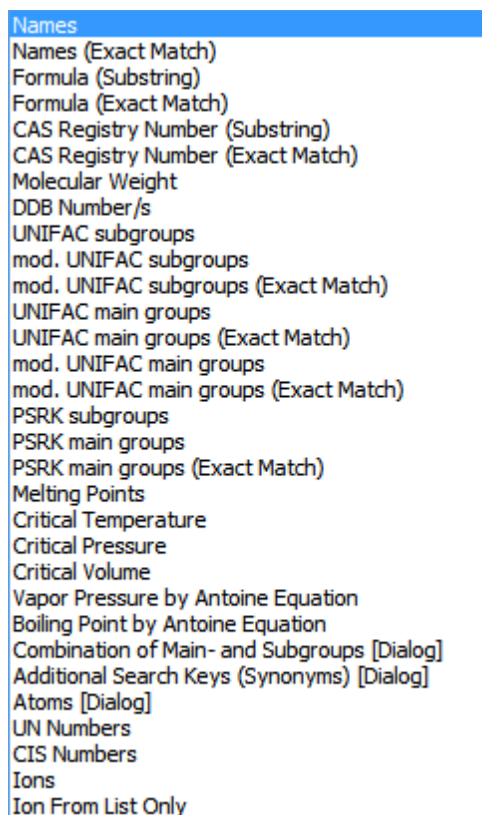


Figure 1: Search Items: Drop-Down Menu

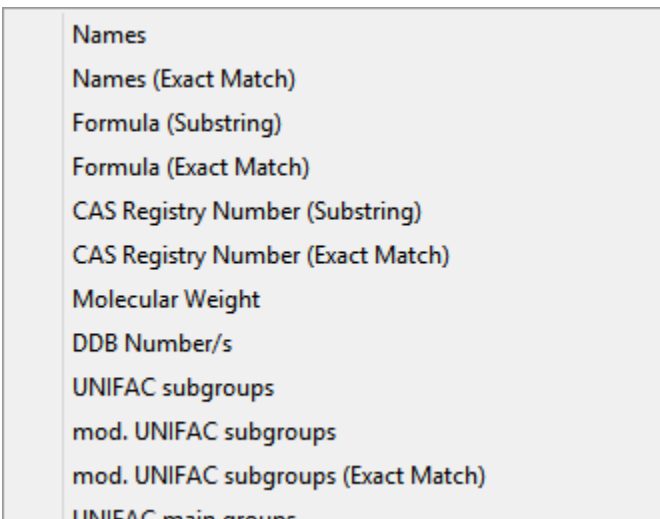
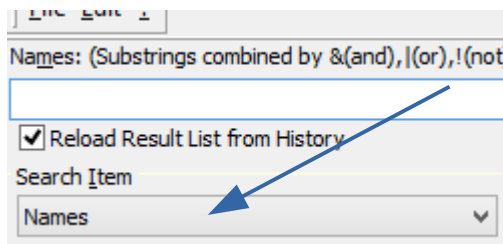


Figure 2: Search Items: Context Menu

a. Search for Names

The search for names can either be a sub-string search or an exact match search. In case of a sub-string search several operators can be used to combine the parts:

| <i>Operator</i> | <i>Used to</i> |
|-----------------|---|
| ! | NOT Excludes strings. If a string is prefixed with the exclamation sign it must not be part of the name |
| & | AND Tells the search routine that both parts before and behind the ampersand must be given. |
| | OR (Pipe symbol) Tells the search routine that either one or the other part or both parts must be present. |

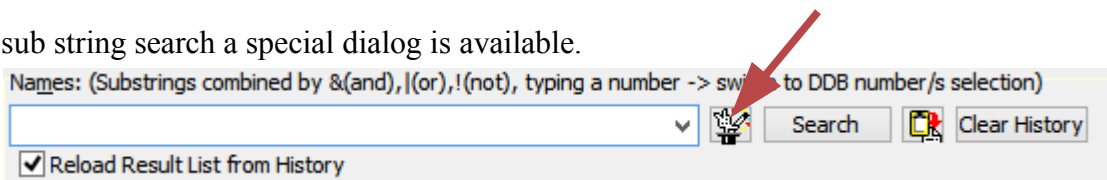
Example searches:

| | |
|-------------|--|
| brom&chlor | Searches for names where both “brom” and “chlor” is present. 2-Bromo-2-chloro-pentane Bromochloromethane [R30B1] |
| brom chlor | Searches for names where “brom” or “chlor” is present. 2-Bromo-pentane 3-Chloro-hexane Chlorine |
| brom&!chlor | Searches for names containing “brom” but “chlor” must not be present. |

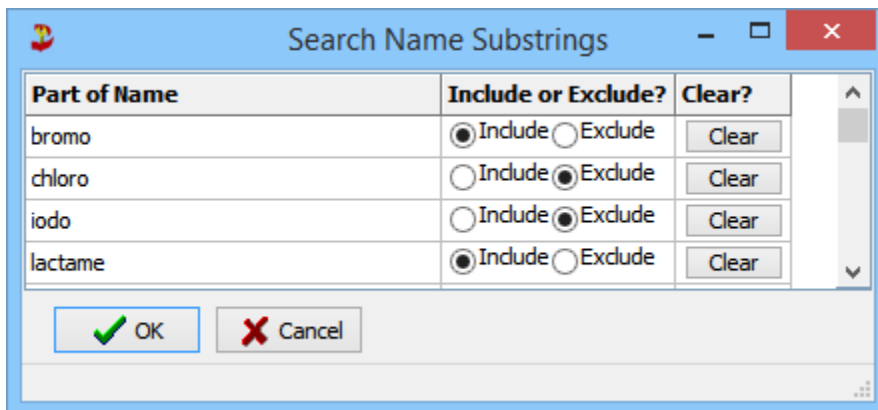
All searches are case-insensitive.

If a substring search finds an exact match the search result list will contain these exact matches as first matches.

For names sub string search a special dialog is available.



The dialog



allows the specification of search strings without the somewhat awkward operators.

b. UNIFAC sub group and main group searches

The group searches allow some kind of structural search because the UNIFAC groups are mostly defined by standard functional groups like ketones, alcohols, etc. The component selection is extended by the selected group list. These numbers have to be entered in the main query edit field:

| UNIFAC Main Groups | |
|--------------------|-------|
| Number | Name |
| 1 | CH2 |
| 2 | C=C |
| 3 | ACH |
| 4 | ACCH2 |
| 5 | OH |
| 6 | CH3OH |
| 7 | H2O |
| 8 | ACOH |
| 9 | CH2CO |
| 10 | CHO |

Main Groups: (Numbers combined by &(and), |(or), !(not))

589

Reload Result List from History

Search

The numbers can be combined with the same operators that have been explained for the sub string search.

c. Empirical Formulas

The search for formulas be performed as sub string or as exact match search.

d. CAS Registry Number

The search for registry numbers be performed as substring or as exact match search. The search requires that the numbers are entered including the hyphens (513-86-0 instead of 513860).

CAS-RN: (CAS registry number, exact match)

75-03-6

Reload Result List from History

Search Clear History

e. Molecular Weight

The molecular weight search requires two numbers separated by blanks: The wanted molecular weight and a value for an acceptable deviation which can be 0.

Molecular Weight: (Weight and maximum deviation)

123 1

Reload Result List from History

Search Clear History

f. DDB Numbers

This search allows to search components directly by the DDB definition numbers (4 for acetone, 31 for benzene, 95 for 2-Propanol, etc.). It is possible to enter multiple numbers. These numbers have to be separated by blanks.

DDB Number/s: (Typing a non-number -> switch to names search)

23 32 36

Reload Result List from History

Search Clear History

g. Critical Temperature, Pressure, Volume

This search require two values separated by blanks: A wanted critical value and an acceptable deviation.

Critical Temperature: (Temperature [K] and maximum deviation)

400 10

Reload Result List from History

h. Vapor Pressure by Antoine

This search allows to find components with a wanted saturated vapor pressure at a given temperature. The component selection program open a special dialog where the data can be entered.

After pressing the Okay button the values are moved to the query edit control and the search can be started.

Vapor Pressure: (P [kPa], maximum deviation in P [kPa], T [K])

150 5 425

Reload Result List from History

Vapor Pressure Search

Pressure [kPa] Allowed Pressure Difference [kPa]

150 5

at Temperature [K]

425

In this example we will find Ethyl benzene which has a vapor pressure of $P=151.6$ kPa at 425 K.

i. Boiling Point by Antoine

This is the reverse search. A dialog opens where a wanted boiling temperature and a pressure can be specified.

Boiling Point Search

Temperature [K] Allowed Temperature Difference [K]

400 5

Pressure [kPa]

101.325

Boiling Point: (T [K], maximum deviation in T [K], P [kPa])

400 5 101.325

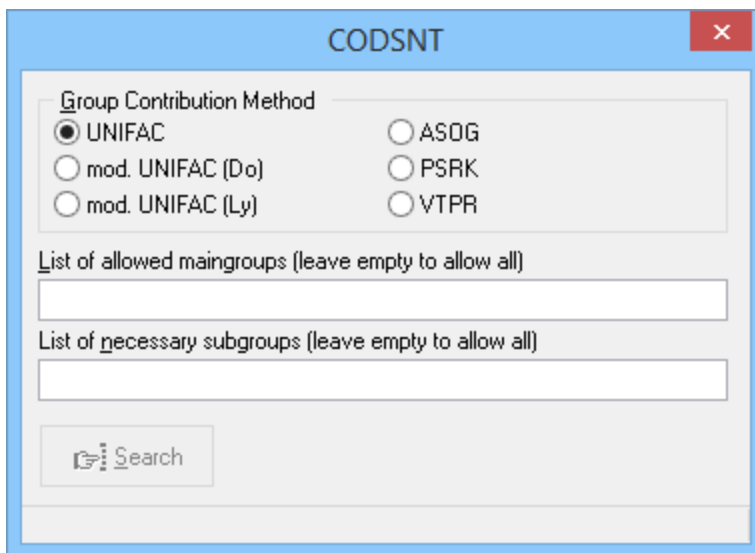
Reload Result List from History

If the pressure is set to 101.325 kPa the search will yield components with normal boiling points near the entered temperature.

The example will return 2-Methyl pyridine which has a normal boiling of $T_B=402$ K.

j. Combination of main and subgroups

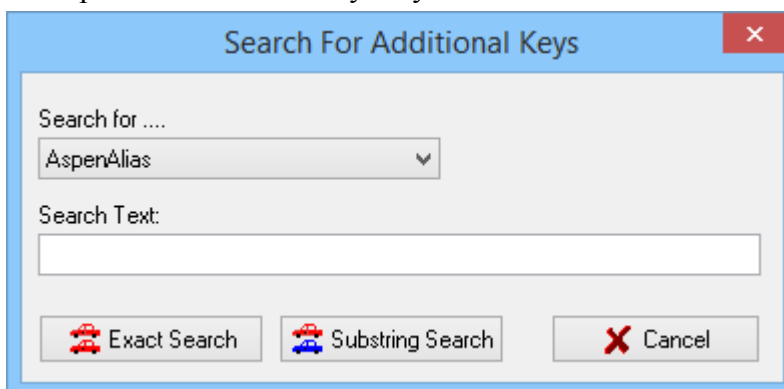
This search opens directly a dialog:



This search allows to search for components with some special combinations of main and sub groups. This search is mainly used internally for the UNIFAC development and is of little use for normal queries.

k. Additional Search Keys (Synonyms)

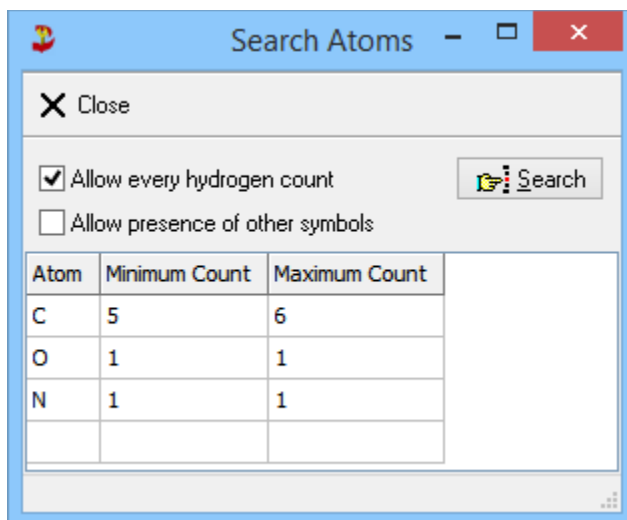
This search allows to search special entries in the synonyms file.



Typically search entries are the Aspen Alias, the Aspen ID, and the Aspen Name.

l. Atoms

This search mode open directly an additional dialog where atoms and their counts can be entered. This search analyzes the empirical formula and searches for components with specified atom types.



The search options are:

- “Allow every hydrogen count”: Hydrogens are not specified in the table and can be present in the component in every number.
- “Allow presence of other symbols”: This option decides whether the search criterion is “exact match” or not.

The example will find ϵ -Caprolactam ($C_6H_{11}NO$).

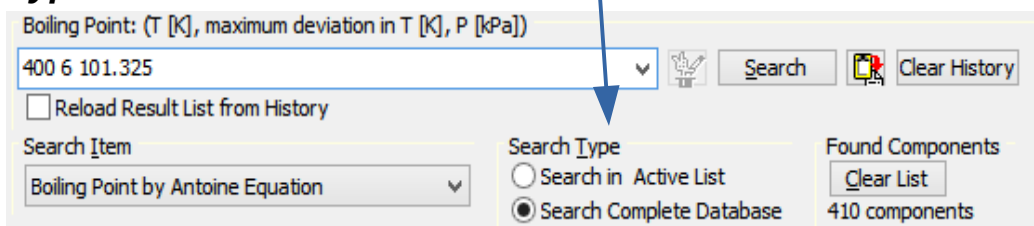
m. UN Numbers

The UN numbers are numbers with four digits specifying some special components and some component class.

n. CIS Numbers

CIS number are specific numbers of the Lonza AG and are only available on request and on special affirmation.

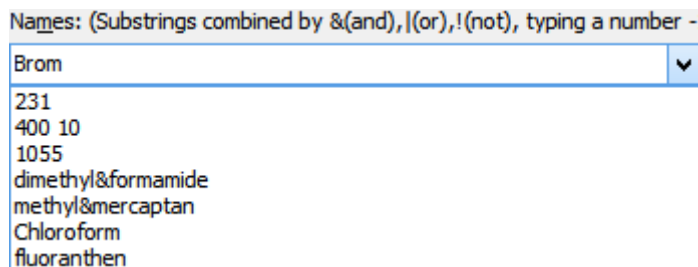
C. Search Type



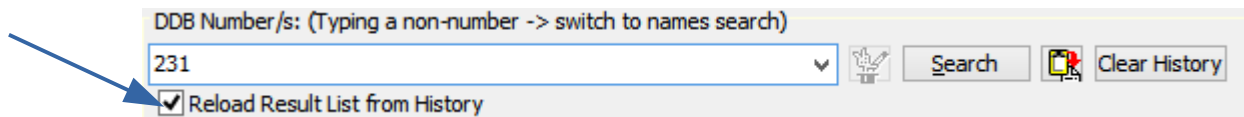
A search can be restricted to the result list of a previous search. This allows to perform different searches sequentially.

D. Search History

The component selection stores the last ten searches. These latest queries are listed in the drop-down menu of the query edit control.



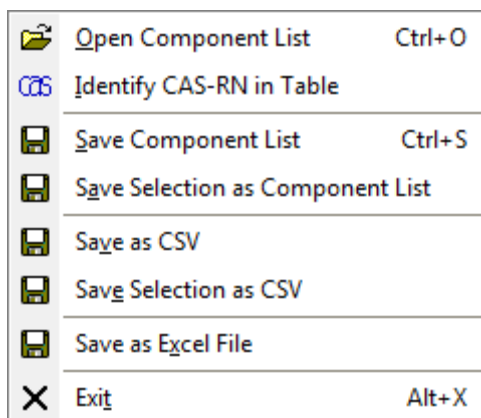
Besides the queries the search result lists are also stored. These list are recovered if the “Reload Result List from History” box is checked.



The complete history can be deleted by the “Clear History” button.

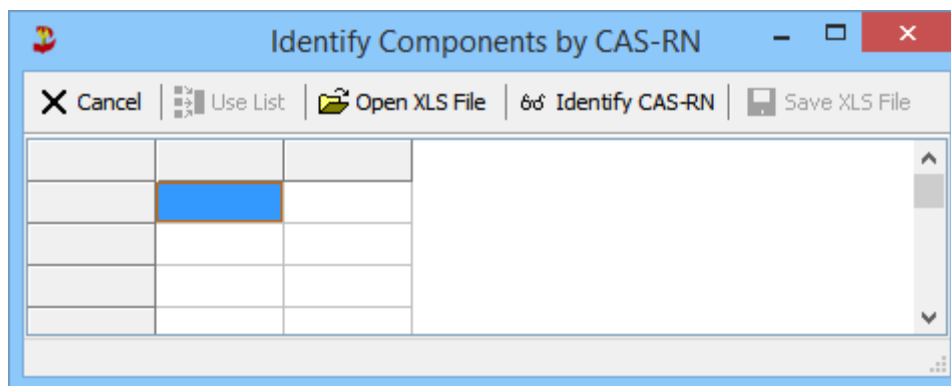
E. The Menus

a. File Menu



The file menu allows to open and save component list in a DDB specific format containing DDB component numbers. A CSV (comma-separated values) will contain the content of the component grid and can be easily loaded in spread sheet programs like Microsoft Excel or OpenOffice/LibreOffice Calc.

For identifying CAS registry numbers a separate dialog is shown where a Microsoft Excel file can be imported.

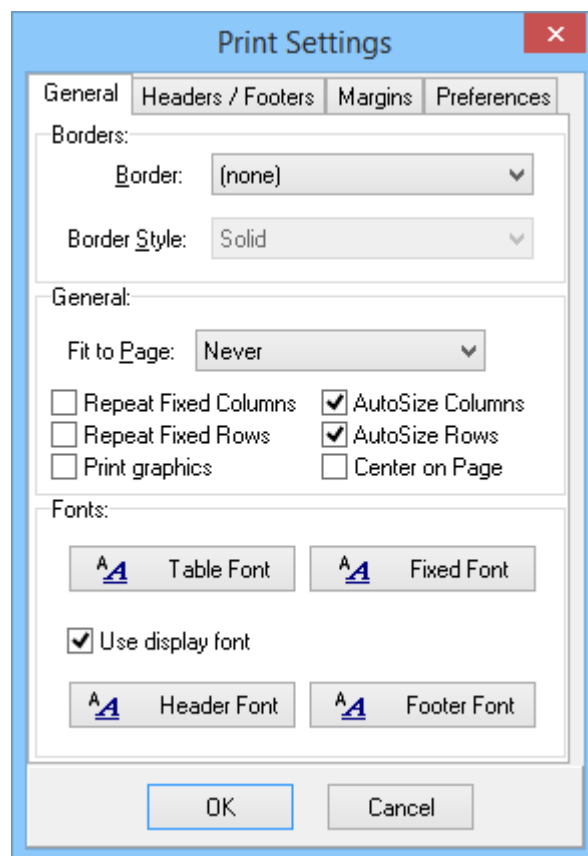
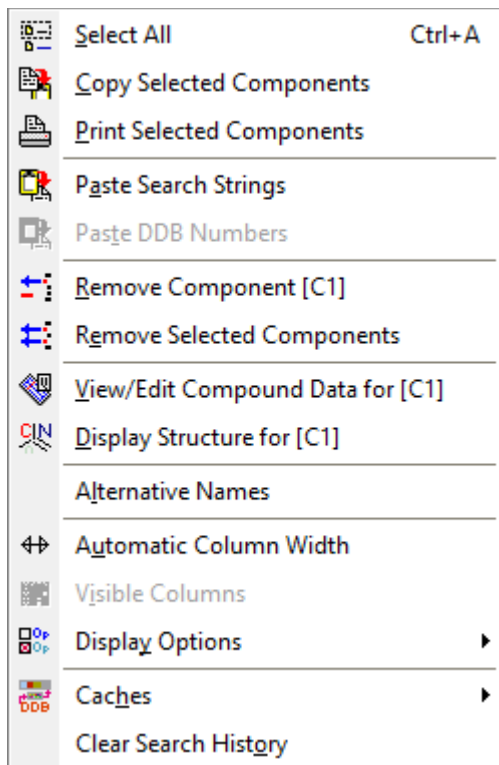


This function searches all grid cells for valid CAS-RN numbers. These cells get a green background and an additional column is added with the DDB numbers of the identified components.

If some components have been identified it is possible to use that list as component list like a search result. The modified table can also be saved a Excel “xls” file.

b. Edit Menu

1. “Select All”
Select all currently shown components (all or result of search)
2. “Copy Selected Components”
Copies the selected lines of the component grid to the Windows clipboard.



3. “Print Selected Components”
Print the selected line of the component grid. The program opens a “Print Settings” dialog where several options are available.
4. “Paste Search Strings”
This dialog can be used to perform multiple searches for strings pasted from the Windows clipboard. A left-click or a right-click in one of the table cells opens a context menu with the different search options.
5. “Remove (Selected) Components”
Removes single or selected lines from the component list

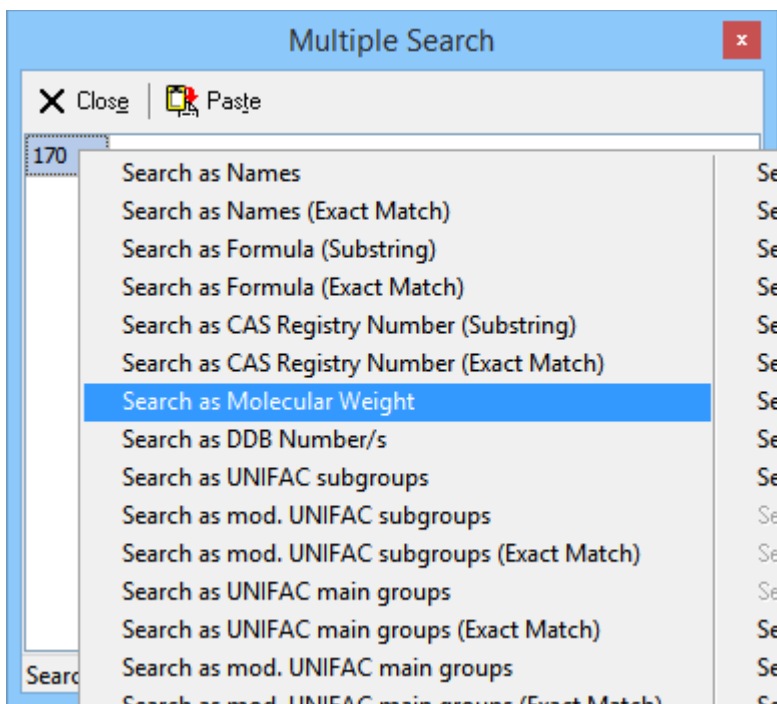
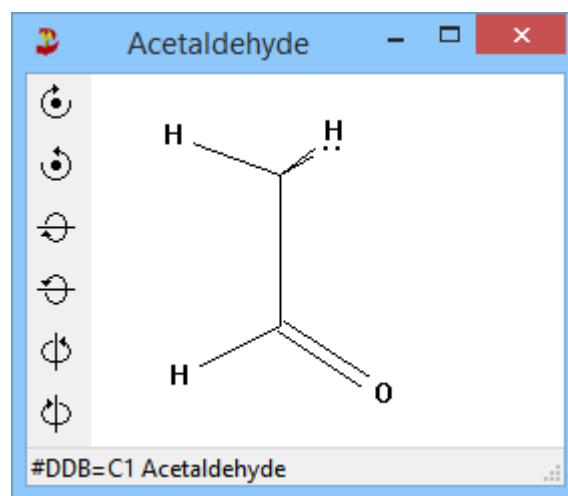
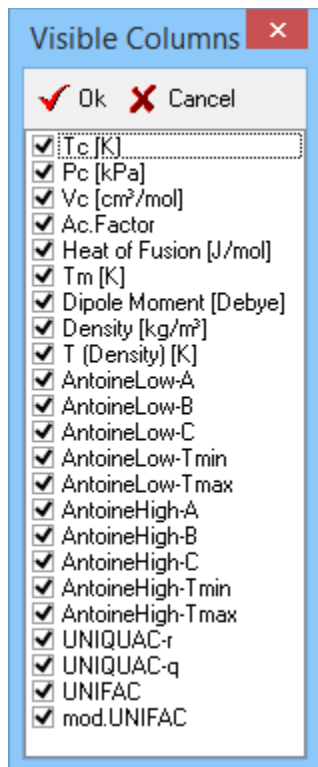


Figure 3: Multiple Search for Pasted Search Strings

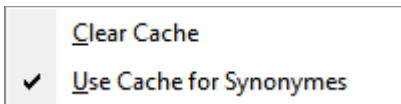
6. “View/Edit Compound Data” for [????]
Starts the component editor.
7. “Display Structure for [????]”
Displays a simple plot of the selected component.
8. “Alternative Names”
The basic component list (without synonyms) contain two names – one main and one alternative (formerly mainly German names)
9. “Automatic Column Widths”
This function adjusts the column widths of the component grid to the size of the contents.
10. “Visible Columns”
If “Complete Data” (see Display Options) is selected this function allows selecting the visible columns.
11. “Display Options”
See chapter “Display Options”.





12. “Caches”

The synonyms cache accelerates the search in the synonyms dramatically but needs a fair amount of memory. Clearing the cache allows to free some memory but mainly it is important if changes done in the main component editor must be visible in the component selection.



13.13. “Clear Search History”

Removes all saved queries.