ChemSep Case Book: Adding Components

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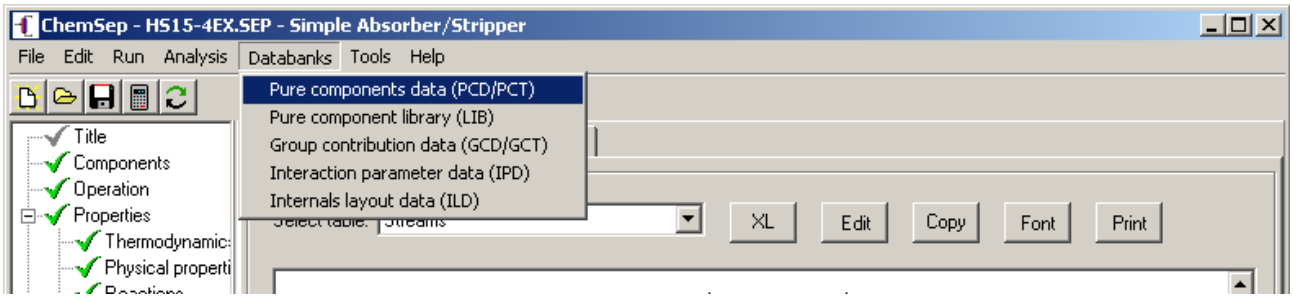
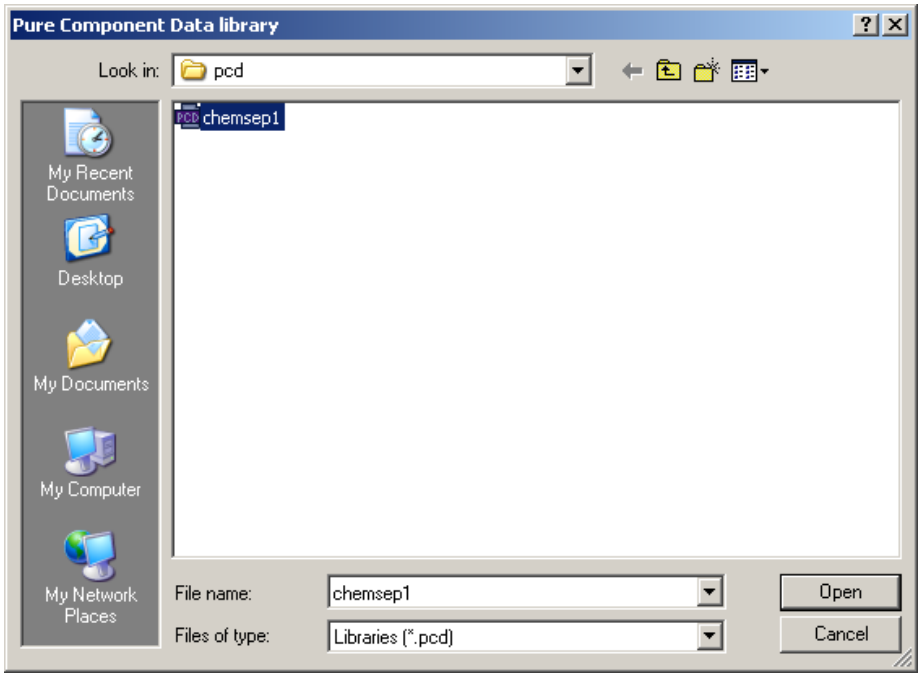
A potentially important drawback of *ChemSep-Lite* is that it comes with a databank of only 53 common compounds. It is, however, possible to add compounds to the databank (or, more sensibly, to create new databanks for additional compounds). We note in passing that the techniques described here can also be used with the full *ChemSep* for Windows. Here we show one way to do this.

Open *ChemSep* and go to the **Databanks** menu. **Select Pure components data (PCD/PCT)** as shown below.

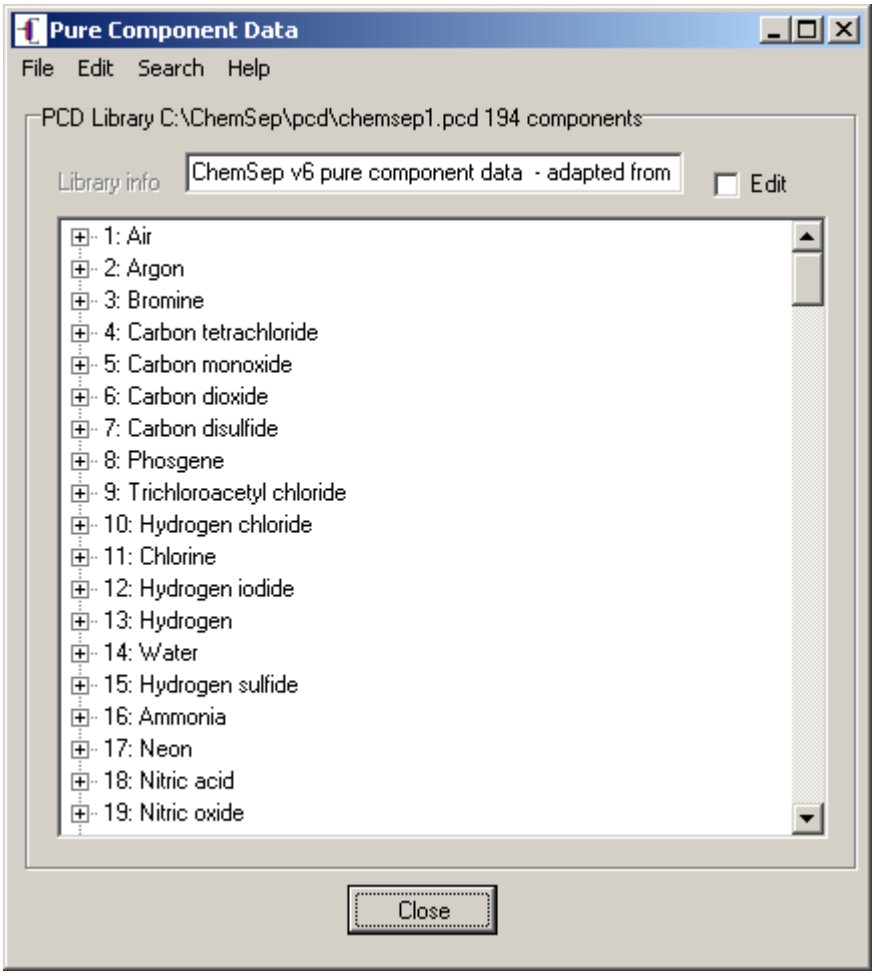


This will bring up a file open window.

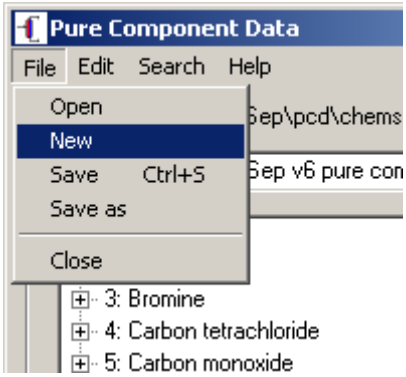


Select a **pcd** file (it does not matter which one – we are going to create a new pcd file, but the program needs to open an existing file first).

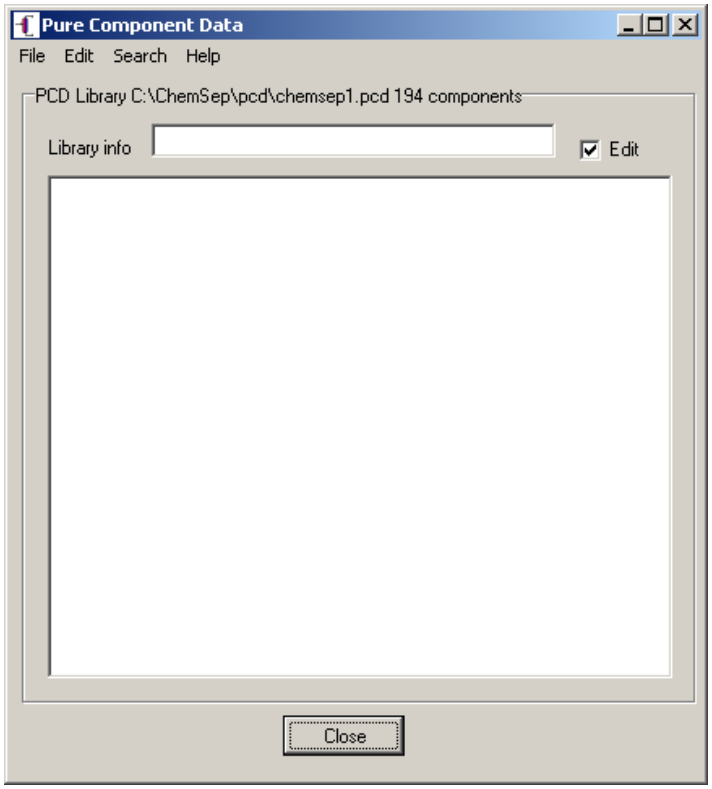
This will open the selected pcd file in a new window:



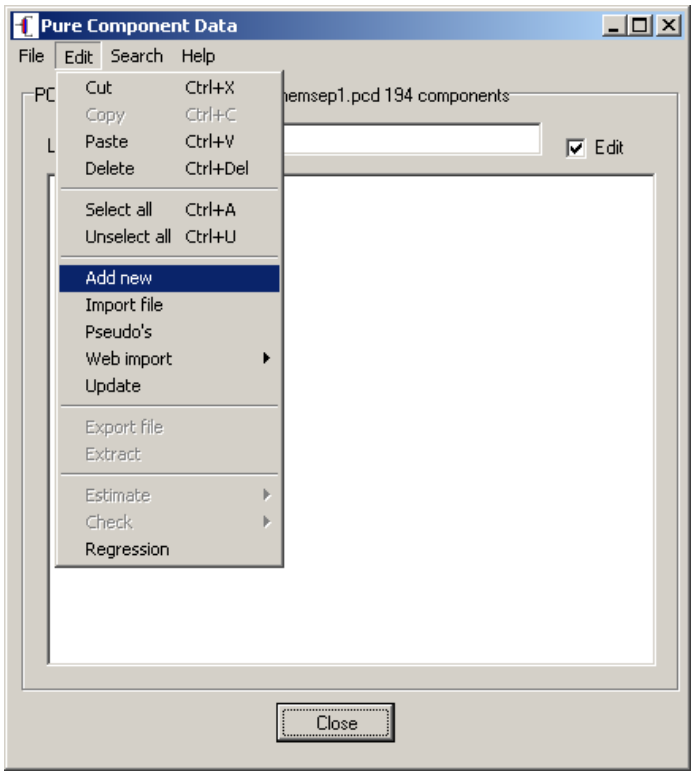
Now, go to the **file** menu and select **New**.



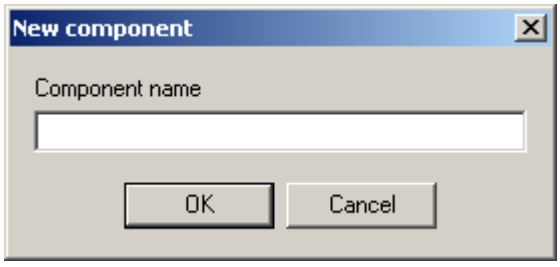
The window will now look like this:



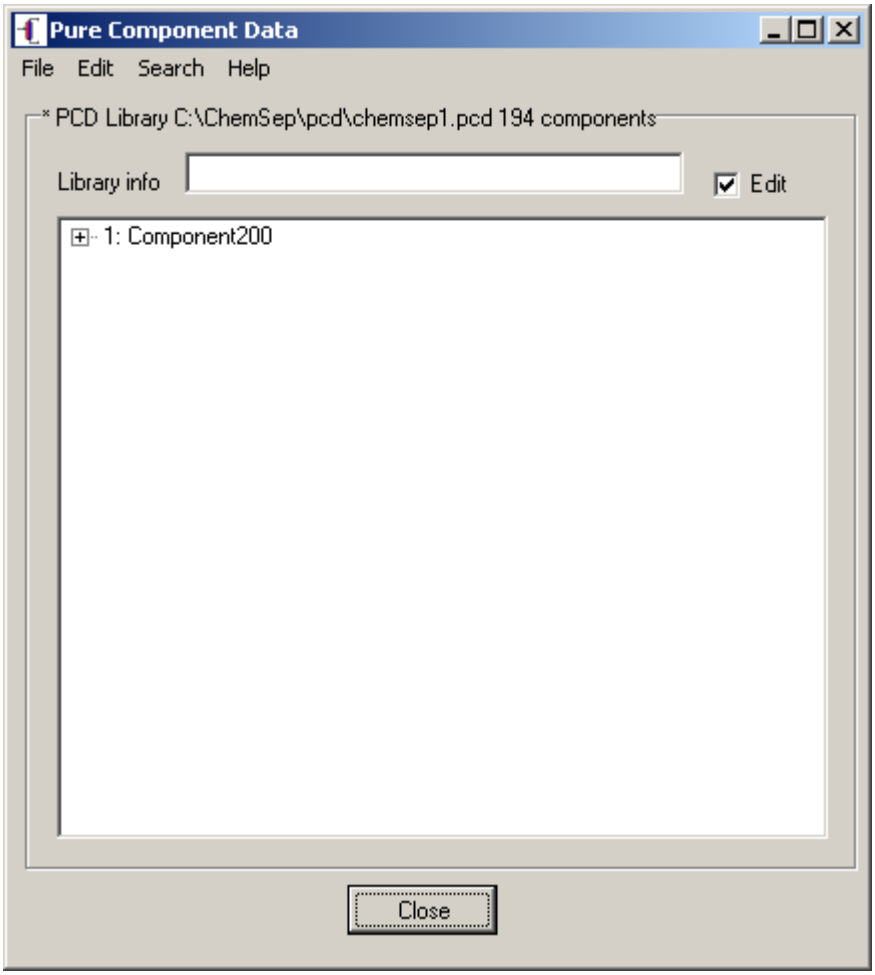
Now go to the **Edit** menu and select **Add new**



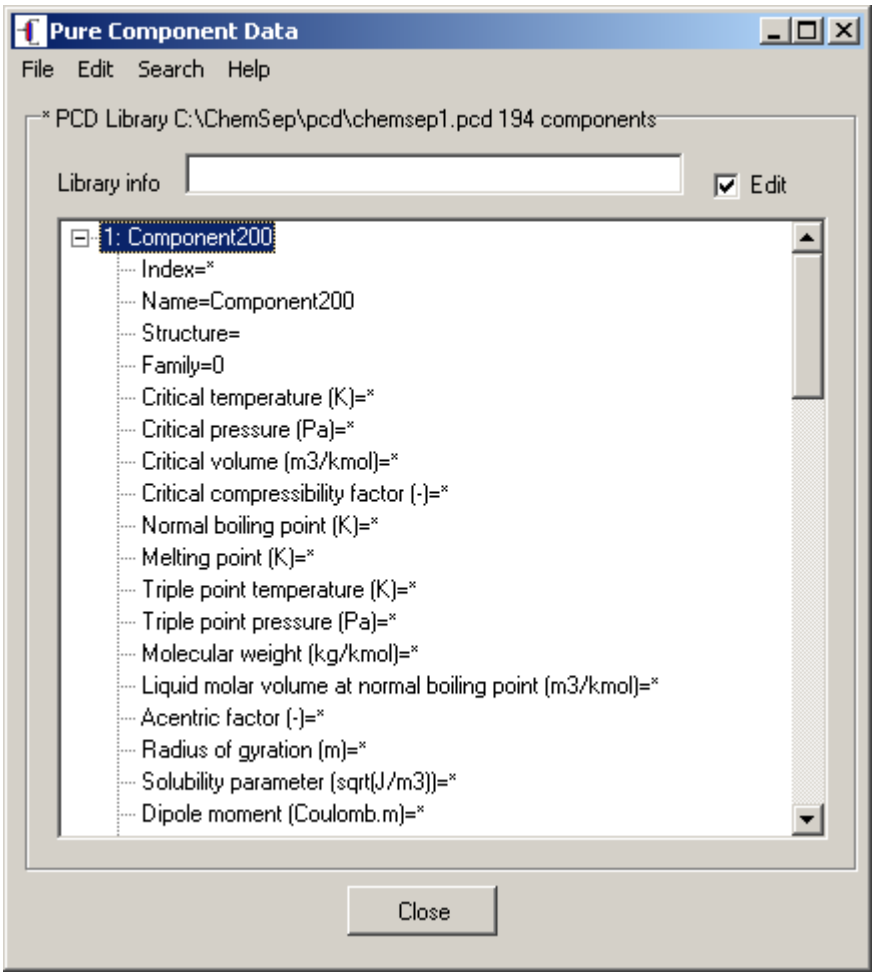
You will be invited to type in the name of a new component:



Type something in the space provided and press **Enter**. You should see something like this.



Click on the + sign by the name of the compound and you will see a long list or property constants (all of which are empty now).



Note the * on each line; this means the parameter has not been entered.

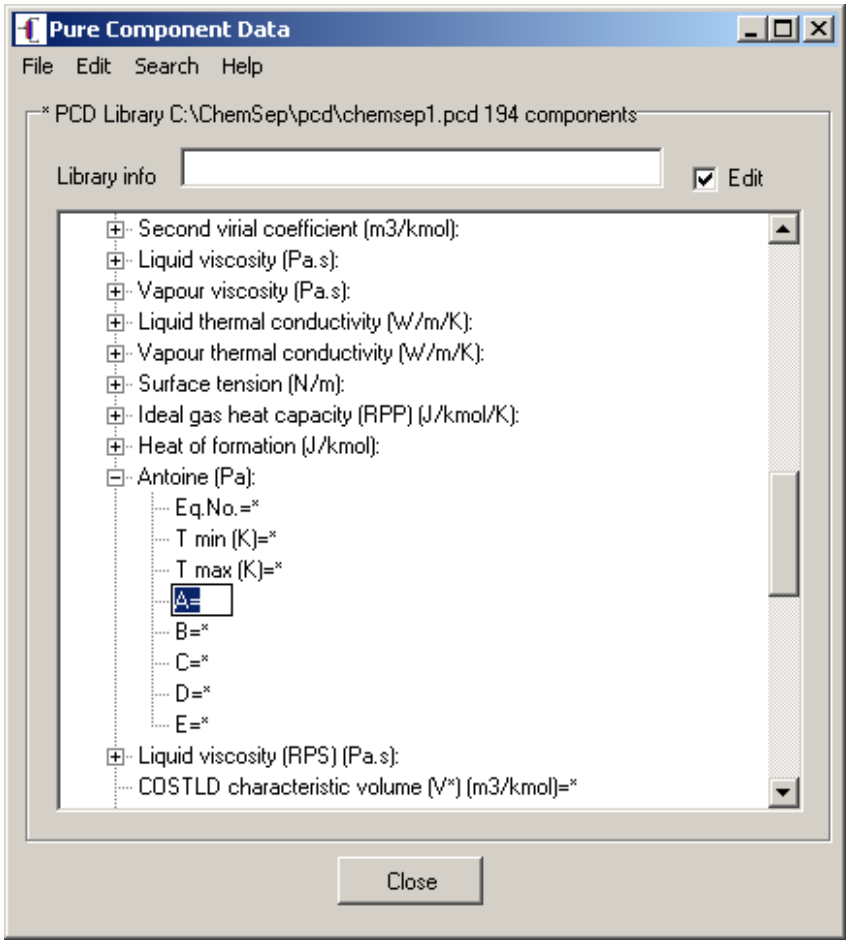
Essential Properties

It is useful to know that you do not need to enter values for all of the missing properties in order to run ChemSep. Here is what you need to enter in the databank:

Index number: anything will do as long as it is high enough (more than 10000 and don't duplicate)
Critical temperature (if you want to use an equation of state)
Critical pressure (ditto)
Acentric factor (advisable for EOS models – program will assume zero if absent)
Ideal gas heat capacity (essential if any enthalpy calculations are to be done)

Many equilibrium calculations can be done with just these parameters. Many other properties can be estimated from just these parameters and even more can be estimated if, in addition, the normal boiling point is provided.

To enter a property constant click on the line of data until you see a box around it as shown below. You may have to click on the line two or three times. Enter the property value to the right of the '=' sign. **Do not delete the '=' sign or anything to the left of it**. **It is essential to use the units specified because the databank editor does not perform unit conversions**.



Do not forget to save the file use (**Save as**) when you have completed the data entry.

Temperature dependent properties

A word of caution about temperature dependent parameters is in order. You can select the equation used to calculate the property as well as enter the limits. The equations available are listed at the end of this article.

All temperature dependent properties require the temperature in Kelvin.

A special note about the Antoine equation which has the following form.

$$\ln P_{sat} = A - \frac{B}{T + C}$$

P_{sat} is the vapor pressure. *ChemSep* requires the temperature to be specified in Kelvin and returns the vapor pressure in Pascals. Parameters from other sources may need to be converted to this form of the equation before being entered in the databank.

Equations in *ChemSep*

100	y = a + b.t + c.t**2 + d.t**3 + e.t**4
101	y = exp(a + b/t + c.ln(t) + d.t**e)
102	y = a.t**b / (1 + c/t + d/t**2)
103	y = a + b.exp(-c/t**d)
104	y = a + b/t + c/t**3 + d/t**8 + e/t**9
105	y = a / b**[1 + (1 - t/c)**d]
106	y = a(1 - t)**[b + c.t + d.t**2 + e.t**3]
107	y = a + b [(c/t) / sinh(c/t)]^2 + d [(e/t) / cosh(e/t)]^2
114	y = a**2/t + b - 2 a c t - a d t**2 - c**2 t^3 / 3 - c d t**4 / 2 - d**2 t**5 / 5
115	y = exp(a + b/t + c.ln(t) + d.t**2 + e/t**2)
116	y = a + b t**0.35 + c t**(2/3) + d t + e t**(4/3)
117	y = a.t + b c / tanh(c/t) - d e / tanh(e/t)
120	y = a - b/(t + c)
121	y = a + b/t + c.ln(t) + d.t**e
122	y = a + b/t + c.ln(t) + d.t**2 + e/t**2
150	y = a + b*T + c*T**2+d*t*+e/T^2;
0	y = a
1	y = a
2	y = a + b.t
3	y = a + b.t + c.t**2
4	y = a + b.t + c.t**2 + d.t**3
5	same as 100
10	same as 207
11	y = exp(a)
12	y = exp(a + b.t)
13	y = exp(a + b.t + c.t**2)
14	y = exp(a + b.t + c.t**2 + d.t**3)
15	y = exp(a + b.t + c.t**2 + d.t**3 + e.t**4)
16	y = a + exp(b/t + c + d.t + e.t**2)
17	y = a + exp(b + c.t + d.t**2 + e.t**3)
45	y = a.t + b.t**2/2 + c.t**3/3 + d.t**4/4 + e.t**5/5
75	y = b + 2.c.t + 3.d.t**2 + 4.e.t**3
207	y = exp[a - b/(t + c)]
208	y = 10**[a - b/(t + c)]
209	y = 10**[a(1/t - 1/b)]
210	y = 10**[a + b/t + c.t + d.t**2]
211	y = a[(b - t) / (b - c)]**d