

Edit Pure Data

Editing / Modifying DDB Pure Component Data



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1 Introduction

This document is a tutorial for storing private pure component data in the Dortmund Databank (DDB).

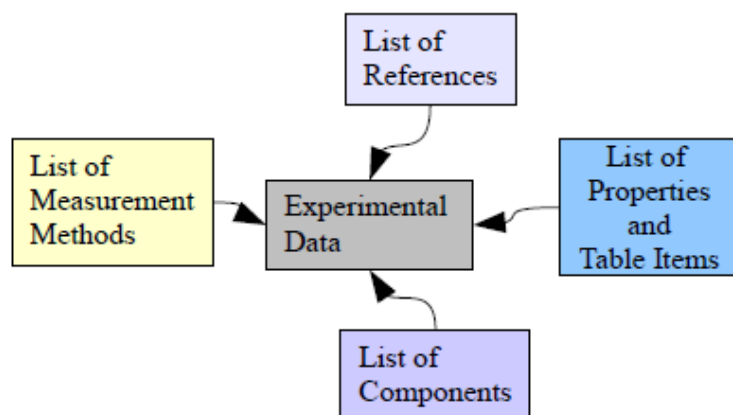


Figure 1: Simplified data bank structure

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

2 Defining the Reference

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

2.1 Adding a New Reference

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

A new reference can be inserted by selecting “*New Private Reference*” in the “Edit” menu. 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.

The literature management (LEAR) documentation contains a detailed description of that dialog.

2.2 Searching for References

If you do not want to create a new reference you have to search the available literature databank for the wanted article or report. A click on the “*Reference Selection*” button opens a search query dialog where the user can specify search parameters like the author(s) name and the publication year (see the literature management documentation for details).

In the search result, use the  button to select the reference.

3 Adding Data Sets to the Current Reference

The data input is reference-centered. All data sets from a single reference can be edited together.

For appending data sets to the current reference select the *New Set* button.

The buttons *Clone*, *Remove* and *Duplicate* allow duplicating the current with data filled set, removing or duplicating the current set. It is also possible to move the current data set to another position (see button and input box above the *Clone*-button).

4 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)

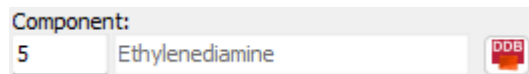
Measurement method

A constant value, its unit and value

Errors for table items with their units

4.1 Component Selection

The key F4 or selecting the button starts the program DDB Components. After a search, you can double-click on a search result line and then the selected component is shown now in the edit field besides the search button.



4.2 Property Selection

Use the Property drop-down control or the pop-up menu to select a property from the list of available properties.

4.3 Specifying Table Entries and Their Units

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

This dialog allows defining 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 from this list opened by a pop-up menu:

LOG: logarithm to the basis 10

LN: natural logarithm

E10: power of 10

EXP: power of e

EINSX: 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 *Add* adds a new column to the table and the button *Modify* 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 *Save as Standard* 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 *Add Standard Column* button. This is useful for editing multiple data sets in a row with the same independent data type like temperature or pressure.

4.4 Purity of the Component

There are several types available for the specification of the purity value.

4.5 Measurement Qualities and Source

Qualities: The data set can be labelled by different Quality marks from several categories.

4.6 International Temperature Standard

There are several possible entries for the specification of the international temperature standard, which defines the (linearized) relationship between resistance and temperature in Platinum resistance thermometers.

4.7 State

This menu is showing the complete list of possible states. The drop-down menu needs some scrolling to see all possible states. A right click on the menu opens a complete overview over all possible states.

DDB Edit Pure Data 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:

DDB Edit Pure Data 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. DDB Edit Pure Data is unfortunately currently not able to check these possible problems.

4.8 Measurement Method

Use the button next to the *Measurement Method* entry to open a new dialog.

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

Open Private resp. *Open Public* allows switching between a public and a private method list.

Use Call → “Measurement Methods Management” from the application main menu to edit the list of (private) methods.

4.9 Constant Property, Value and Unit

In the *Constant Property* area, it is possible to define one optional constant value or error for a data set.

4.10 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 [K] Factor: 1 Error: 0 [K] <input type="button" value="Remove"/>	VIS [mPas] Factor: 1 Error: 0 [mPas] <input type="button" value="Remove"/>
323	2.15
328.84	2.04

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

Figure 2: Example input


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 *Plot* 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 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 “Scale” allows switching between the display of “x vs. y” and “1000/x vs. log y”.

The “*Polynomial Fit Deviations*” button () 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.

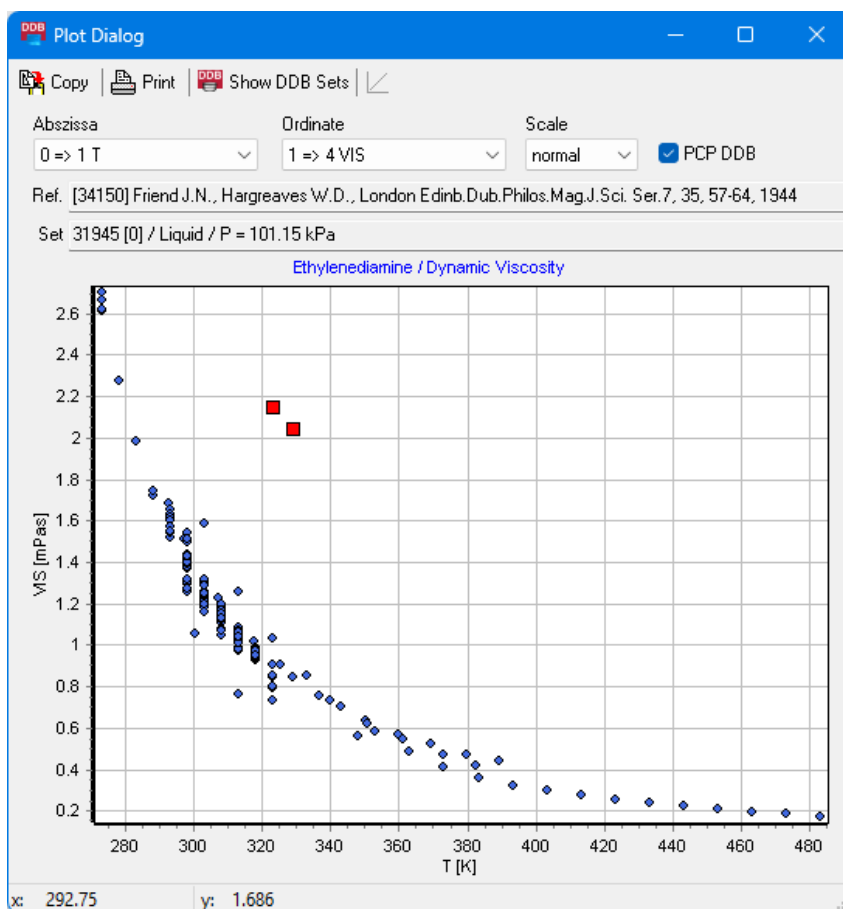


Figure 3: Plot

The buttons *Copy* and *Paste* allow to copy and paste the data grid to and from the Windows clipboard – for modifying data outside DDB Edit Pure Data e. g. in a spread-sheet.

The data grid has a context (pop-up) menu with some additional functions. These only manipulate the content of the grid, not the column header.

5 Saving Data to File

The “Input by” field must not be empty. Enter two letters (representing the user) into the field. The application remembers the setting.

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

The filename extension must be “.ol”.

DDB Edit Pure Data 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 DDB Edit Pure Data automatically stores another file with the same name but different extension.

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

6 Adding Data Sets to the Private Databank

Use the “Add to PCP” to open a new dialog. Use the following steps to add datasets to the pure component properties databank.

First Step: Select “QRX” or “QR” 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 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 or overwrite existing datasets.

Append: All datasets found in the 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 4 Data set list – append mode).

Datasets					Comments
Number	Component	Points	Ref.	Store at	
<input checked="" type="checkbox"/> 1	68	1	140196	Append	<input checked="" type="checkbox"/> Select All <input type="checkbox"/> Select None Display Datasets to be replaced
<input checked="" type="checkbox"/> 2	157	1	140196	Append	
<input checked="" type="checkbox"/> 3	149	2	140196	Append	
<input checked="" type="checkbox"/> 4	31	2	140196	Append	
<input checked="" type="checkbox"/> 5	47	1	140196	Append	
<input checked="" type="checkbox"/> 6	84	1	140196	Append	

Figure 4: Data set list – append mode

Replace (Specify Sets): The datasets will replace existent datasets. The user has to specify the dataset number (see Figure 5 Data set list – replace mode).


Datasets					Comments
Number	Component	Points	Ref.	Store at	
<input checked="" type="checkbox"/> 1	68	1	140196	1	<input checked="" type="checkbox"/> Select All <input type="checkbox"/> Select None Display  Datasets to be replaced
<input checked="" type="checkbox"/> 2	157	1	140196	2	
<input checked="" type="checkbox"/> 3	149	2	140196	3	
<input checked="" type="checkbox"/> 4	31	2	140196	17	
<input checked="" type="checkbox"/> 5	47	1	140196	166	
<input checked="" type="checkbox"/> 6	84	1	140196	233	

Figure 5: Data set list – replace mode

Third Step: “Check data sets to be replaced” (replacement mode only)

The button *Display Data Sets to be replaced* starts the database retrieval program and displays the data sets selected for replacement.

Fourth Step: Add data sets

After the data sets have been added DDB Edit Pure Data 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.

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

7 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. Only private data sets can be modified.

Press the “Edit PCP Dataset” button, enter the data set numbers in to the input field of the new appearing dialog, and click the “Display” button.

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

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.

The grid has a context menu with many helpful functions.

Use the „Save“ button to store the modified data set in the database.

Use the „Discard” button to close the dialog without any modifications.