

Pure Data Editing

Editing/Modifying DDB Pure Component Data

DDBSP - Dortmund Data Bank Software Package



DDBST

DORTMUND DATA BANK
SOFTWARE & SEPARATION
TECHNOLOGY

DDBST Software & Separation Technology GmbH

Marie-Curie-Straße 10

D-26129 Oldenburg

Tel.: +49 (0) 441 361819 0

Fax: +49 (0) 441 361819 10

E-Mail: support@ddbst.com

Web: www.ddbst.com

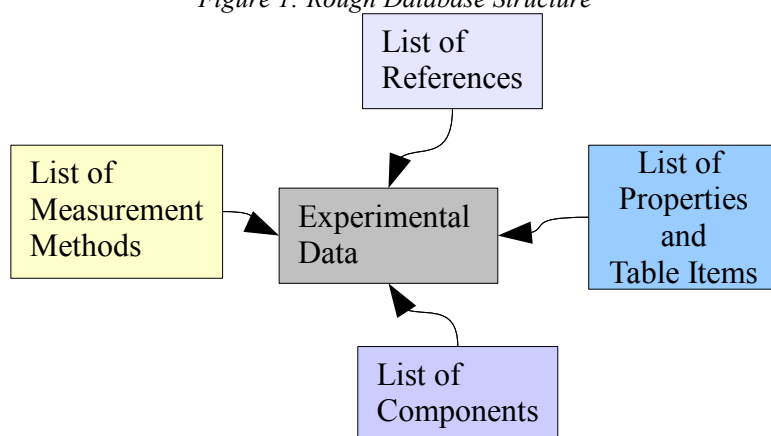
Contents

Introduction.....	3
Starting the program	3
Defining the Reference.....	4
Adding a New Reference.....	4
Searching for References.....	5
Adding Datasets to the Current Reference	6
Adding Necessary Specifications for Single Sets.....	7
Component Selection.....	7
Property Selection.....	9
Specifying Table Entries and Their Units.....	9
Purity of the Component.....	10
Measurement Quality.....	10
International Temperature Standard.....	11
State.....	11
Measurement Method.....	12
Constant Value, Unit, Value.....	12
Data Input.....	12
Saving Data to File.....	14
Adding Datasets to the Private Databank.....	15
Modifying Datasets in the Database.....	17

Introduction

This document is intended as a tutorial for entering private, customer-owned pure component data in the Dortmund Databank (DDB).

Figure 1: Rough Database Structure



The pure component properties database contains experimental data plus additional data like references, measurement methods, a component specification and some other related information.

Components, measurement methods and references are stored separately from the experimental data. It is necessary to update these external lists before (new) references, methods, or components can be selected.

Properties and table items are also defined outside this editor in a definition file.

EditPureData (normally) does not edit sets in the database directly. Instead it works on files which can be added to the database. This working mode allows to keep originals of the edited data whereas the database only contains recalculated and even somewhat “trimmed” data.

Editing data bank sets directly is possible though and will be explained at the end of this tutorial.

Starting the program

The program for editing pure component properties is “EditPureData” and can be found in the “Editors” program folder.

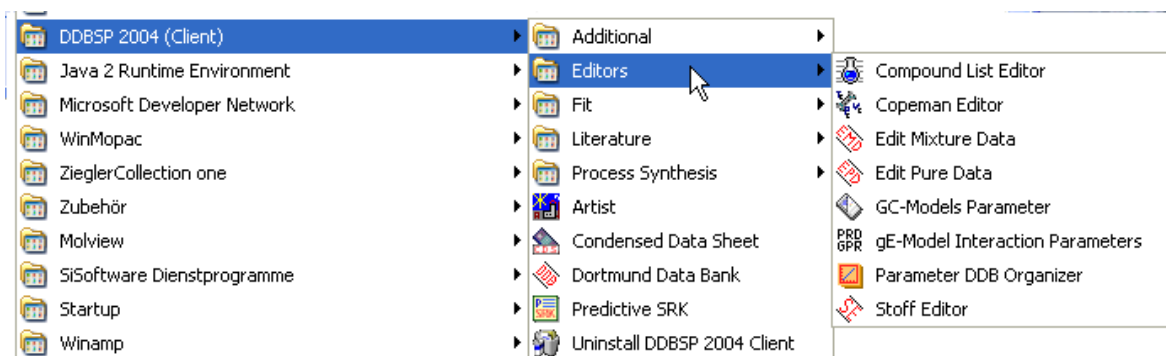


Figure 2 Program Folder

The programs start with a screen showing only some edit fields regarding literature information:

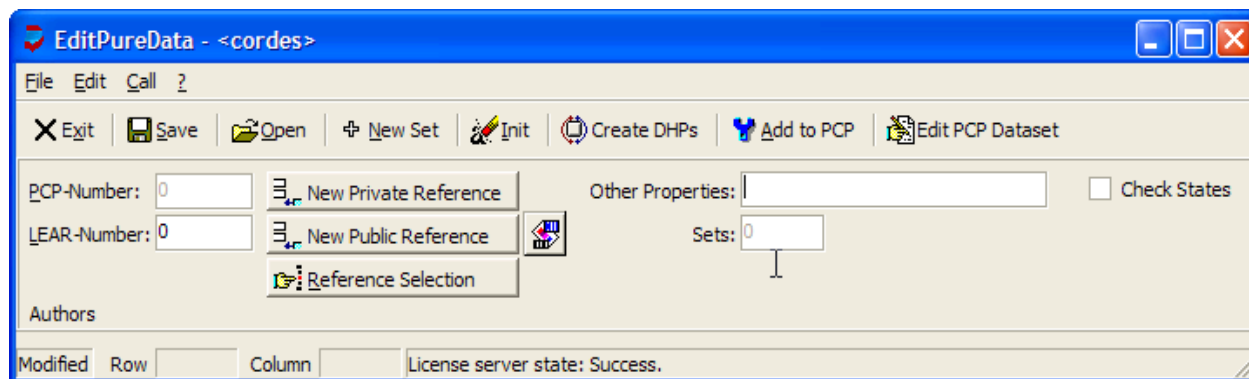



Figure 3 Initial Dialog

This document tries a stepwise introduction in the usage of this programs. It starts with the necessary prerequisite for all DDB datasets.

Defining the Reference

Every dataset in the DDB is referenced. The reference is normally an article from a scientific journal but might be also a thesis or a report.

Adding a New Reference

For new private datasets it is normally recommended to create a new private reference. A reference can be insert by selecting the button  - a menu item in the "Edit" is also available. If no private literature databank is present the program asks if it shall create a new one.

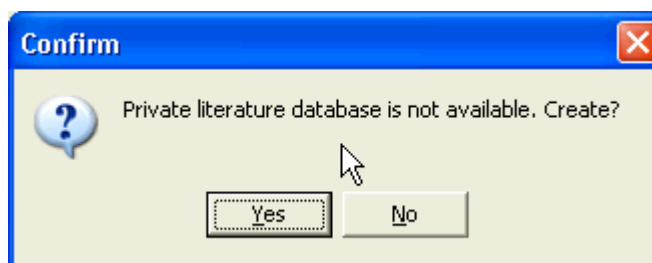


Figure 4 New Reference - Database Creation

After confirming with "Yes" the literature management program displays the edit dialog for a new reference (see below).

Figure 5 New Reference - Editor

None of the entries are necessary to enter, even the completely empty sheet can be saved. But it is recommended to define at least authors.

The next question is

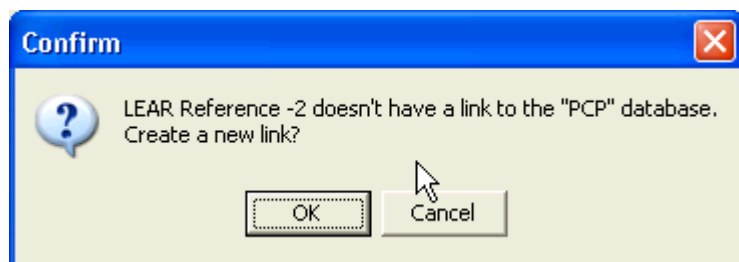
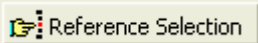


Figure 6 New Reference - Link Creation

You **have** to select “OK” if you want to use the new reference. “Links” are obligatory keywords in the literature database for determining the databases – in case of EditPureData the pure component properties database - where the reference is in use.

A more detailed description of the literature management program (LEAR) is available.

Searching for References

If you don't want to create a new reference you have to search the available literature databank for the wanted article or report. After selecting the  Reference Selection button a search query dialog is opened.

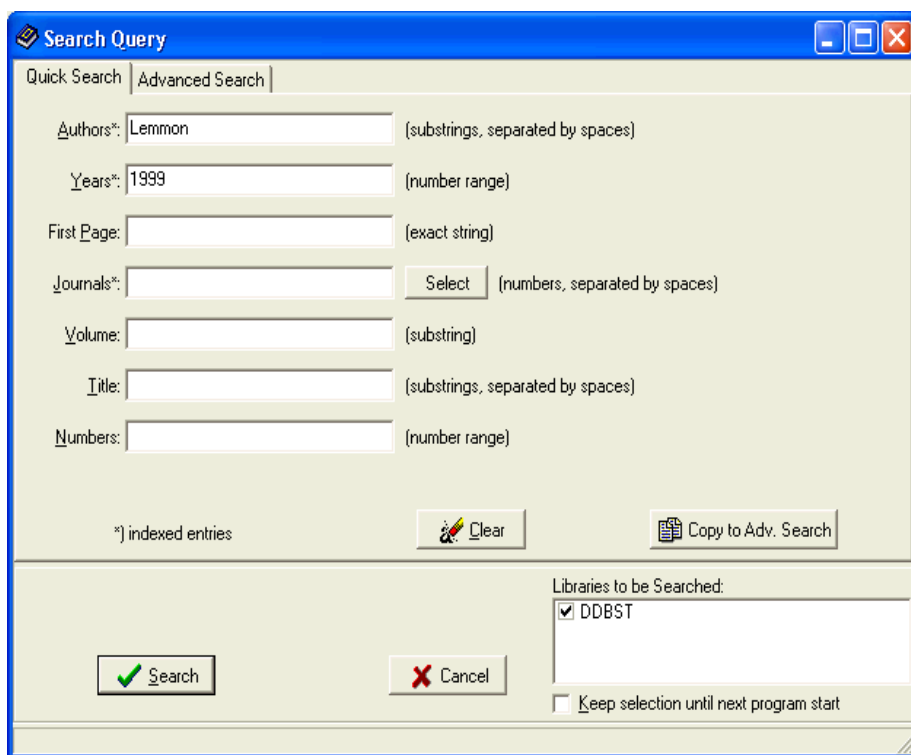


Figure 7 Reference Search - Search Query

The result for the given example is

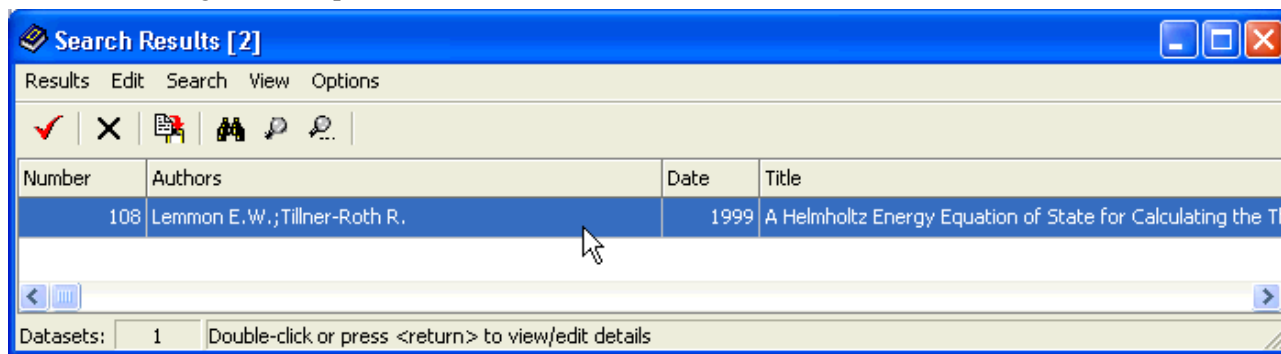

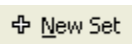


Figure 8 Reference Search - Search Result

Select  to select the reference. If a PCP link is missing it will be created like for new datasets.

Adding Datasets to the Current Reference

EditPureData works reference-centered. All datasets from a single reference can be edited together.

For appending (empty) datasets to the current reference select the  button. Using it twice EditPureData shows the following screen:

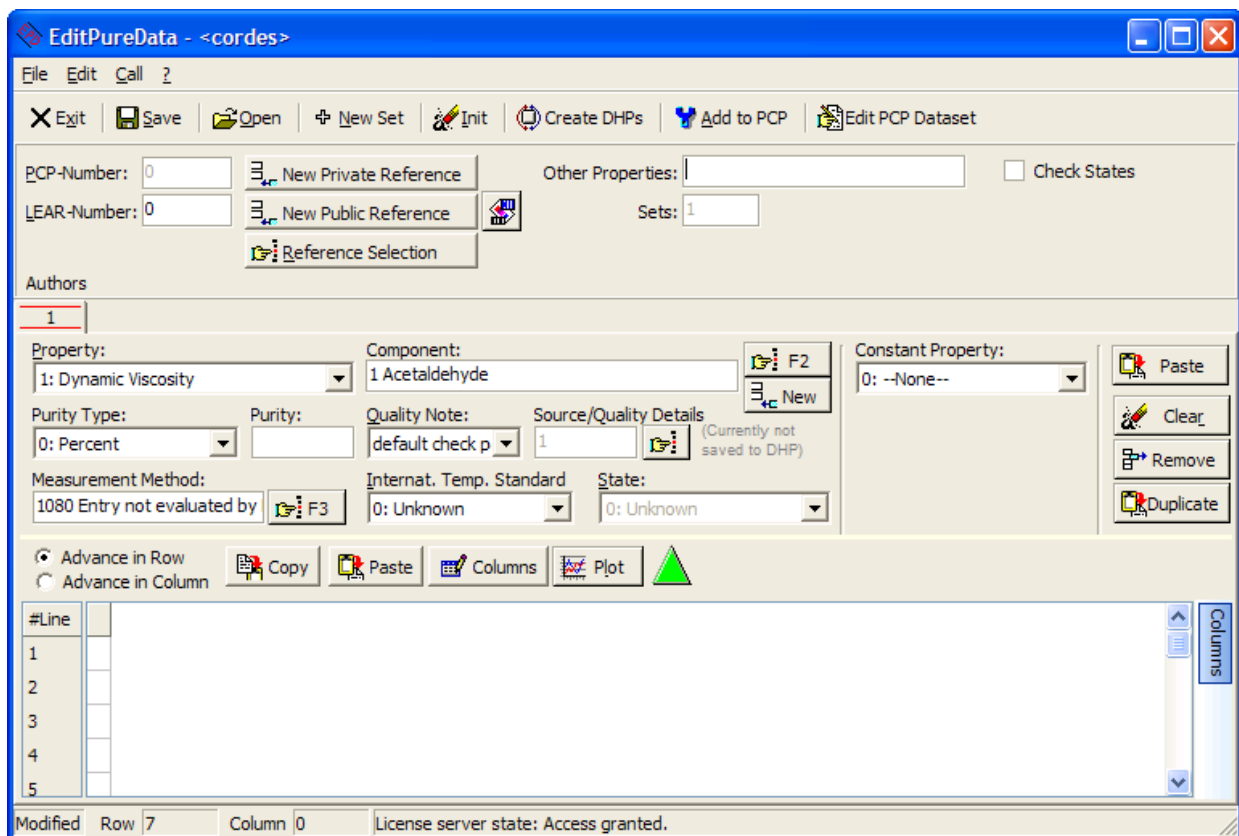
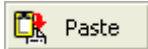
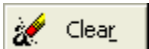
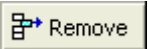


Figure 9 Adding Datasets

The buttons , ,  allow to paste selected entries from other sheets, clear the current sheet or to remove the current set.

Adding Necessary Specifications for Single Sets

Necessary specifications are

1. Component
2. Property
3. Table entries
4. Units of table entries

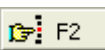
Additional specifications are

1. Purity of the component
2. Quality of the measurement or data
3. Used internal temperature standard
4. State ('Unknown' is possible)
5. Measurement method
6. A constant value, its unit and value
7. Errors for table items with their units

Component Selection

Component:
1 Acetaldehyde

 F2
 New

F2 or selecting the  button starts the program
ComponentSelection:

This program displays the entire list of components available in the DDB. For this tutorial it is sufficient to double-click line number 5 (Ethylenediamine).

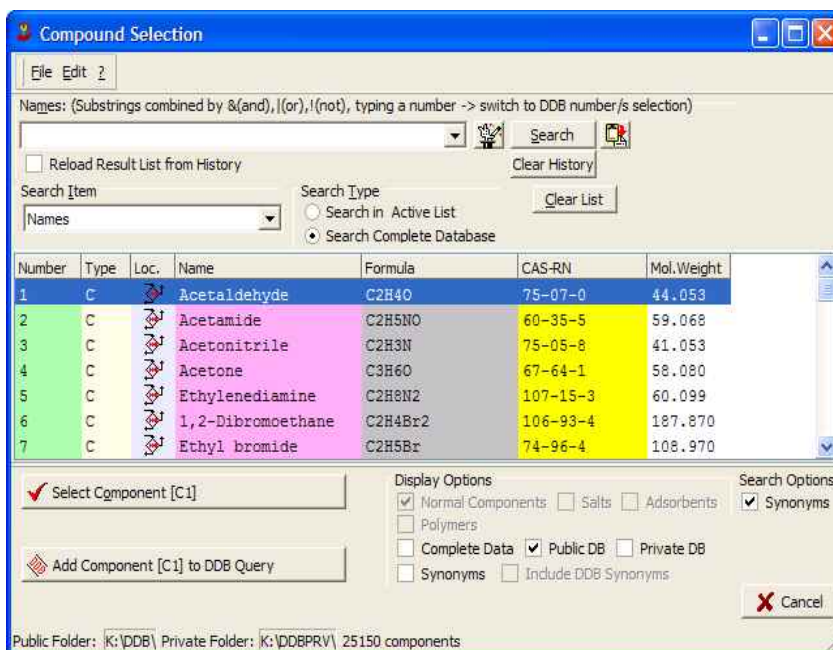
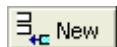


Figure 10 Component Selection

The selected component is shown now in the edit field besides the search button:

Component:
5 Ethylenediamine

If you have a new component you can enter quickly a new one by selecting the



button.

The “New Component” dialog allows to enter two different names a CAS registry code, a molecular weight and the empirical formula.

Almost all entries are necessary mainly for calculation purposes.

The new component can either be stored in the public DDBST database or (recommended) in the private customer's database.

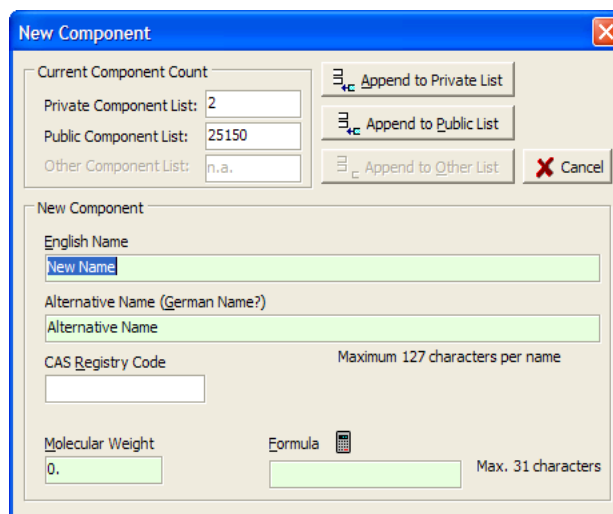


Figure 11 New Component

Property Selection

Property:
 1: Viscosity

EditPureData provides a list of available and editable properties.

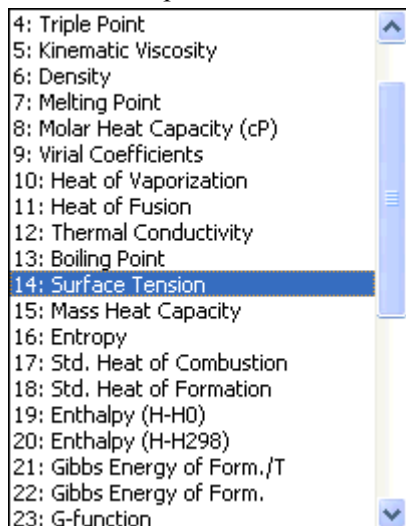


Figure 13 Property Selection - Dropdown Menu

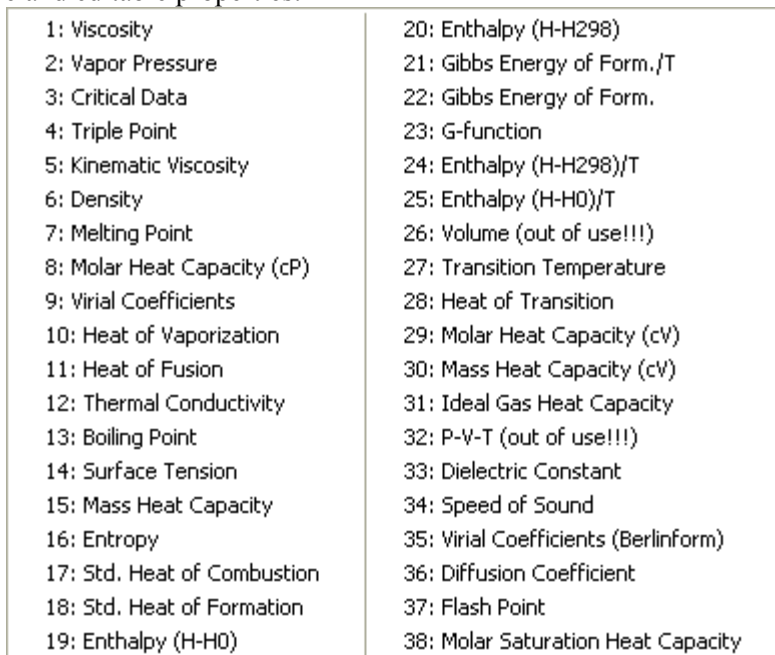


Figure 12 Property Selection - Popup Menu

The list of properties is controlled by a definition file named PURSEL.DEF in the public DDB folder. It is intentionally not described here since it **must** not be modified by users. If there is an urgent demand for further properties please contact DDBST.

Specifying Table Entries and Their Units

The table entries and units dialog is a docked dialog at the right side of the data grid. The complete dialog is opened only by moving the mouse above the “Columns” button.

This dialog allows to define a single column in the data table. The table item can be either selected from the drop-down menu or from a pop-up-menu. The pop-up menu is somewhat more concise since it displays the complete list of table items at a glance.



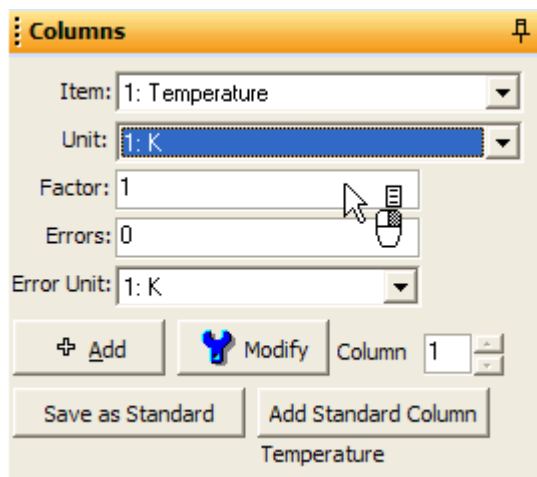


Figure 14 Table Entry Specification

The unit drop-down menu only contains the units for the currently selected table item.

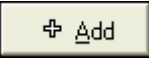
The factor might be a numerical value but can also be one of the list:


LOG	EXP
LN	EINSX
E10	TAUX

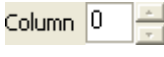
Figure 15 Non-numerical "Factors"

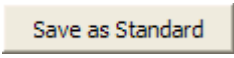
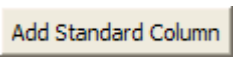
LOG: logarithm to the basis 10
 LN: natural logarithm
 E10: power of 10
 EXP: power of e
 EINS: Divided by 1
 TAUX: Divided by 1000

Additionally it is possible to add an error for the entire column. It is also possible to specify a different unit which is only valid for the error (necessary for percent errors).

The button  adds a new column to the table and the

button  would change the specified column. The "Modify" button is only enabled if a column in

the main edit window has been selected. The "Column" spin-edit  displays the selected column. EditPureData allows currently only up to six columns. If constant errors are used the column count decreases by the number of constant errors.

The  button allows defining a single table item to be set as a standard which then can be added by a single mouse click of the  button. This is useful for editing multiple data sets in a row with the same independent data type like temperature or pressure.

Purity of the Component

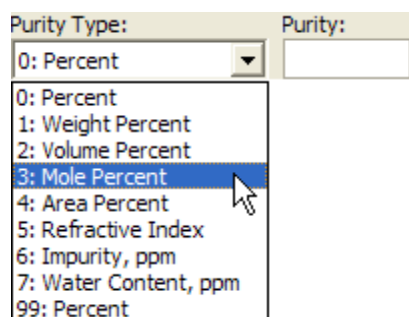


Figure 16 Purity

Both values 0 and 99 refer to an unspecified percentage.

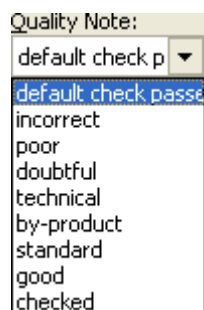
Measurement Quality

Figure 17
Quality

“default check passed” means that only a first glance test has been made during the import or input but no concrete judgment was possible. The other words are simply descriptions for notes from 1 (=bad or even incorrect) to 9 (=excellent).

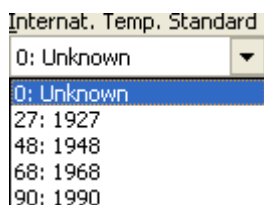
International Temperature Standard

Figure 18 Temperature
Standard

Five possible entries are possible like shown.

The ITS defines the (linearized) relationship between resistance and temperature in Platinum resistance thermometers.

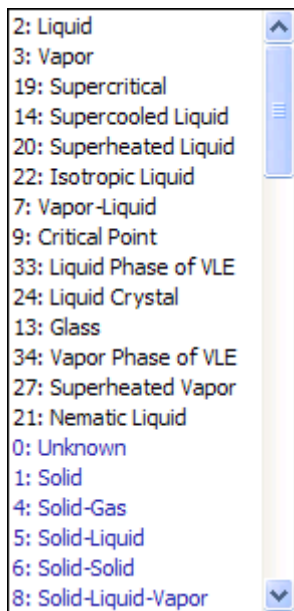
State

Figure 19 States Drop
down Menu

Both menus are showing the complete list of possible states. The drop-down menu needs some scrolling to see all possible states.

2: Liquid	0: Unknown	47: Crystal 2 > Crystal 3
3: Vapor	1: Solid	48: Ideal Gas
19: Supercritical	4: Solid-Gas	49: Supercooled Solid
14: Supercooled Liquid	5: Solid-Liquid	50: Crystal 4 > Liquid
20: Superheated Liquid	6: Solid-Solid	51: Metastable Solid
22: Isotropic Liquid	8: Solid-Liquid-Vapor	52: Stable Solid
7: Vapor-Liquid	10: Crystal 1	53: Crystal 3-Vapor
9: Critical Point	11: Crystal 2	54: Metastable Solid-Liquid-Vapor
33: Liquid Phase of VLE	12: Crystal 3	55: Crystal 4
24: Liquid Crystal	15: Plastic	56: Smectic Liquid > Isotropic Liquid
13: Glass	16: Crystal 2 > Crystal 1	57: Crystal > Rotator
34: Vapor Phase of VLE	17: Crystal 3 > Crystal 2	58: Rotator > Liquid
27: Superheated Vapor	18: Gas-Liquid	59: Crystal 5 > Liquid
21: Nematic Liquid	23: PVT-Range	60: Liquid > monotropic liquid crystal
	25: Metastable Crystal	61: Crystal 1 > unspecified Solid
	26: Mesomorphic Liquid	62: Solid > Smectic Liquid
	28: Liquid > Glass	63: Smectic Liquid > Nematic Liquid
	29: Crystal 2 > Liquid	64: Solid > monotropic liquid crystal
	30: Crystal 3 > Liquid	65: Smectic Liquid A > Smectic Liquid B
	31: Metastable Solid > Liquid	66: Solid1-Liquid-Vapor
	32: Glass > Crystal	67: Solid2-Liquid-Vapor
	35: Crystal 3 > Crystal 1	68: Solid1-Solid2-Liquid
	36: Crystal 1 > Nematic Liquid	69: Solid1-Solid2-Vapor
	37: Nematic Liquid > Isotropic Liquid	70: Crystal > Smectic Liquid A
	38: Solid Phase of SLE	71: Crystal > Plastic
	39: Liquid Phase of SLE	72: Crystal > Smectic Liquid C
	40: Crystal 1-Vapor	73: Solid > Isotropic Liquid
	41: Crystal 2-Vapor	74: Crystal 3 > Glass
	42: Supercooled Liquid - Solid	75: Crystal 2 > Glass
	43: Crystal 4 > Crystal 3	76: Glass > cholesteric liquid crystal
	44: Crystal 1 > Liquid	77: cholesteric liquid crystal
	45: Supercooled Liquid > Vapor	78: cholesteric liquid crystal > isotropic liquid
	46: Crystal 5 > Crystal 4	

Figure 20 State Popup Menu

EditPureData has an internal list which states are suitable for a given property. These states are sorted to the front of the list. The selection of other state description is still possible, though.

Possible Pitfalls:

EditPureData allows selecting the state “Unknown” but since this entry is sometimes essential for a correct property identification it is very recommended to select the correct state.

Another possible pitfall is the consistency between the selected property and the state. Please be aware that some properties need special states. For example the states “vapor-liquid” or “solid-vapor” have to be used for heats of vaporization. Other states are incorrect. EditPureData is unfortunately currently not able to check these possible problems.

Measurement Method

The list of methods for the pure component properties data bank is extremely long since it more a collection of random strings imported from many sources than a man-made validated list of methods.

Measurement Method:

1080 Entry not evaluated by



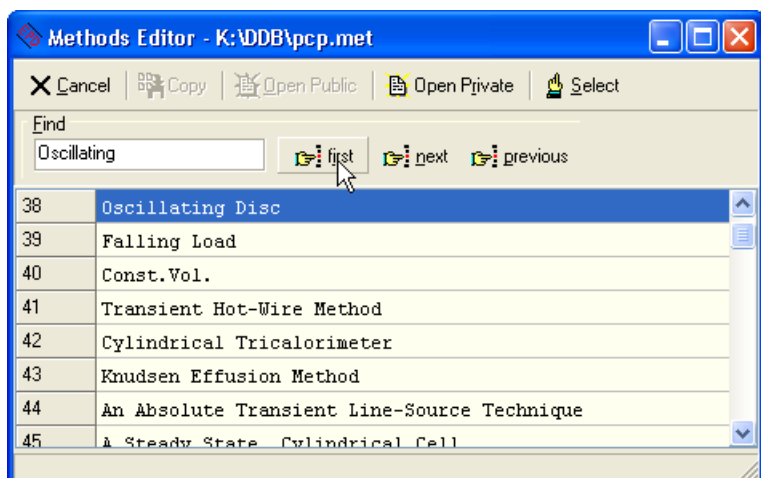
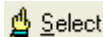

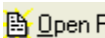


Figure 21 Measurement Methods

A method can be selected by the  **Select** button or by double-clicking the line.

 **Open Private** resp.  **Open Public** allow to switch a public and a private method's list.

Constant Value, Unit, Value

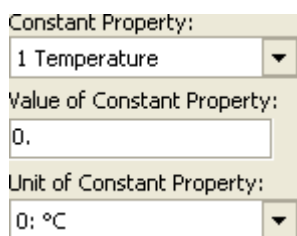


Figure 22 Constant

It is possible to define exactly zero or one constant value for a dataset.

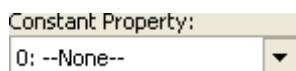


Figure 23 No Constant

Data Input

Data input can be started after all columns have been defined. The specified table entries are displayed in the top rows of the columns together with their units, factors, and column errors.




T [°C] Factor: 1 Error: 0 [°C] <input type="button" value="Remove"/>	VIS [G/MS] Factor: 1 Error: 0 [G/MS] <input type="button" value="Remove"/>
323	2.15 
328.84	2.04 


Figure 24 Example Input

In this example we have two columns – a temperature and a viscosity column.

The options “Advance in Row” and “Advance in Column” change the behavior of the return/enter key for the “auto-advance mode” of the grid. After typing a value and hitting the enter/return key the cursor jumps to the next cell either in the next row (“Advance in Row”) or the next column (“Advance in Column”).

The button  allows to display a quick plot of the currently edited dataset. If there are already datasets available in the pure component properties data bank these data are plotted together with the new set.

The new data points are red squares, the PCP data points are black stars.

The diagram can be copied (as metafile) and printed. The  button starts the Dortmund Data Bank program and displays the data sets already available in the DDB.

The “Scales” allows to switch between the display of “x vs. y” and “1000/x vs. log y”.

The “Polynomial Fit Deviations” can be used to take a quick look if the experimental data points are lined up properly – which is obviously a suitable criterion only for some properties.

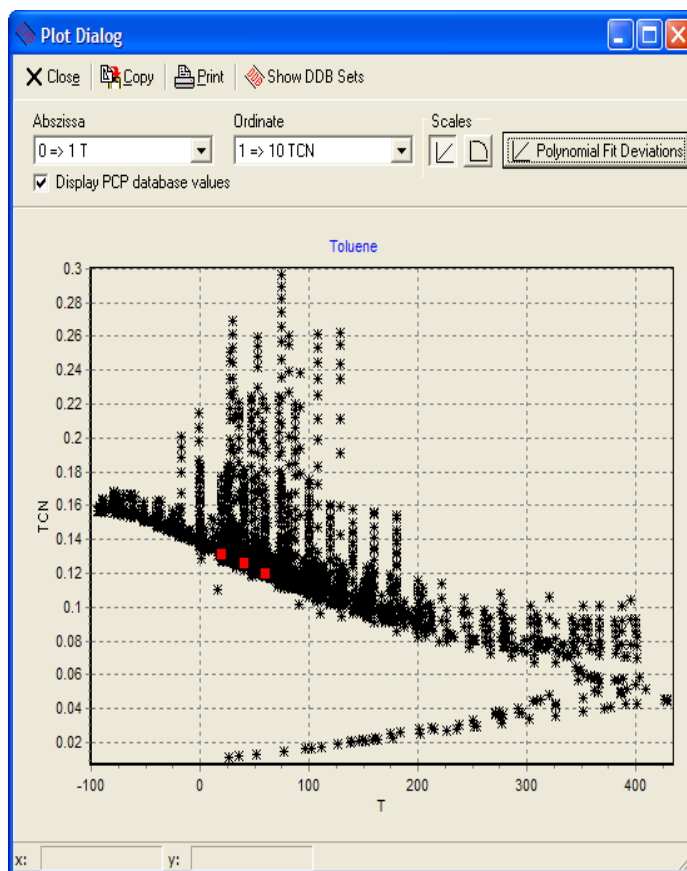

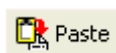



Figure 25 Plot

The buttons  and  allow to copy and paste the data grid to and from the Windows clipboard – for modifying data outside EditPureData e. g. in a spread-sheet.

The button  is used to get the table entries (Figure 14 Table Entry Specification) dialog to front. This is only necessary if that dialog is hidden by the main window.

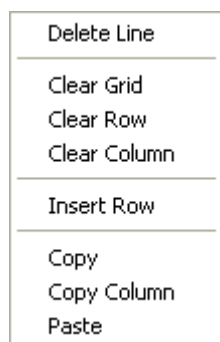


Figure 26 Data Grid Context Menu

The data grid has a context (pop-up) menu with some additional functions. These function do not change the column specifications, they only manipulate the grid content.

Saving Data to File

After selecting the  Save button a standard Windows save dialog is used to determine a filename.

The filename extension must be “.ol”.

EditPureData has not stored any data in the database yet. The stored file contains the originally typed data and is a common text file where the single entries are identified with tags.

It is recommended to store and archive these files for future maintenance. Only these files can be reloaded.

In the background EditPureData automatically stores two other files with the same name but different extensions.

The “DHP” files contains recalculated data and will be used to append the data to the pure component properties database.

The “PCP” files contains almost the same data as the DHP file and was intended to be used in the databank retrieval program. This format is written only for compatibility reasons.

Adding Datasets to the Private Databank

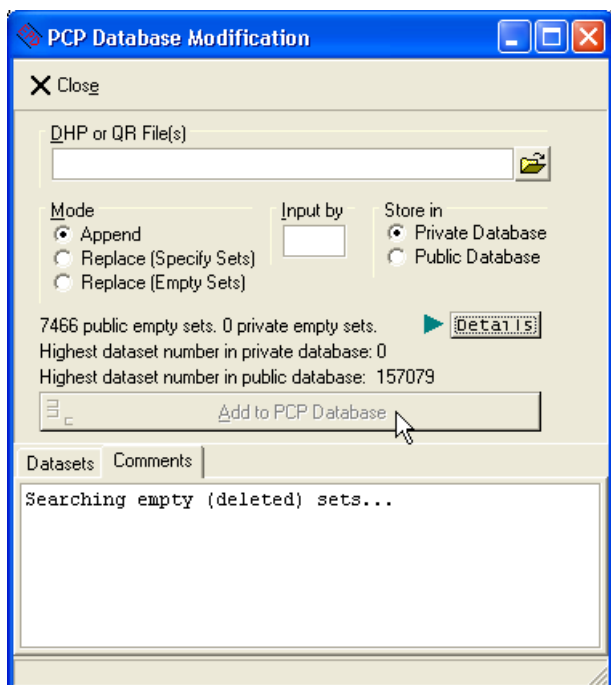


Figure 27 Adding Datasets to the Data Bank

This dialog might need some seconds to be responsive because the program searches initially for deleted sets.

The list of deleted sets is necessary because EditPureData offers an options to overwrite previously removed datasets.

The following steps are necessary to add datasets to the pure component properties databank.

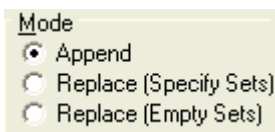
First Step: Select “DHP” files (see page 15 for a short description of DHP files)



The program uses a standard Windows open dialog. After the datasets have been loaded the program display the number of datasets found (“DHP File contains 15 dataset(s)”) in the “Comments” page and the complete list of sets in the “Datasets” page.

Second Step: Select update mode

It is possible to append new data, overwrite existent datasets or overwrite already deleted datasets.



1. **Append:** All datasets found in the DHP file will be appended at the end of the databank
It is possible to select only some of the loaded datasets by setting or removing the check marks in the “Datasets” page (see Figure 28 Dataset List - Append Mode).
2. **Replace (Specify Sets):** The datasets will replace existent datasets. The user has to specify the dataset number (see Figure 29 Dataset List - Replace Mode).
3. **Replace (Empty Sets):** The new datasets will replace previously removed datasets. It is possible to select only some of the loaded datasets by setting or removing the check marks in the “Datasets” page (see Figure 28 Dataset List - Append Mode).

Third Step: “Input by” specification


Number	Component	Points	Ref.	Store at
1	867	1	18017	Append
2	17359	1	18017	Append
3	9189	1	18017	Append
4	17360	1	18017	Append
5	867	8	18017	Append
6	867	8	18017	Append
7	867	8	18017	Append

Figure 28 Dataset List - Append Mode

Number	Component	Points	Ref.	Store at
1	867	1	18017	1
2	17359	1	18017	2
3	9189	1	18017	3
4	17360	1	18017	4
5	867	8	18017	5
6	867	8	18017	6
7	867	8	18017	7

Figure 29 Dataset List - Replace Mode

Every dataset has a two character signature for the specifying the editor of the datasets.

The buttons  starts the database retrieval program and displays the datasets selected for replacement.

Fourth Step: Select database

It is possible to store data in the public database (from DDBST) and a customer's database (private). Adding datasets to or replacing datasets in the public database is not recommended since future delivery would overwrite these changes.

Fifth Step: Add datasets

A last question has to be answered:

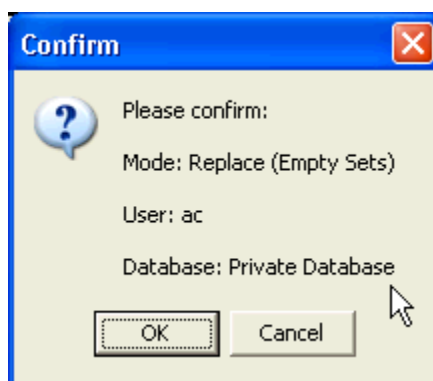


Figure 30 Confirm Write Access

After the datasets have been added EditPureData displays a protocol which shows the old dataset count and some details of the new datasets like the reference and component number, the property code and the datasetnumber.

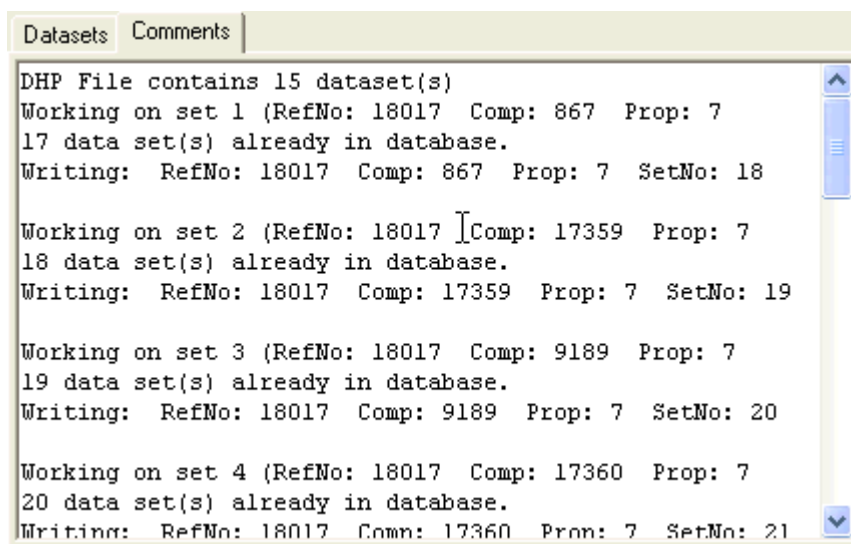
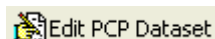


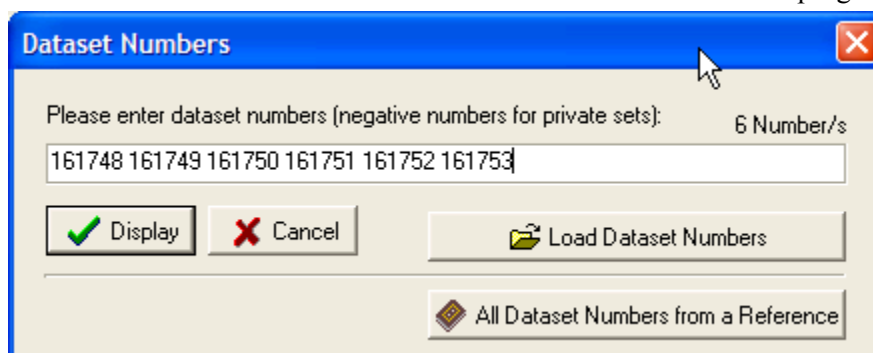
Figure 31 Update log

After this step the datasets are stored in the pure component properties database.

Modifying Datasets in the Database



If the "ol" might not be available or for a quick repair it is possible to modify datasets in the data bank directly. You have to know the dataset number which can be obtained in the database retrieval program.



The program opens a separate edit window for every data set entered in this dialog.

Modify Single Set: 111925 [0]

Component: 3 Acetonitrile

Property: 6: Density

State: 2: Liquid

Reference No.: 5504

Constant Property: 0 --None--

Constant Value: 0

Measurement Method: 284

Purity: 99.80000305 Purity Type: 0: Percent

Quality: 0: default check passed

Internat. Temp. Standard: 0: Unknown

Input By: OP

Original Number: 5240

Table Items

1: 1: Temperature 2: 2: Pressure

3: 5: Density 4: 55: Error in Density

5: -1: nothing 6:

Location: public

Dataset Number: 111925

Save Discard Delete

T	P	DEN	±DEN
[K]	[kPa]	[kg/m3]	[kg/m3]
302.95	133000.000	877.193	18.472
309.15	144600.000	877.193	18.472
314.15	152600.000	877.193	18.472
319.95	163100.000	877.193	18.472
326.15	172500.000	877.193	18.472
333.55	182200.000	877.193	18.472
341.15	192800.000	877.193	18.472
348.95	204800.000	877.193	18.472

Comment:

Figure 32 Direct Database Editor

The main difference is that the databank contains recalculated datasets with standard units and some few other restrictions. The editor does not allow to change units and the dataset can not be loaded from file or stored to disk.

Most other properties can be changed like it has been done in the normal file-oriented editor. Additional feature can be found in the context menu of the data grid.

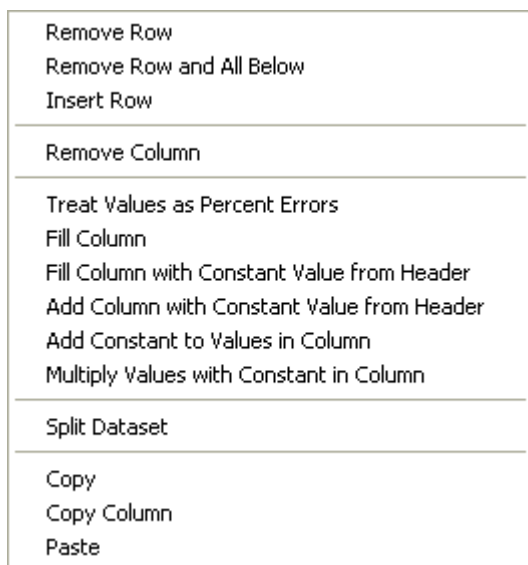
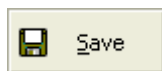


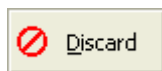
Figure 33 Data Grid Context Menu

Several functions have been introduced due to common errors in the database.

The three buttons perform the following actions:



Save the modified datasets in the database.



Discard any modification



Delete the current dataset from

the databank. Deleted datasets are not completely erased only their reference number is set to zero. The behavior is described in the confirmation dialog presented before actually removing the dataset.

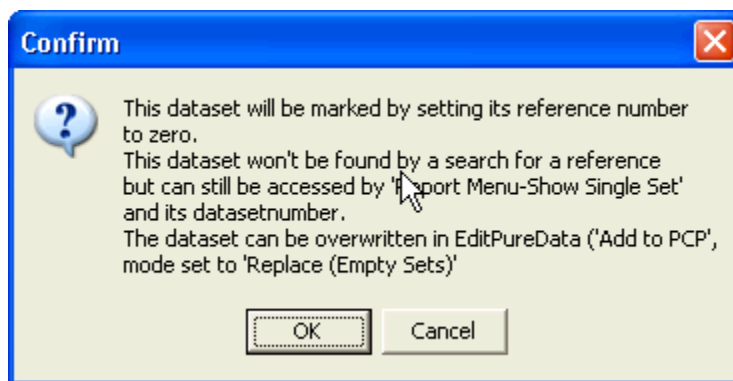


Figure 34 Confirmation of Dataset Removal