

Pure Data Editing

Editing / Modifying DDB Pure Component Data

DDBSP - Dortmund Data Bank Software Package



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1 Introduction

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

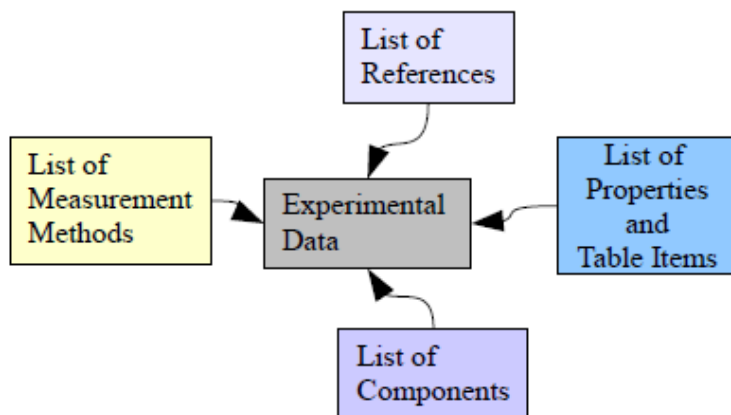


Figure 1: Simplified data bank structure

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 keeping 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.

2 Starting the Program

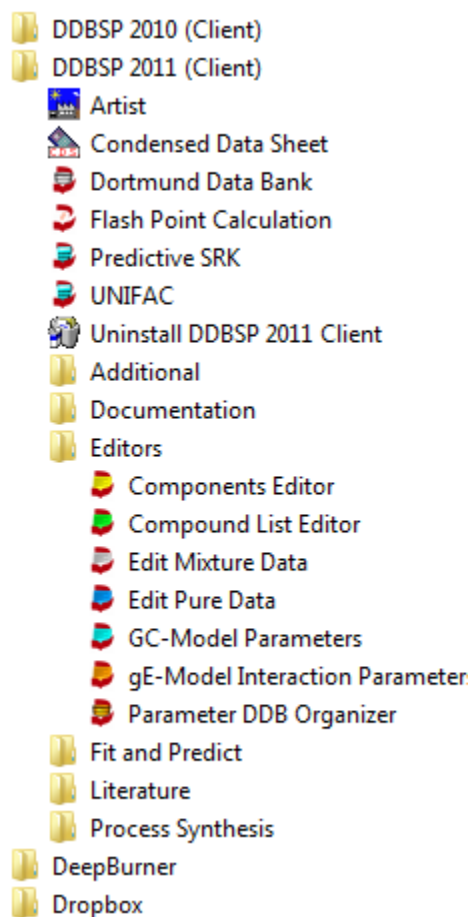


Figure 2: Program folder

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

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

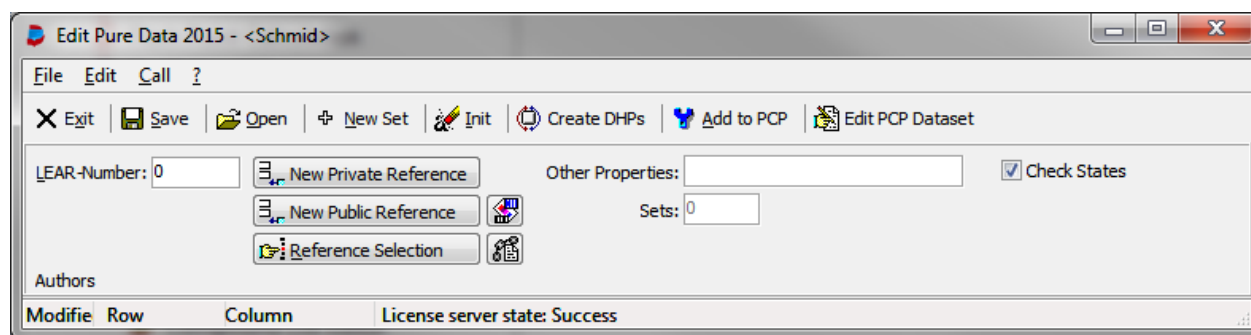


Figure 3: Initial dialog

This document is a stepwise introduction in the usage of this program. It starts with the necessary prerequisite for all DDB data sets.

3 Defining the Reference

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

3.1 Adding a New Reference

For new private data sets it is normally recommended to create a new private reference.

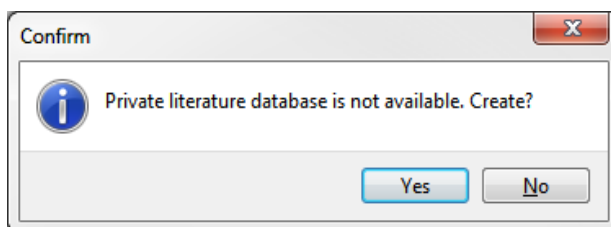



Figure 4: New reference data base creation.

A new reference can be inserted by selecting the button  **New Private Reference** - a menu item in the “Edit” menu is also available. If no private literature databank is present, the program asks if it shall create a new one. After confirming with “Yes” the literature management program displays the edit dialog for a new reference (see below).

The 'New Entry [DDBST/p]' dialog box includes the following fields and controls:

- Literature Kind:** A dropdown menu set to 'Article in Journal'.
- Dataset Number:** A text field containing 'New Entry'.
- User defined Number:** An empty text field.
- Title:** A large text area with a Google search icon.
- Authors:** A text field with a Google search icon.
- Pages:** A field with 'to' and a dropdown.
- Volume:** A text field.
- Issue:** A text field.
- Series:** A text field.
- Year:** A field with 'to' and a dropdown.
- Journal:** A dropdown menu set to '750'.
- Currently Undefined In Source List:** A button.
- Publ. Progr.:** A text field.
- ISSN:** A text field.
- Shelfmark:** A text field.
- ZDB-ID:** A text field.
- Publisher/Place:** A text field.
- Language:** A dropdown menu.
- Keywords:** A text field with a search icon.
- Entered at:** A date field showing '07.03.2014'.
- By:** A text field showing 'schmid'.
- Location:** A text field.
- Status:** A dropdown menu set to 'available'.
- Comments:** A large text area.
- URLs:** A table with one row containing '1' and buttons 'Open', 'Del', and 'New'.
- DOI:** A text field with a search icon.
- Links:** A text field with a search icon.
- Buttons:** 'Save' and 'Close' at the bottom.

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

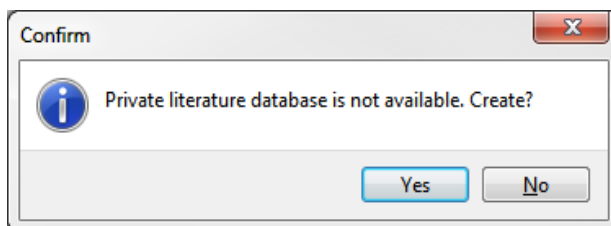



Figure 6: New reference – link creation.

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.

3.2 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.

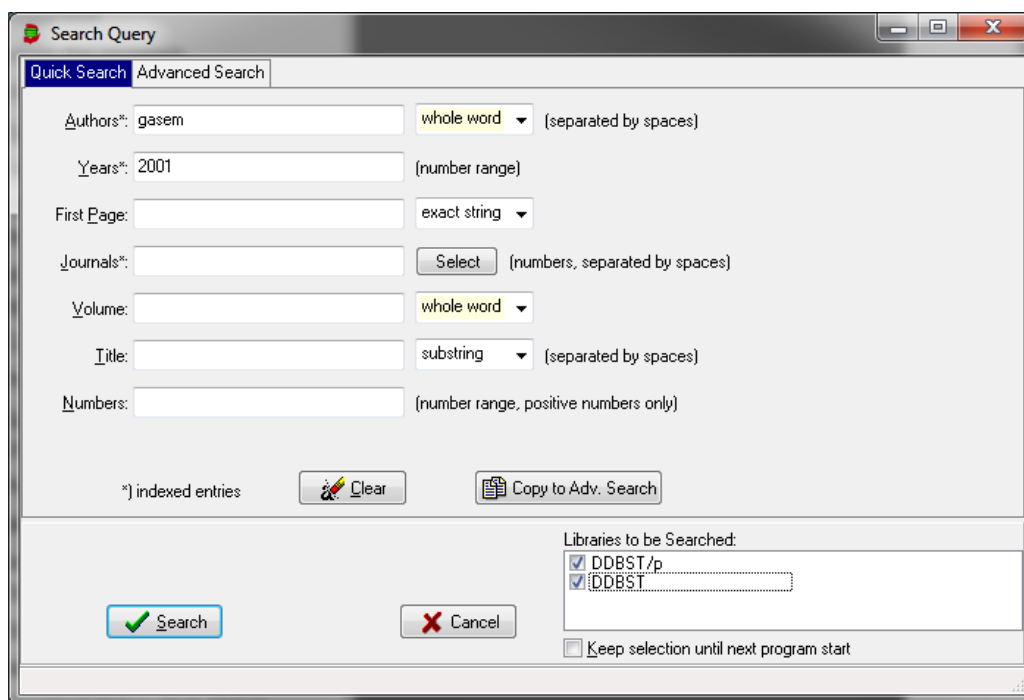
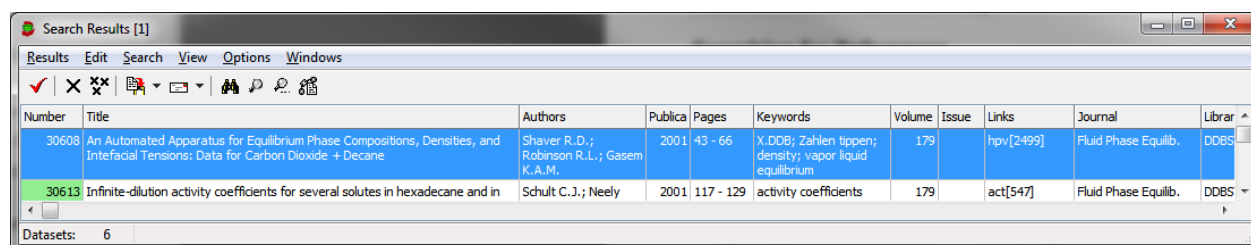


Figure 7: Reference search – search query.


The result for the given example is



Number	Title	Authors	Publica	Pages	Keywords	Volume	Issue	Links	Journal	Librar
30608	An Automated Apparatus for Equilibrium Phase Compositions, Densities, and Interfacial Tensions: Data for Carbon Dioxide + Decane	Shaver R.D.; Robinson R.L.; Gasem K.A.M.	2001	43 - 66	X.DDB; Zahlen tippen; density; vapor liquid equilibrium	179		hqv[2499]	Fluid Phase Equib.	DDBS
30613	Infinite-dilution activity coefficients for several solutes in hexadecane and in	Schult C.J.; Neely	2001	117 - 129	activity coefficients	179		act[547]	Fluid Phase Equib.	DDBS

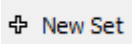
Datasets: 6

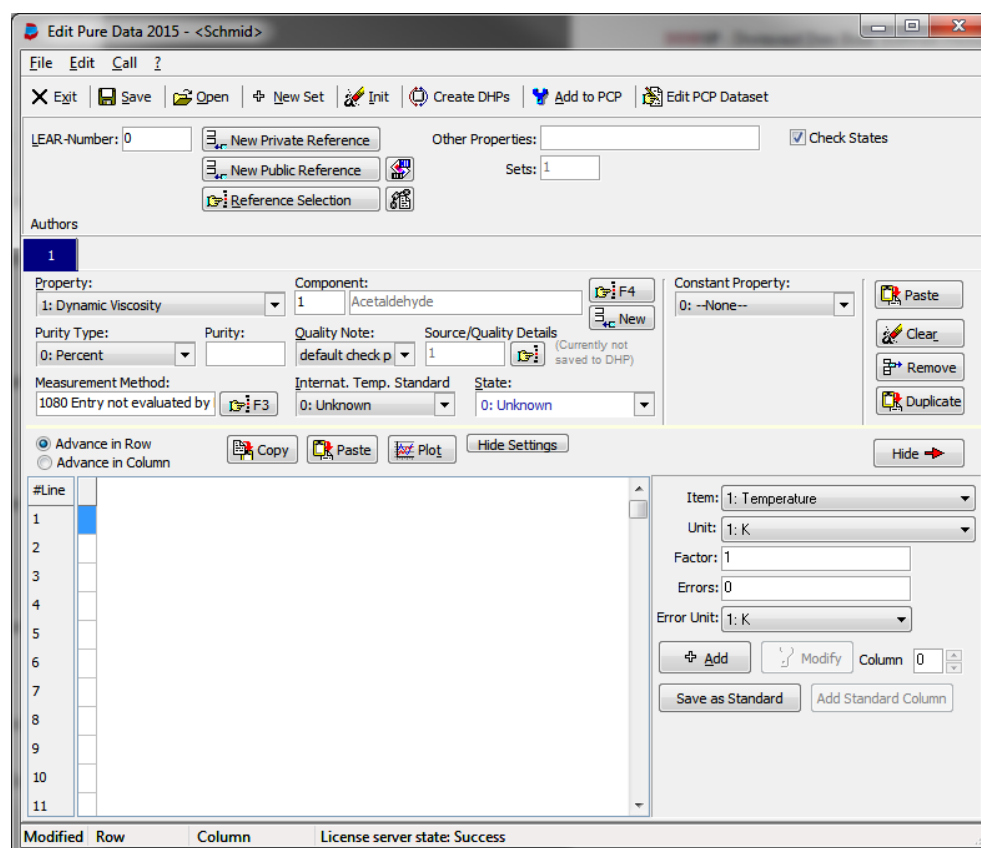
Figure 8: Reference search – search results.

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

4 Adding Datasets to the Current Reference

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

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



File Edit Call ?

Exit Save Open New Set Init Create DHPs Add to PCP Edit PCP Dataset

LEAR-Number: 0 New Private Reference Other Properties: Check States

New Public Reference Sets: 1

Reference Selection

Authors

1

Property: 1: Dynamic Viscosity Component: 1 Acetaldehyde F4

Purity Type: Purity: Quality Note: Source/Quality Details (Currently not saved to DHP)

Measurement Method: 1080 Entry not evaluated by F3 Internat. Temp. Standard State: 0: Unknown

Constant Property: 0: --None-- Paste

Clear Remove Duplicate

Advance in Row Advance in Column Copy Paste Plot Hide Settings

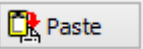
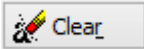
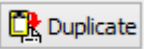
#Line	Modified	Row	Column	License server state
1				
2				
3				
4				
5				
6				
7				
8				
9				
10				
11				

Item: 1: Temperature Unit: 1: K Factor: 1 Errors: 0 Error Unit: 1: K

Add Modify Column 0 Save as Standard Add Standard Column

Modified Row Column License server state: Success

Figure 9: Adding data sets

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

5 Adding Necessary Specifications for Single Sets

Necessary specification are

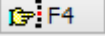
- Component
- Property
- Table entries
- Units of table entries

Additional specifications are

- Purity of the component
- Quality of the measurement or data
- Used internal temperature standard
- State ('Unknown' is possible)
- Measurement method
- A constant value, its unit and value
- Errors for table items with their units

5.1 Component Selection



The key F4 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).

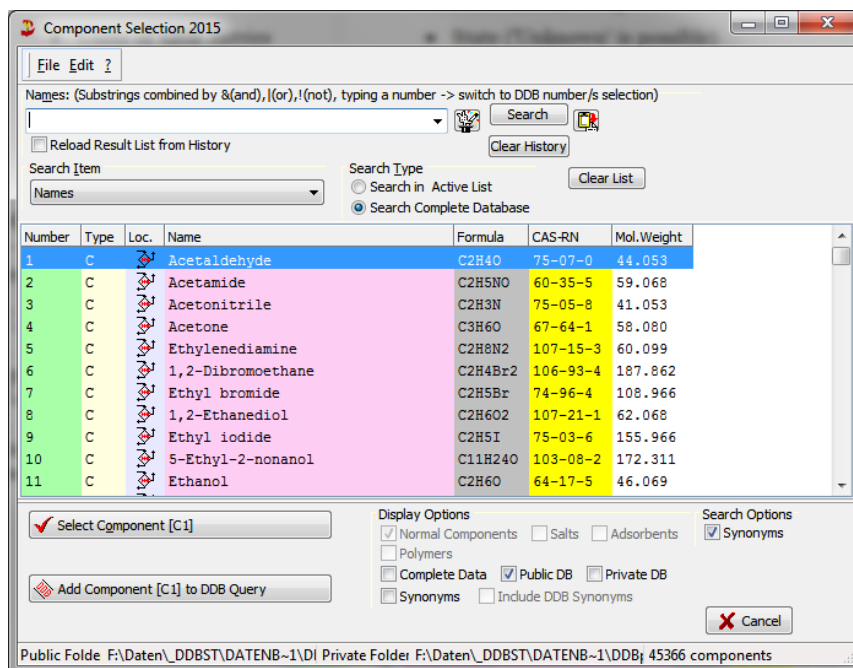


Figure 10: Component selection

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

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





button.

The “New Component” dialog allows entering 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.

 A screenshot of the 'New Component' dialog box. It contains fields for 'Current Component Count', 'Private Component List' (with value 1), 'Public Component List' (with value 45366), and 'Other Component List' (with value n.a.). There are buttons for 'Append to Private List', 'Append to Public List', 'Append to Other List', and 'Cancel'. Below these is the 'New Component' section with fields for 'English Name' (containing 'New Name'), 'Alternative Name (German Name?)', 'Alternative Name', 'CAS Registry Code' (with a note 'Maximum 127 characters per name'), 'Molecular Weight [g/mol]' (with value 0 and a calculator icon), and 'Formula' (with a note 'Max. 31 characters'). At the bottom are checkboxes for 'Is Ionic Liquid', 'Is Carbohydrate', 'Is Polymer', 'Is Pharmaceutical', 'Biodiesel', and 'Oil & Gas'.

Figure 11: New component

5.2 Property Selection

EditPureData provides a list of available and editable properties.

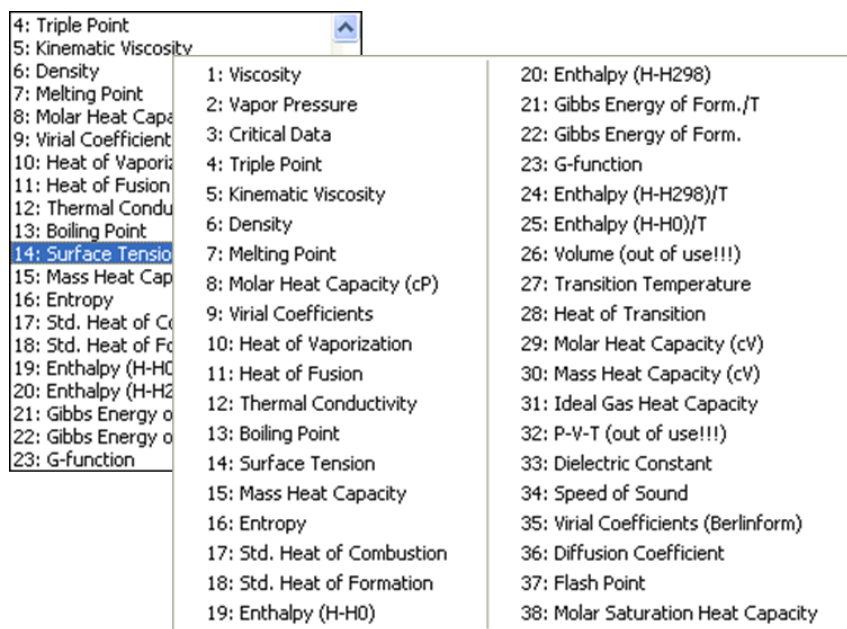


Figure 12: Property selection: Drop down and pop up menu

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.

5.3 Specifying Table Entries and Their Units

The table entries and units dialog is a docked dialog at the right side of the data grid.

Figure 13: Table entry specifications

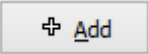

This dialog allows to define a single column in the data table. The table item can be either selected from the drop-down menu or from a pop-up-menu. The pop-up menu is somewhat more concise since it displays the complete list of table items at a glance.


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

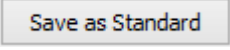
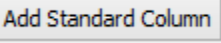
The factor might be a numerical value but can also be one of the list:

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

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.

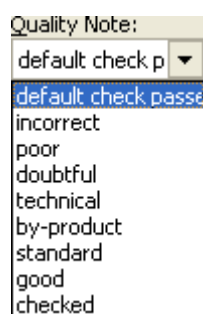
The  button allows defining a single table item to be set as a standard which then can be added by a single mouse click of the  button. This is useful for editing multiple data sets in a row with the same independent data type like temperature or pressure.

5.4 Purity of the Component

Figure 14: Purity

Both values 0 and 99 refer to an unspecified percentage.

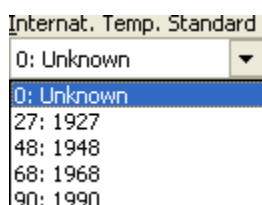
5.5 Measurement Quality



“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).

Figure 15: Quality

5.6 International Temperature Standard

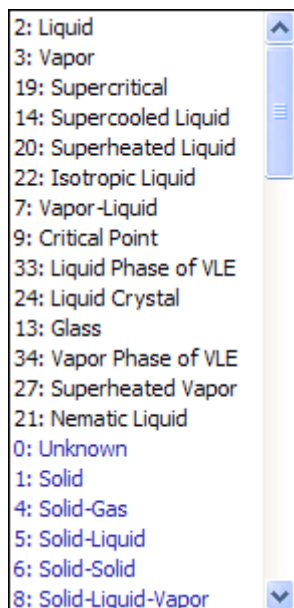


Five possible entries are possible like shown.

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

Figure 16: Temperature standard

5.7 State



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

Figure 17: States drop down menu

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 18: State pop up menu

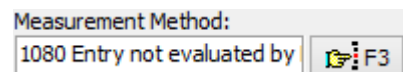
EditPureData has an internal list which states are suitable for a given property. These states are sorted to the front of the list. The selection of other state description is still possible, though.

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.

5.8 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.

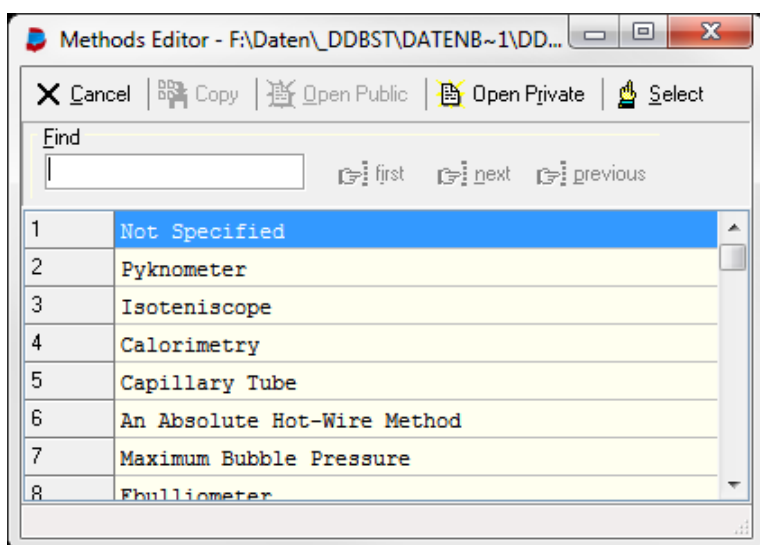





Figure 19: Measurement methods

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.

5.9 Constant Property, Value and Unit

Constant Property:
1 Temperature ▼

Value of Constant Property:
0.

Unit of Constant Property:
0: °C ▼

Figure 20: Constant

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

Constant Property:
0: --None-- ▼

Figure 21: No constant

5.10 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 22: 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 displaying a quick plot of the currently edited data set. If there are already data sets 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

 Show DDB Sets button starts the Dortmund Data Bank program and displays the data sets already available in the DDB.

The “Scales” allows switching 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.

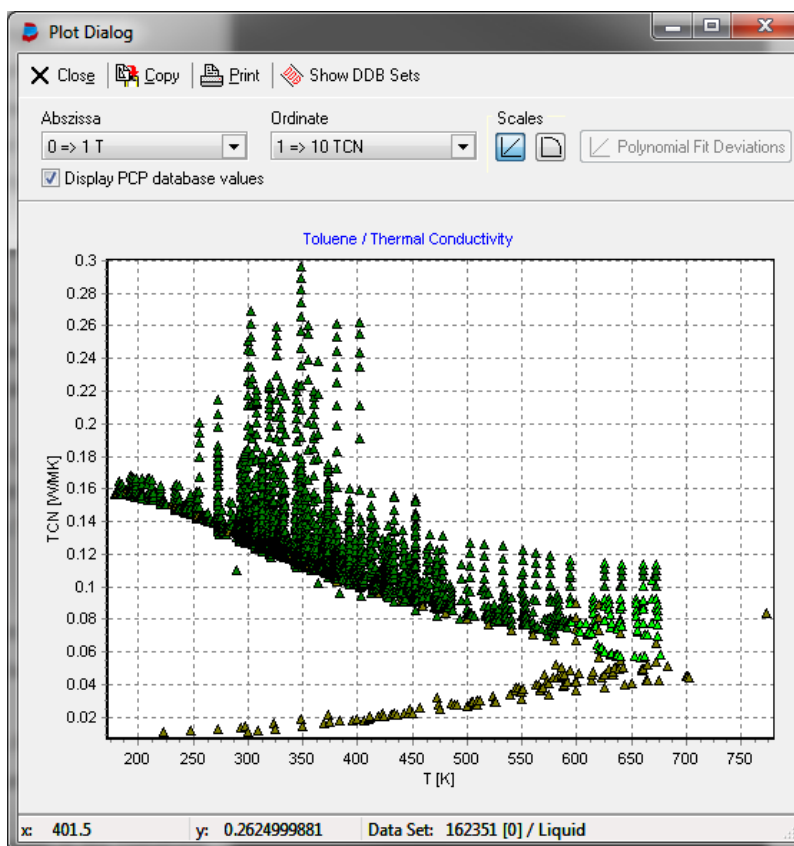




Figure 23: Plot

The buttons  Copy and  Paste 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.

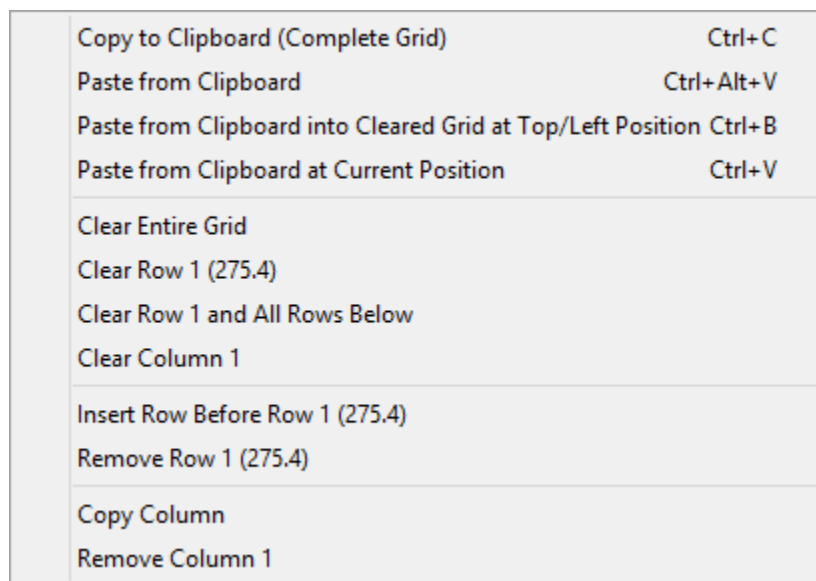


Figure 24: Data grid context menu

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.

6 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.

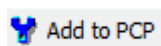
It is recommended to store and archive these files for future maintenance. Only these files can be reloaded.

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.

7 Adding Data Sets to the Private Databank



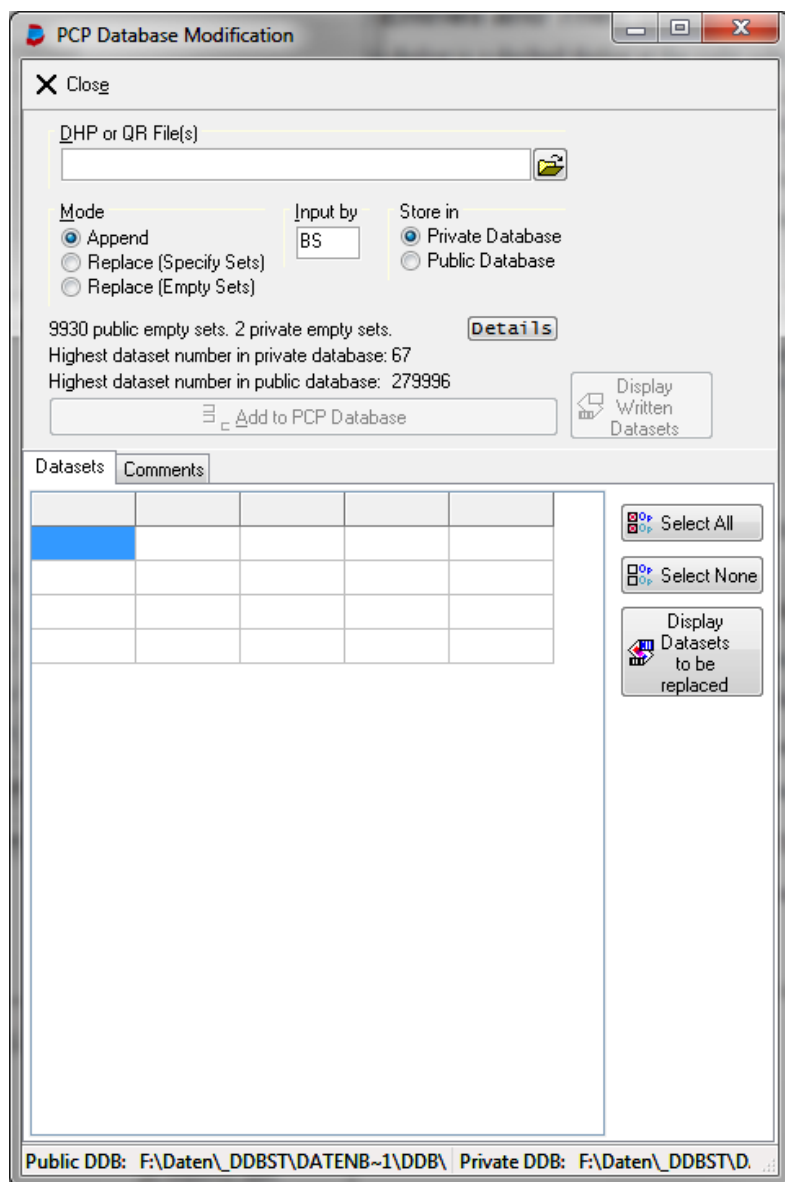
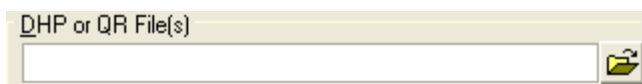


Figure 25: Adding data sets to the data bank.

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 data sets have been loaded the program displays the number of data sets found (“DHP File contains 15 data set(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.

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 option to overwrite previously removed data sets.

Mode

☒ Append

☐ Replace (Specify Sets)

☐ Replace (Empty Sets)

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 data sets by setting or removing the check marks in the “Data sets” 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 Data Set 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).

Datasets					Comments
Number	Component	Points	Ref.	Store at	
<input checked="" type="checkbox"/> 1	867	1	18017	Append	
<input checked="" type="checkbox"/> 2	17359	1	18017	Append	
<input checked="" type="checkbox"/> 3	9189	1	18017	Append	
<input checked="" type="checkbox"/> 4	17360	1	18017	Append	
<input checked="" type="checkbox"/> 5	867	8	18017	Append	
<input checked="" type="checkbox"/> 6	867	8	18017	Append	
<input checked="" type="checkbox"/> 7	867	8	18017	Append	

Select All

Select None

Display Datasets to be replaced

Figure 27: Data set list – append mode

Datasets					Comments
Number	Component	Points	Ref.	Store at	
<input checked="" type="checkbox"/> 1	867	1	18017	1	
<input checked="" type="checkbox"/> 2	17359	1	18017	2	
<input checked="" type="checkbox"/> 3	9189	1	18017	3	
<input checked="" type="checkbox"/> 4	17360	1	18017	4	
<input checked="" type="checkbox"/> 5	867	8	18017	5	
<input checked="" type="checkbox"/> 6	867	8	18017	6	
<input checked="" type="checkbox"/> 7	867	8	18017	7	

Select All

Select None


Display Datasets to be replaced

Figure 26: Data set list – replace mode

Third Step: “Input by” specification.

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



The buttons  starts the database retrieval program and displays the data sets 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 data sets to or replacing data sets in the public database is not recommended since future delivery would overwrite

these changes.

Fifth Step: Add data sets

A last question has to be answered:



Figure 28: Confirm write access

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

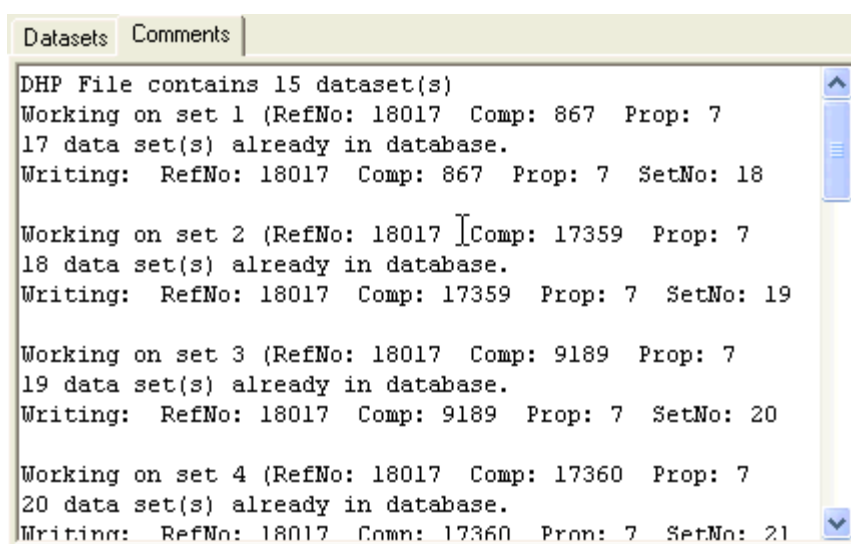


Figure 29: Update log

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

8 Modifying Datasets in the Database

If the original “ol” is not available or for a quick repair it is possible to modify data sets in the data bank directly. You have to know the data set number which can be obtained in the database retrieval program.

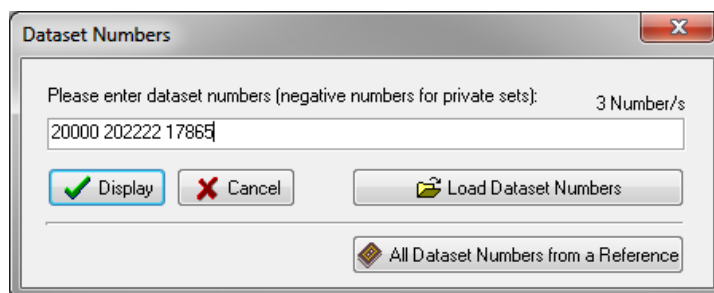


Figure 30: Edit window

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

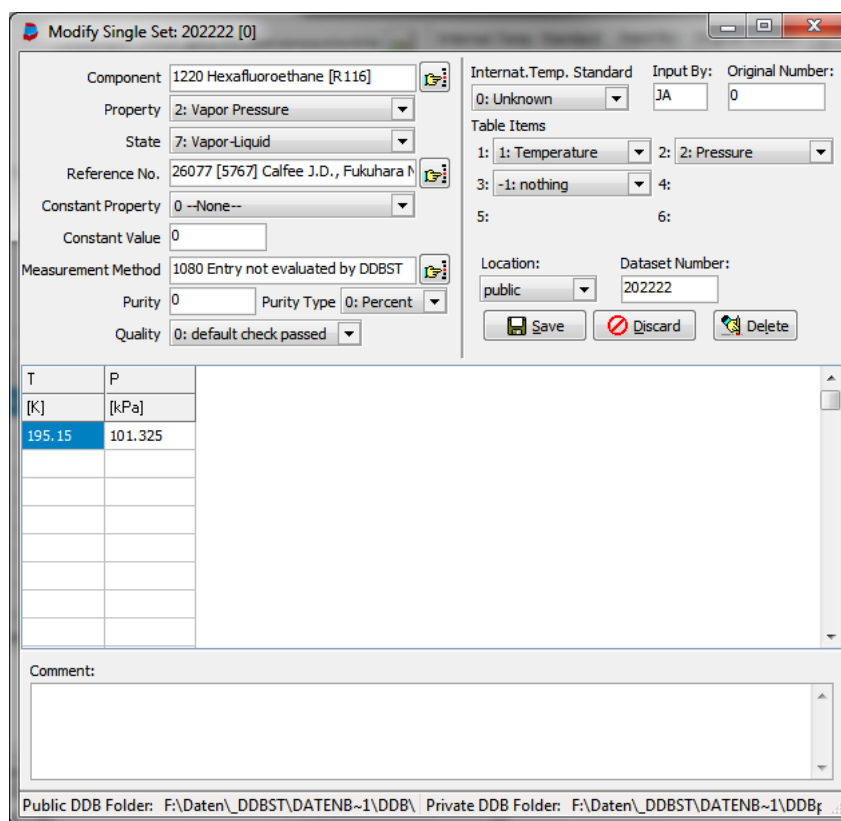


Figure 31: Direct database editor

The main difference is that the databank contains recalculated data sets with standard units and some few other restrictions. The editor does not allow to change units and the data set cannot 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.

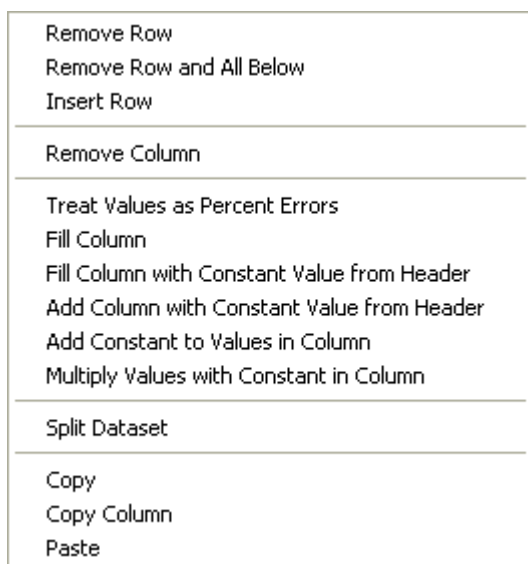
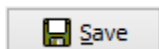


Figure 32: Data grid context menu

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

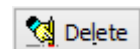
The three buttons perform the following actions:



Save the modified data sets in the database.



Discard any modification



Delete the current data set from the databank. Deleted data sets 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 data set.

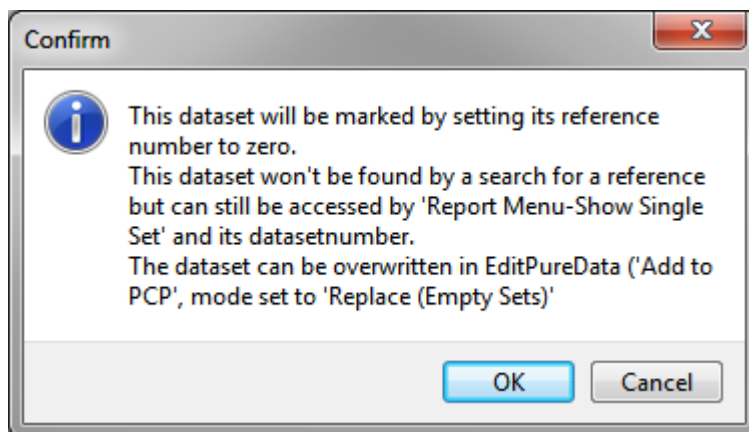


Figure 33: Confirmation of data set removal