The *View Data* module

Use ***View Data*** to examine stored compound data (H, S, $C_p(T)$, G, etc.) in ***Compound*** type databases and list solutions and their constituents in ***Solution*** type databases.

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(continued)

Table of contents (continued)

The *View Data* module

1° **Click** on ***View Data*** in the main ***FactSage*** window.

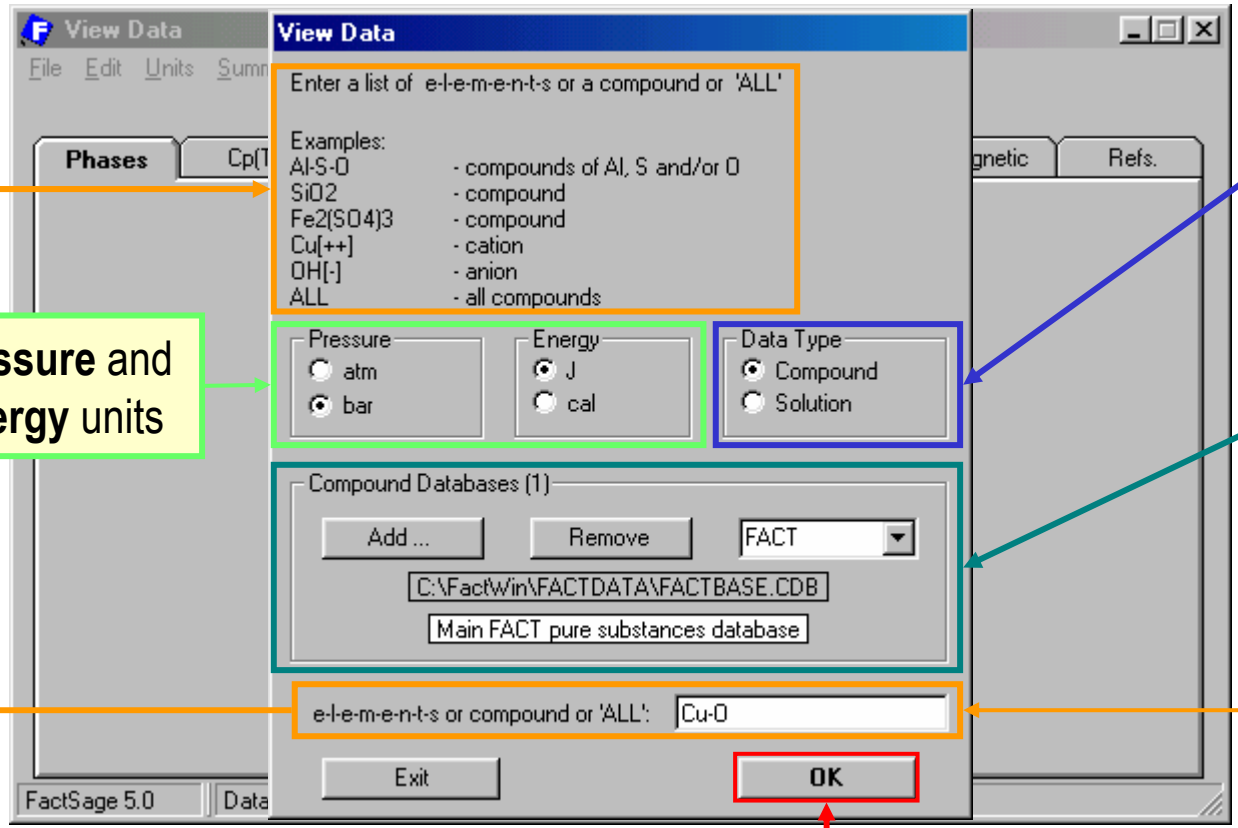
View Data of a Compound Database

The following two slides show how a search for a list of compounds in a given system is prepared and executed.

The resulting list of species is shown and the various options in the Menu bar are indicated.

Note that the search can also be for a single compound with a given formula. The appropriate entry formats are shown in the first of the two slides.

View Data of a Compound Database



Pressure and **Energy** units

Compound Database

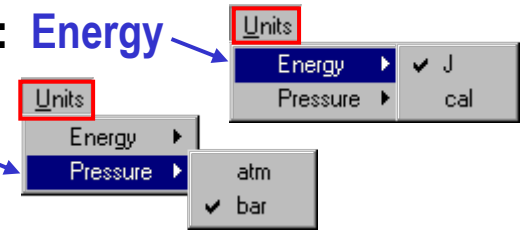
Possibility to add other databases in the data search - see slide 18

For example, the elements **Cu** and **O**

Click on «OK» to scan the **Main *FACT* pure substance database** for all species of **Cu** and **O**

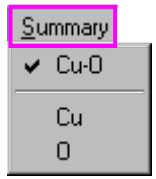
The Menu Bar

Units Menu: **Energy**



Pressure

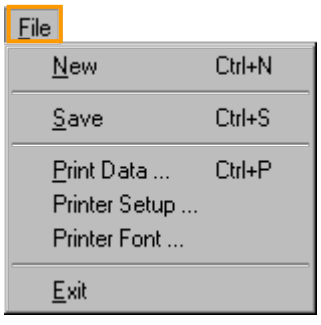
Summary Menu:

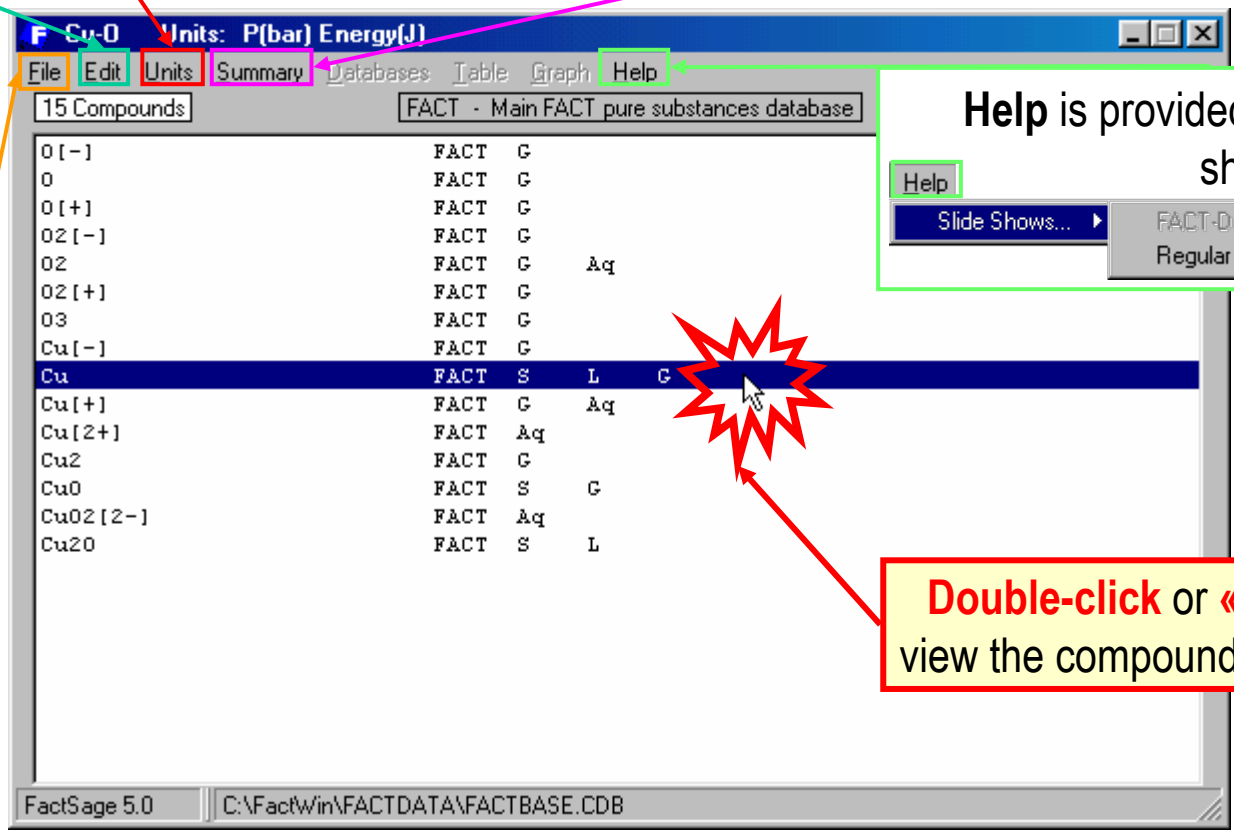


- **All species containing Cu and O**
- **All species containing Cu**
- **All species containing O**

Edit Menu:

File Menu:





Help is provided through a slide show presentation

Double-click or **«Enter»** to view the compound data of **Cu**

Phases and References of a compound

The following two slides show the display window with the basic information on a particular compound.

The substance name and the molecular weight are shown.

The Phases Tab in the display window is related to the phases and the temperature ranges for which data are available.

The second slide shows the result when clicking on the Refs. Tab.

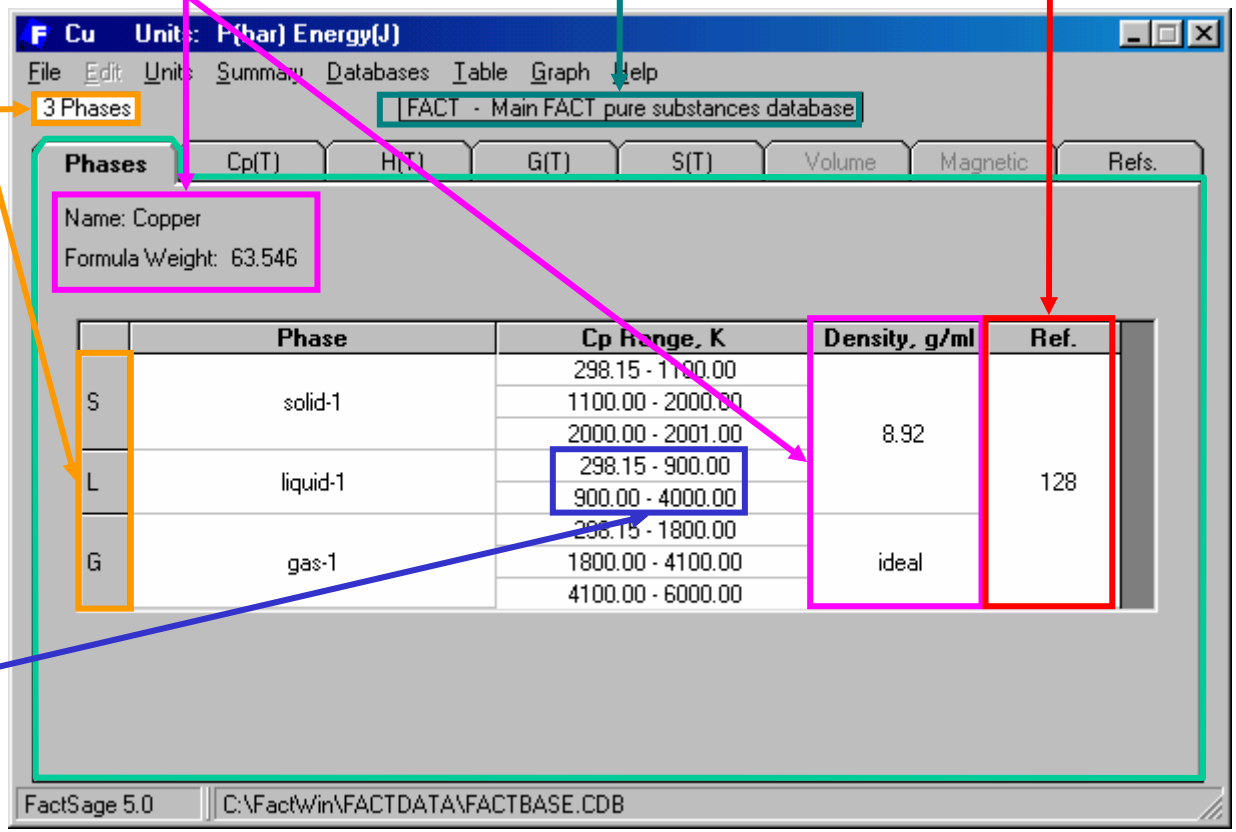
Phases

Retrieval of data on Cu from the Main ***FACT*** pure substances database.

Species name, formula weight and density

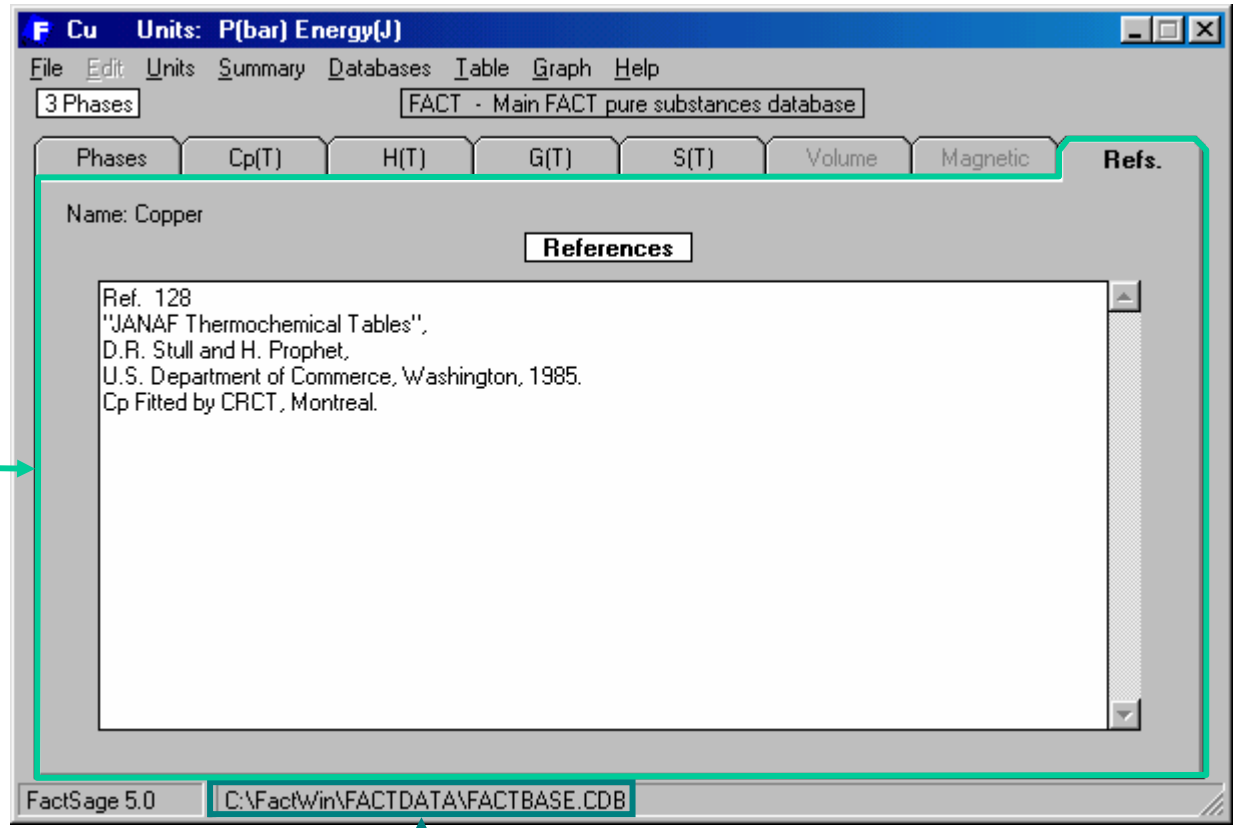
References

Cu has 3 phases – **S**, **L** and **G**.



There are 2 temperature ranges for Cu (liq) – each has its own C_P expression.

References



Bibliographic data

The full name of the database appears in the Status Bar: [C:\FactWin\FACTDATA\FACTBASE.CDB].

The basic compound data: H_{298}, S_{298} and C_p coefficients

The following slide shows the basic data that are stored for any compound in a database. These are:

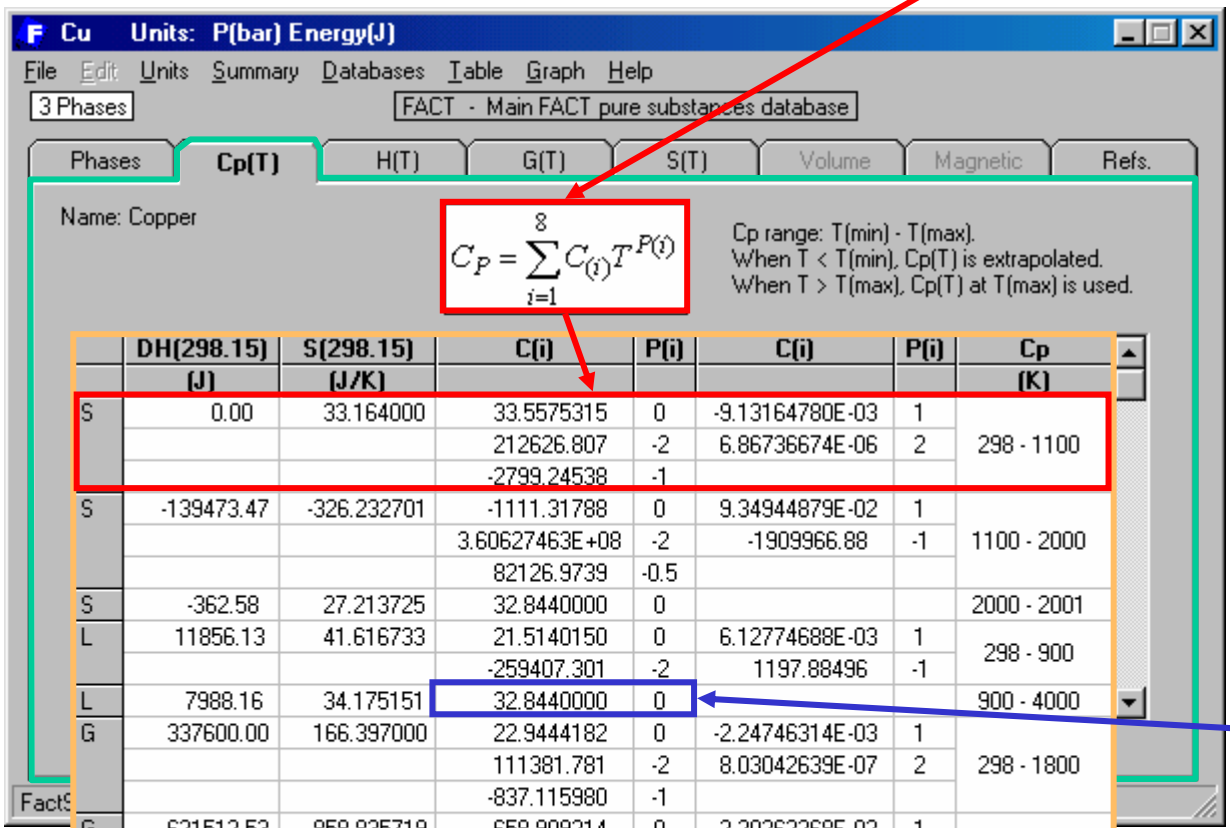
- the enthalpy of formation DH_{298},
- the entropy S_{298} and
- the coefficients of the C_p-polynomial

In many cases it is necessary to use more than one set of coefficients of C_p in order to describe the C_p-curve with sufficient accuracy. Furthermore, if a compound undergoes phase changes with increase of temperature, each new phase will have at least one new C_p-polynomial.

Heat capacity expressions – $C_p(T)$

The heat capacity expression of solid copper between 298 K and 1100K is:

$C_p(T) = [33.5575315 - 9.13164780 \times 10^{-3}\, T + 212626.807\, T^{-2} + 6.86736674 \times 10^{-6}\, T^2 - 2799.24538\, T^{-1}]$ (J/mol·K)



	DH(298.15) (J)	S(298.15) (J/K)	C(i)	P(i)	C(i)	P(i)	Cp (K)
S	0.00	33.164000	33.5575315	0	-9.13164780E-03	1	
			212626.807	-2	6.86736674E-06	2	298 - 1100
			-2799.24538	-1			
S	-139473.47	-326.232701	-1111.31788	0	9.34944879E-02	1	
			3.60627463E+08	-2	-1909966.88	-1	1100 - 2000
			82126.9739	-0.5			
S	-362.58	27.213725	32.8440000	0			2000 - 2001
L	11856.13	41.616733	21.5140150	0	6.12774688E-03	1	298 - 900
			-259407.301	-2	1197.88496	-1	
L	7988.16	34.175151	32.8440000	0			900 - 4000
G	337600.00	166.397000	22.9444182	0	-2.24746314E-03	1	
			111381.781	-2	8.03042639E-07	2	298 - 1800
			-837.115980	-1			
G	621512.53	858.835719	658.909214	0	-2.20262268E-02	1	
			-4.41758515E+08	-2	1658224.92	-1	1800 - 4100
			-58679.2292	-0.5			
G	666782.42	786.762822	11.4516407	0	-81355891.4	-2	4100 - 6000
			-148798.790	-1	3843.93389	-0.5	

Note that the 2nd C_p expression for the liquid is constant at temperatures over 900 K.

Different derived thermodynamic functions: H(T), S(T) and G(T)

The basic data DH_{298}, S_{298} and $C_p(T)$ can be used to derive the temperature dependence of the enthalpy, H(T), the entropy, S(T) and, most important, the Gibbs energy, G(T).

$$H(T) = DH_{298} + \int_{298}^{T} Cp(T)dT$$

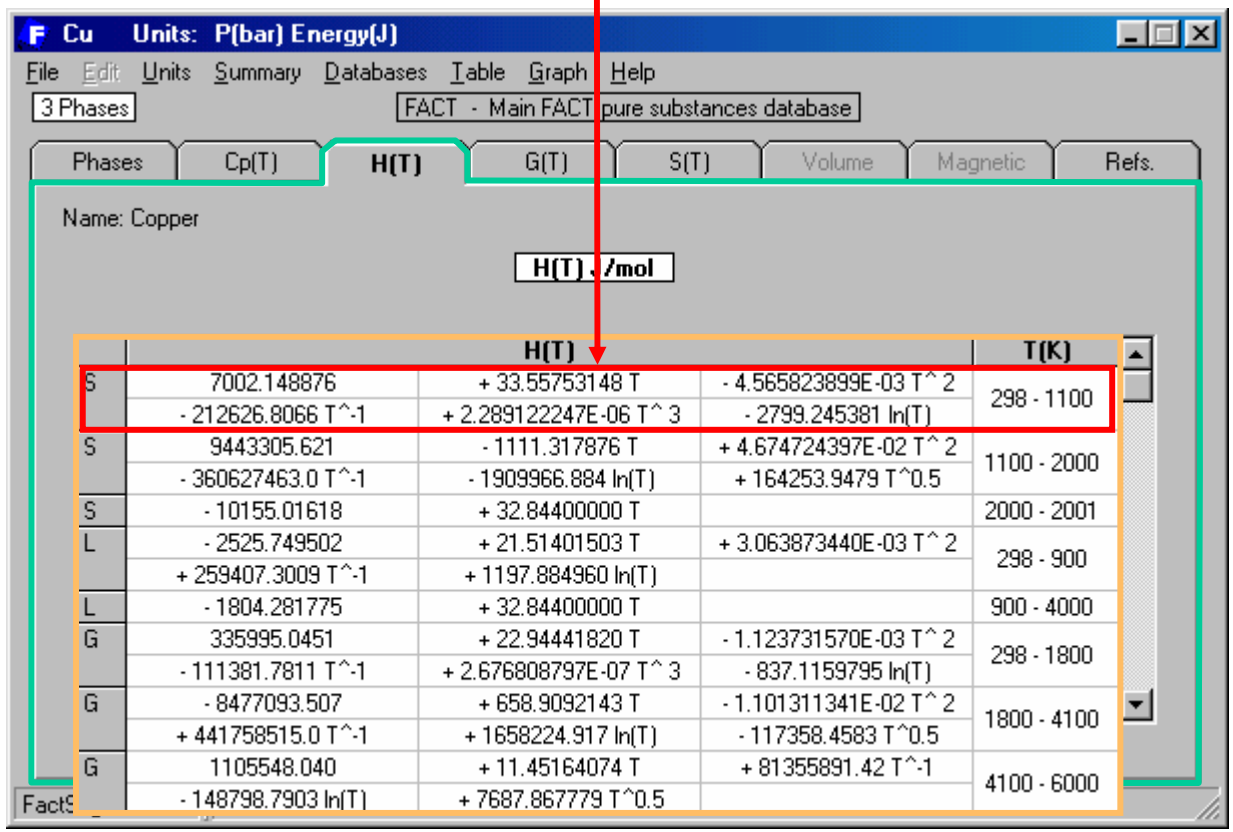
$$S(T) = S_{298} + \int_{298}^{T} Cp(T)/T dT$$

Combined in the Gibbs-Helmholtz equation:

$$G(T) = H(T) - T \cdot S(T)$$

Enthalpy expressions – H(T)

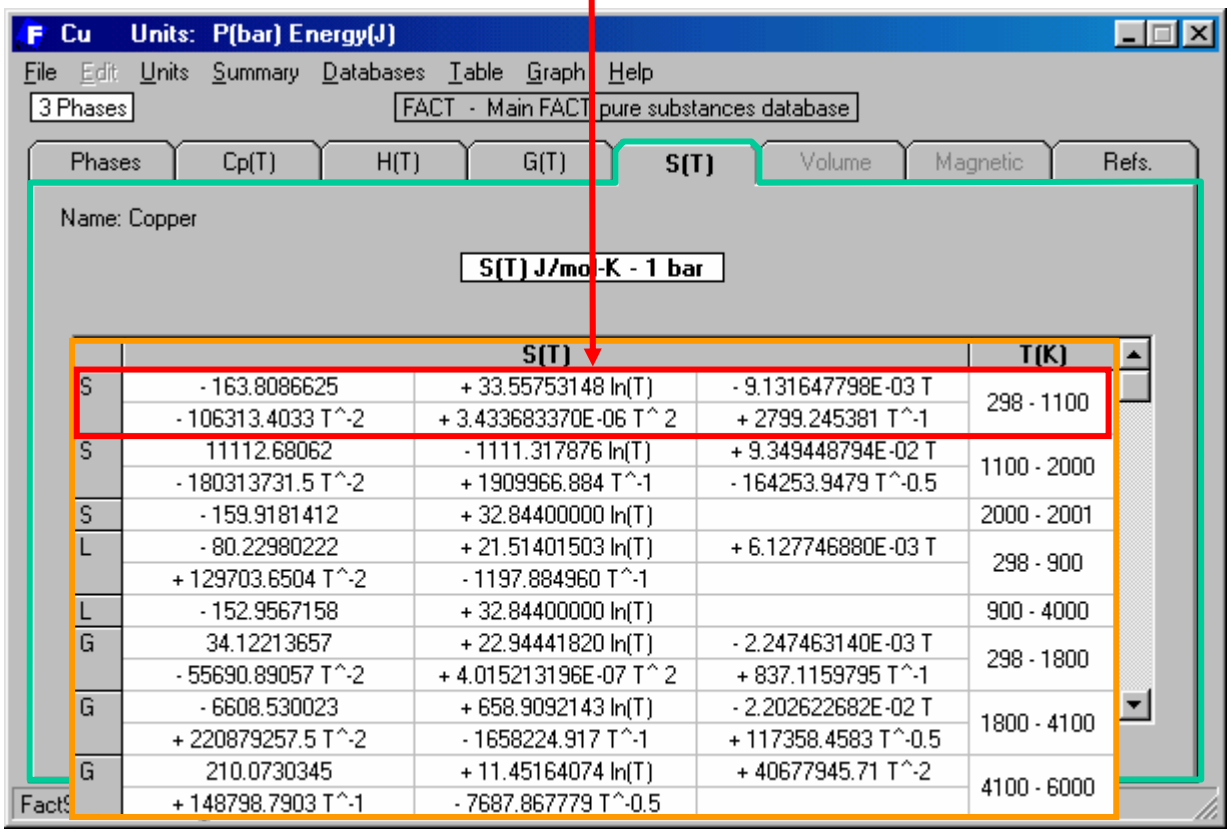
$$H(T) = [\,7002.148876 + 33.55753148\,T - 4.565823899 \times 10^{-3}\,T^2 - 212626.8066\,T^{-1} + 2.289122247 \times 10^{-6}\,T^3 - 2799.245381\,\ln T]\ \text{(J/mol)}$$



	H(T)			T(K)
S	7002.148876	+ 33.55753148 T	- 4.565823899E-03 T^ 2	298 - 1100
	- 212626.8066 T^-1	+ 2.289122247E-06 T^ 3	- 2799.245381 ln(T)	
S	9443305.621	- 1111.317876 T	+ 4.674724397E-02 T^ 2	1100 - 2000
	- 360627463.0 T^-1	- 1909966.884 ln(T)	+ 164253.9479 T^0.5	
S	- 10155.01618	+ 32.84400000 T		2000 - 2001
L	- 2525.749502	+ 21.51401503 T	+ 3.063873440E-03 T^ 2	298 - 900
	+ 259407.3009 T^-1	+ 1197.884960 ln(T)		
L	- 1804.281775	+ 32.84400000 T		900 - 4000
G	335995.0451	+ 22.94441820 T	- 1.123731570E-03 T^ 2	298 - 1800
	- 111381.7811 T^-1	+ 2.676808797E-07 T^ 3	- 837.1159795 ln(T)	
G	- 8477093.507	+ 658.9092143 T	- 1.101311341E-02 T^ 2	1800 - 4100
	+ 441758515.0 T^-1	+ 1658224.917 ln(T)	- 117358.4583 T^0.5	
G	1105548.040	+ 11.45164074 T	+ 81355891.42 T^-1	4100 - 6000
	- 148798.7903 ln(T)	+ 7687.867779 T^0.5		

Entropy expressions – S(T)

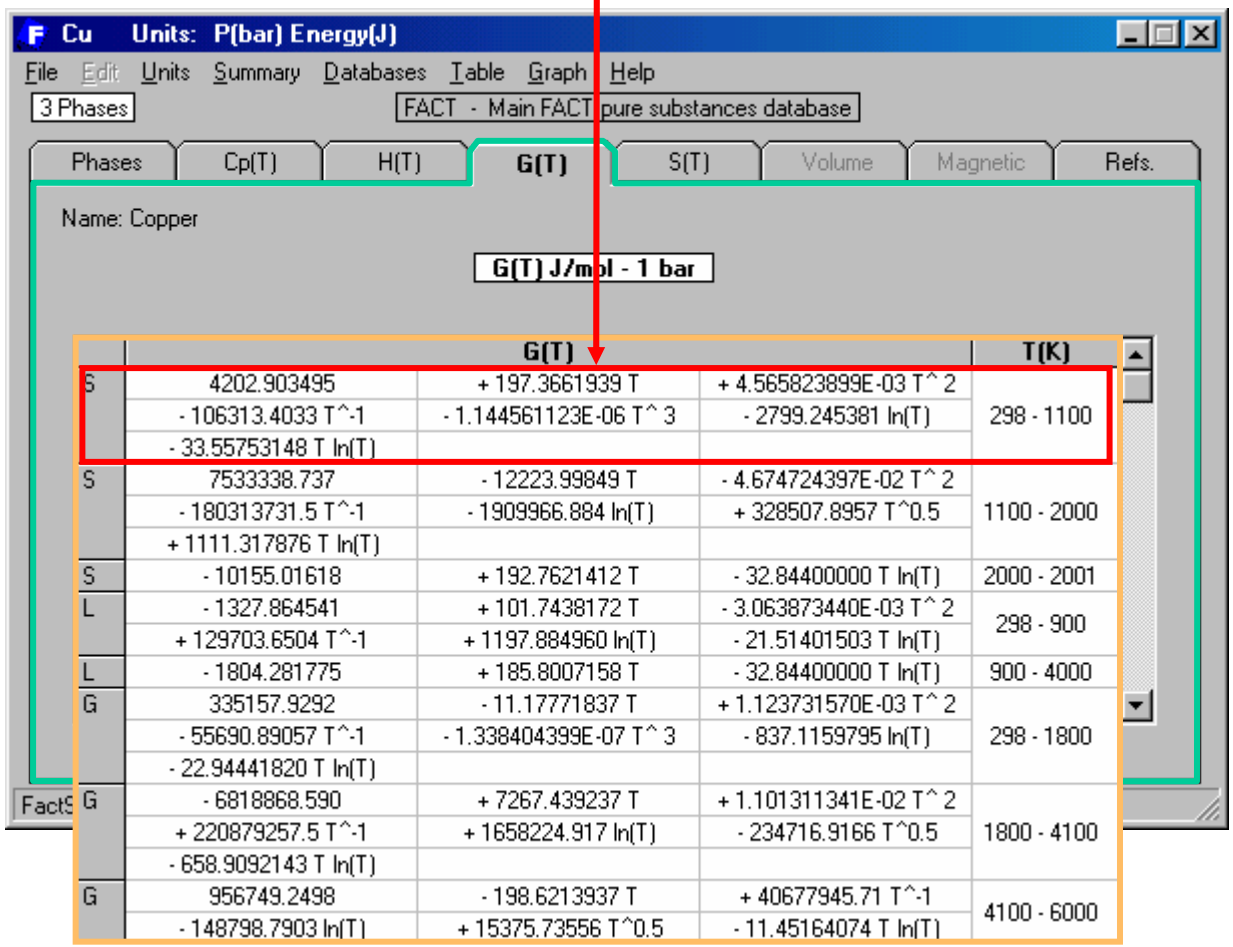
$$S(T) = [-163.8086625 + 33.55753148 \ln T - 9.131647798 \times 10^{-3} T - 106313.4033 T^{-2} + 3.433683370 \times 10^{-6} T^{2} + 2799.245381 T^{-1}] \text{ (J/mol·K) at 1 bar}$$



	S(T)			T(K)
S	- 163.8086625	+ 33.55753148 ln(T)	- 9.131647798E-03 T	298 - 1100
	- 106313.4033 T^-2	+ 3.433683370E-06 T^ 2	+ 2799.245381 T^-1	
S	11112.68062	- 1111.317876 ln(T)	+ 9.349448794E-02 T	1100 - 2000
	- 180313731.5 T^-2	+ 1909966.884 T^-1	- 164253.9479 T^-0.5	
S	- 159.9181412	+ 32.84400000 ln(T)		2000 - 2001
L	- 80.22980222	+ 21.51401503 ln(T)	+ 6.127746880E-03 T	298 - 900
	+ 129703.6504 T^-2	- 1197.884960 T^-1		
L	- 152.9567158	+ 32.84400000 ln(T)		900 - 4000
G	34.12213657	+ 22.94441820 ln(T)	- 2.247463140E-03 T	298 - 1800
	- 55690.89057 T^-2	+ 4.015213196E-07 T^ 2	+ 837.1159795 T^-1	
G	- 6608.530023	+ 658.9092143 ln(T)	- 2.202622682E-02 T	1800 - 4100
	+ 220879257.5 T^-2	- 1658224.917 T^-1	+ 117358.4583 T^-0.5	
G	210.0730345	+ 11.45164074 ln(T)	+ 40677945.71 T^-2	4100 - 6000
	+ 148798.7903 T^-1	- 7687.867779 T^-0.5		

Gibbs Energy expressions – G(T)

$$G(T) = [\,4202.903495 + 197.3661939\,T - 4.565823899 \times 10^{-3}\,T^2 - 106313.4033\,T^{-1} + 1.144561123 \times 10^{-6}\,T^3 - 2799.245381\,\ln T - 33.55753148\,T\ln T\,] \text{ (J/mol) at 1 bar}$$



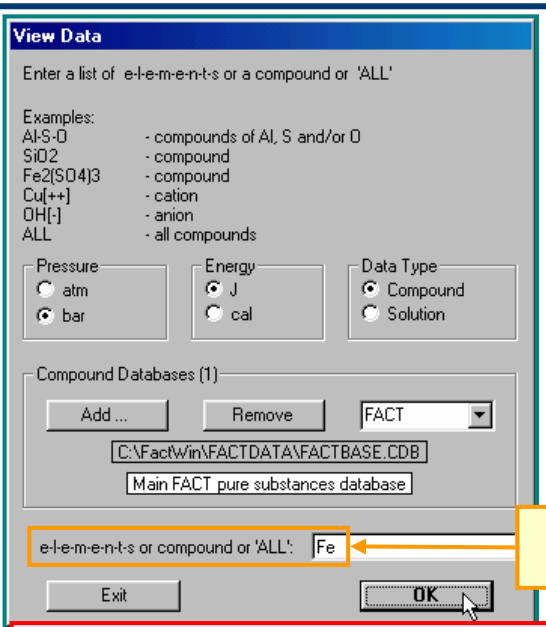
	G(T)			T(K)
S	4202.903495	+ 197.3661939 T	+ 4.565823899E-03 T^ 2	298 - 1100
	- 106313.4033 T^-1	- 1.144561123E-06 T^ 3	- 2799.245381 ln(T)	
	- 33.55753148 T ln(T)			
S	7533338.737	- 12223.99849 T	- 4.674724397E-02 T^ 2	1100 - 2000
	- 180313731.5 T^-1	- 1909966.884 ln(T)	+ 328507.8957 T^0.5	
	+ 1111.317876 T ln(T)			
S	- 10155.01618	+ 192.7621412 T	- 32.84400000 T ln(T)	2000 - 2001
L	- 1327.864541	+ 101.7438172 T	- 3.063873440E-03 T^ 2	298 - 900
	+ 129703.6504 T^-1	+ 1197.884960 ln(T)	- 21.51401503 T ln(T)	
L	- 1804.281775	+ 185.8007158 T	- 32.84400000 T ln(T)	900 - 4000
G	335157.9292	- 11.17771837 T	+ 1.123731570E-03 T^ 2	298 - 1800
	- 55690.89057 T^-1	- 1.338404399E-07 T^ 3	- 837.1159795 ln(T)	
	- 22.94441820 T ln(T)			
G	- 6818868.590	+ 7267.439237 T	+ 1.101311341E-02 T^ 2	1800 - 4100
	+ 220879257.5 T^-1	+ 1658224.917 ln(T)	- 234716.9166 T^0.5	
	- 658.9092143 T ln(T)			
G	956749.2498	- 198.6213937 T	+ 40677945.71 T^-1	4100 - 6000
	- 148798.7903 ln(T)	+ 15375.73556 T^0.5	- 11.45164074 T ln(T)	

Additional basic data of a compound

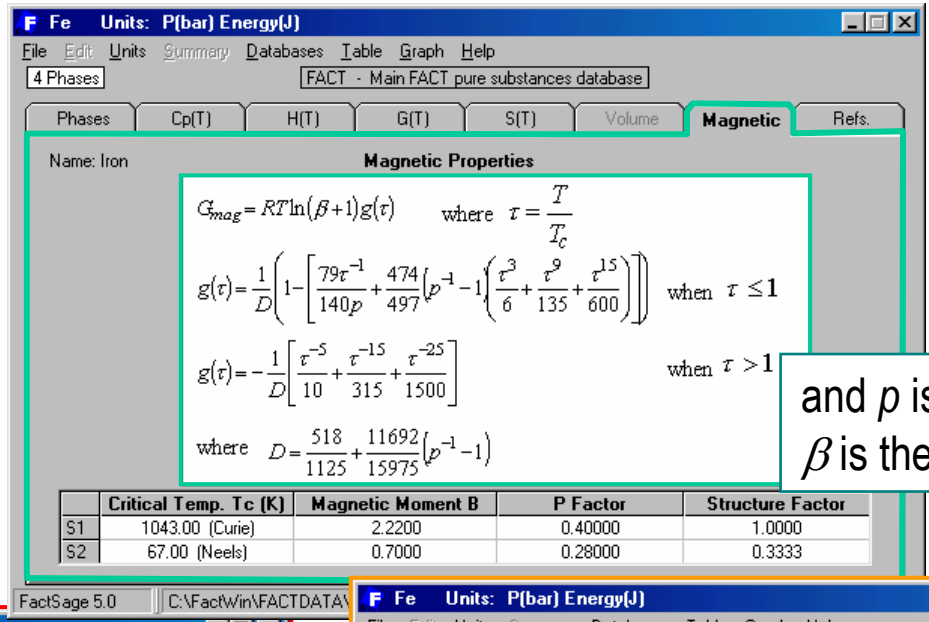
The compound database format permits not only the storage of the standard data shown in the previous slides.

It is also possible to enter data for the magnetic Gibbs energy of a solid compound, basic data the permit the calculation of virial coefficients of gaseous compounds, and data to treat the pressure dependence of the Gibbs energy of condensed compounds according to the Birch-Murnaghan approach.

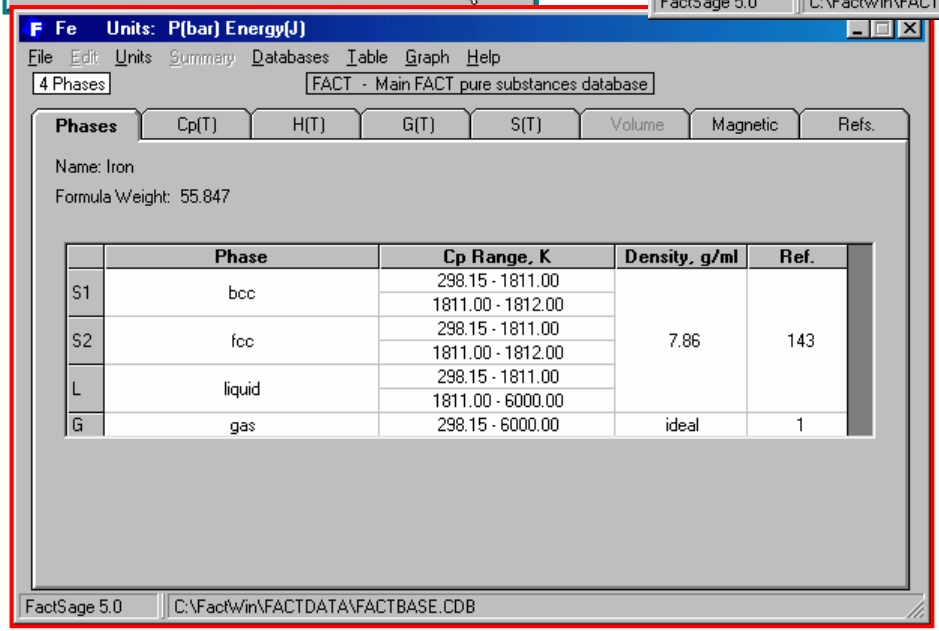
Magnetic data and C_p expressions for Fe

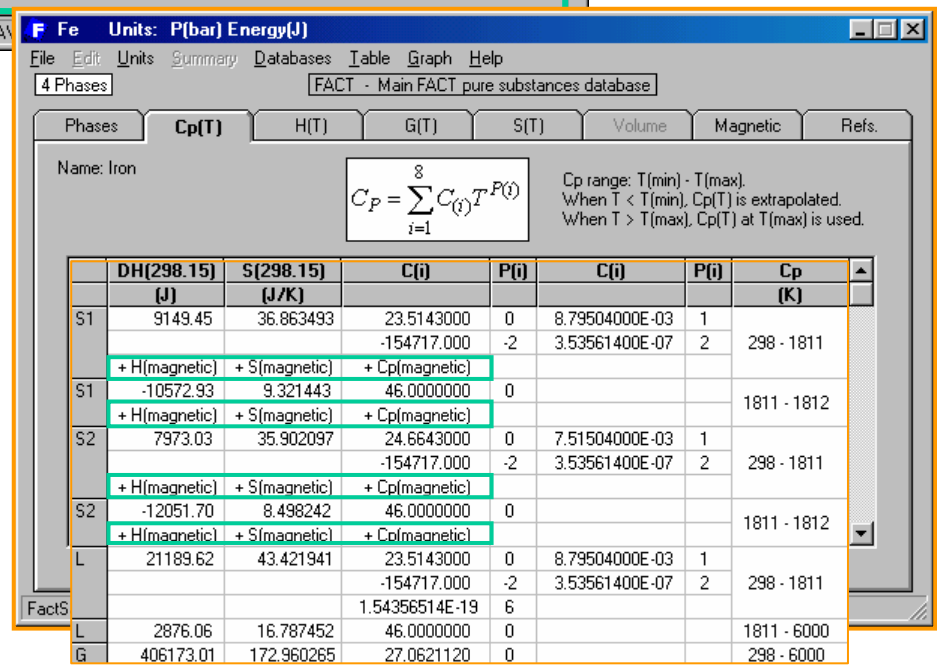


Fe

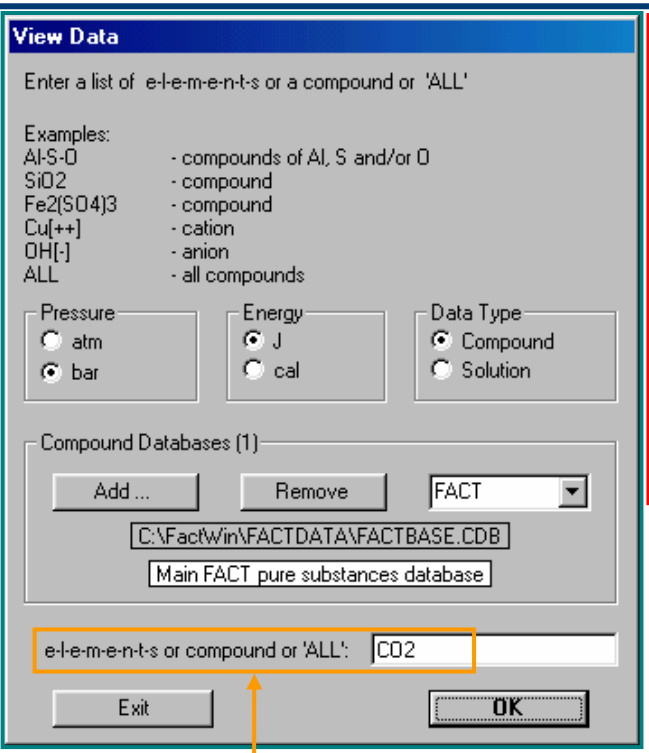


and p is the P Factor and β is the Structure Factor





Real gas coefficients for carbon dioxide CO_2



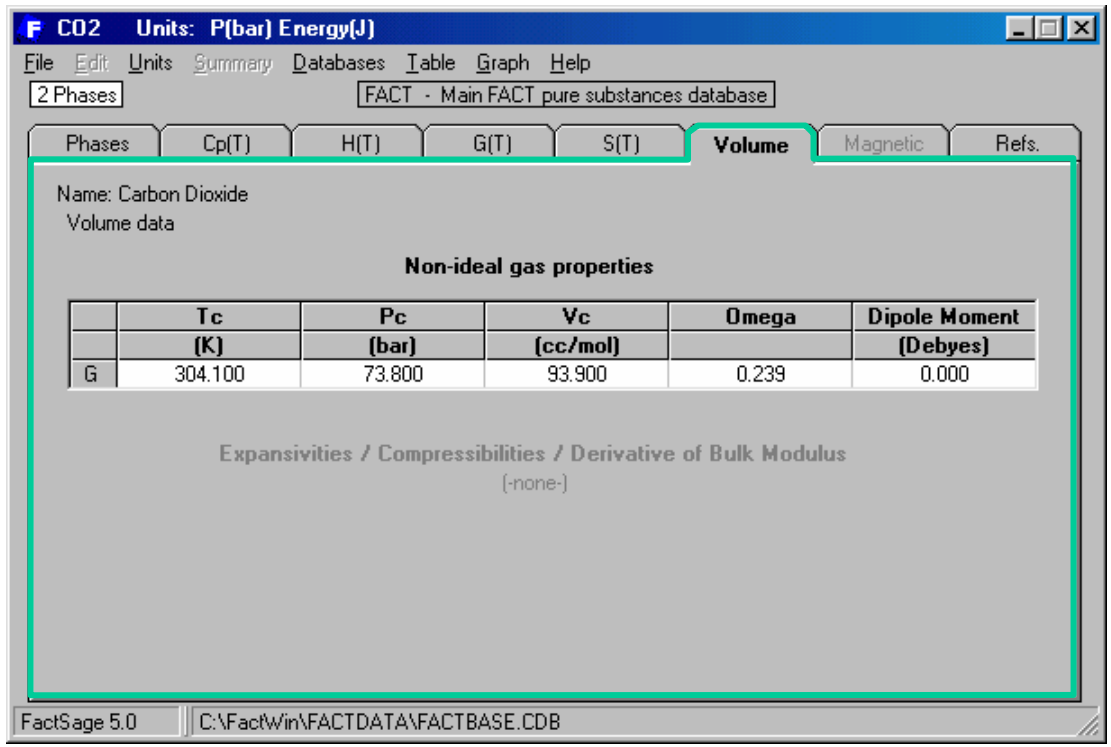
For example, CO_2

The truncated virial equation of state is employed to treat real gases:

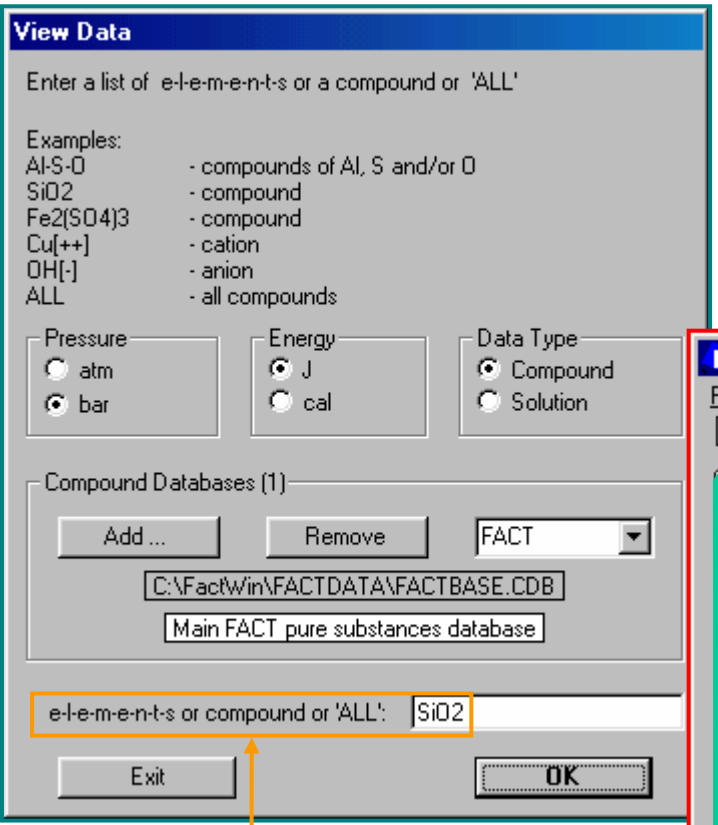
$$\frac{PV}{RT} = 1 + \frac{BP}{RT}$$

B is estimated (for pure gases and mixtures) by the Tsonopoulos method* from P_c, T_c and omega (the acentric factor) for the pure gases. Gases are treated as non-polar. For ideal gases, the value of **B** is zero.

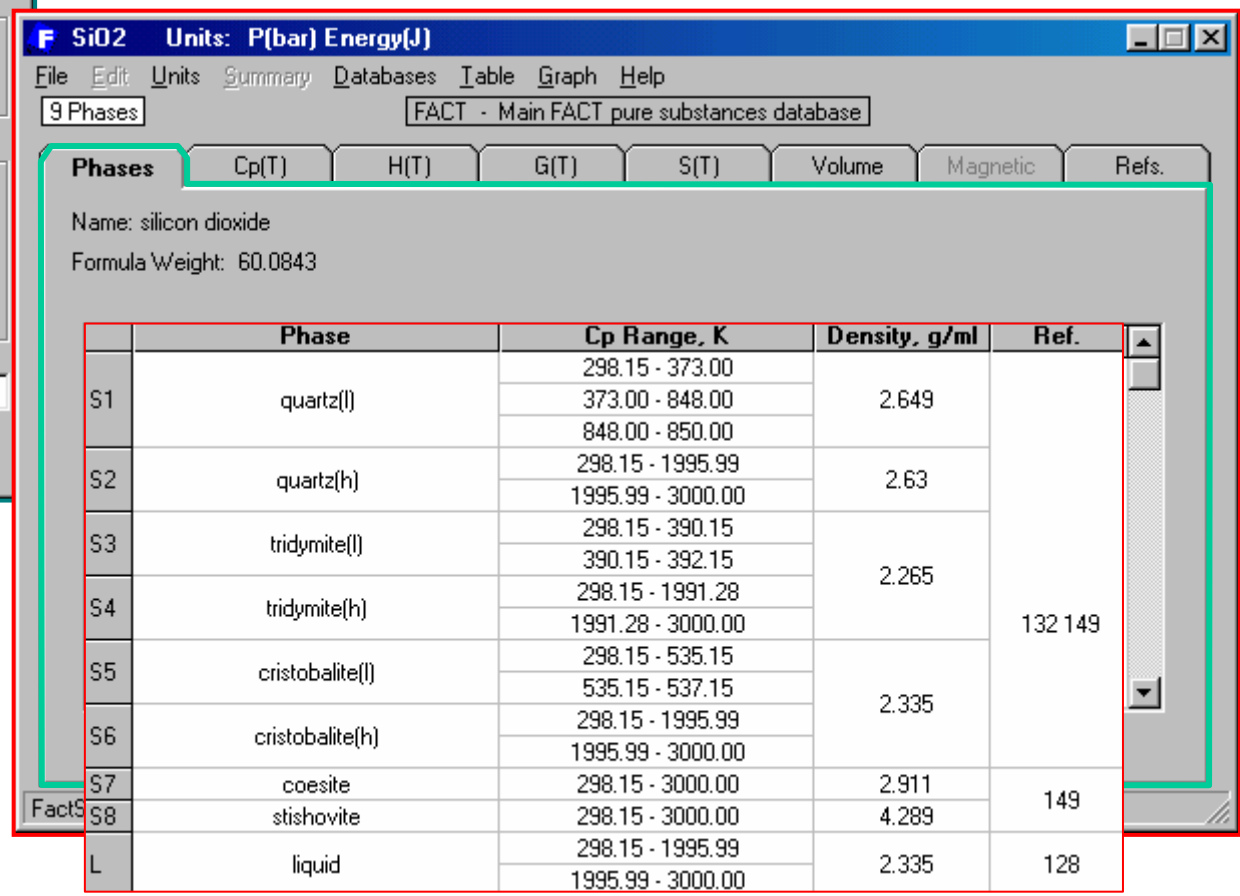
* «*An Empirical Correlation of Second Virial Coefficients*» by C. Tsonopoulos, AIChE Journal, vol. 20, No 2, pp. 263-271, 1974.



Data for SiO_2

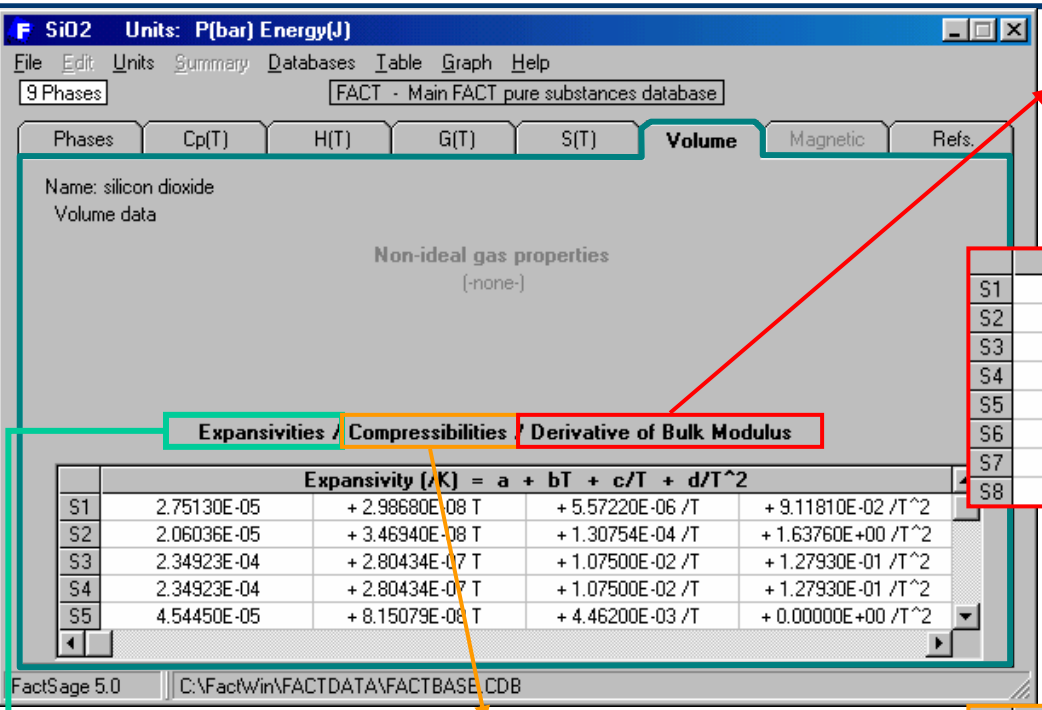


For example, SiO_2



	Phase	Cp Range, K	Density, g/ml	Ref.
S1	quartz(l)	298.15 - 373.00	2.649	132 149
		373.00 - 848.00		
		848.00 - 850.00		
S2	quartz(h)	298.15 - 1995.99	2.63	
		1995.99 - 3000.00		
S3	tridymite(l)	298.15 - 390.15	2.265	
		390.15 - 392.15		
S4	tridymite(h)	298.15 - 1991.28		
		1991.28 - 3000.00		
S5	cristobalite(l)	298.15 - 535.15	2.335	
		535.15 - 537.15		
S6	cristobalite(h)	298.15 - 1995.99		
		1995.99 - 3000.00		
S7	coesite	298.15 - 3000.00	2.911	149
S8	stishovite	298.15 - 3000.00	4.289	
L	liquid	298.15 - 1995.99	2.335	128
		1995.99 - 3000.00		

Volume data - expansivities, compressivities and derivative of bulk modulus



Derivative of the bulk modulus expression:

$$a + bT \ln T$$

	Derivative of Bulk Modulus = a + bT ln(T)	
S1	6.40000E+00	+ 0.00000E+00 T ln(T)
S2	5.34600E+00	+ 0.00000E+00 T ln(T)
S3	6.00000E+00	+ 1.00000E-03 T ln(T)
S4	6.00000E+00	+ 1.00000E-03 T ln(T)
S5	6.00000E+00	+ 0.00000E+00 T ln(T)
S6	6.00000E+00	+ 0.00000E+00 T ln(T)
S7	8.40000E+00	+ 0.00000E+00 T ln(T)
S8	6.00000E+00	+ 1.00000E-03 T ln(T)

	Expansivity (/K) = a + bT + c/T + d/T^2			
S1	2.75130E-05	+ 2.98680E-08 T	+ 5.57220E-06 /T	+ 9.11810E-02 /T^2
S2	2.06036E-05	+ 3.46940E-08 T	+ 1.30754E-04 /T	+ 1.63760E+00 /T^2
S3	2.34923E-04	+ 2.80434E-07 T	+ 1.07500E-02 /T	+ 1.27930E-01 /T^2
S4	2.34923E-04	+ 2.80434E-07 T	+ 1.07500E-02 /T	+ 1.27930E-01 /T^2
S5	4.54450E-05	+ 8.15079E-08 T	+ 4.46200E-03 /T	+ 0.00000E+00 /T^2

Compressibility expression (compressibilities):

$$a + bT + cT^2 + \frac{d}{T^3} \quad \left[Mbar^{-1}\right]$$

	Compressibility (/Mbar) = a + bT + cT^2 + dT^3			
S1	2.55600E-06	+ 1.15570E-11 T	+ 1.01280E-16 T^2	+ 8.89179E-19 /T^3
S2	1.39700E-06	+ 2.41191E-09 T	+ 2.15180E-12 T^2	+ 6.45430E-16 /T^3
S3	3.80000E-06	+ 0.00000E+00 T	+ 0.00000E+00 T^2	+ 0.00000E+00 /T^3
S4	3.80000E-06	+ 0.00000E+00 T	+ 0.00000E+00 T^2	+ 0.00000E+00 /T^3
S5	5.13000E-06	+ 0.00000E+00 T	+ 0.00000E+00 T^2	+ 0.00000E+00 /T^3
S6	5.13000E-06	+ 0.00000E+00 T	+ 0.00000E+00 T^2	+ 0.00000E+00 /T^3
S7	1.05000E-06	+ 1.00000E-10 T	+ 0.00000E+00 T^2	+ 0.00000E+00 /T^3
S8	2.95400E-07	+ 8.96100E-11 T	+ 3.29000E-14 T^2	+ 2.33100E-17 /T^3

Thermal expansion expression (expansivities):

$$a + bT + \frac{c}{T} + \frac{d}{T^2} \quad \left[K^{-1}\right]$$

	Expansivity (/K) = a + bT + c/T + d/T^2			
S1	2.75130E-05	+ 2.98680E-08 T	+ 5.57220E-06 /T	+ 9.11810E-02 /T^2
S2	2.06036E-05	+ 3.46940E-08 T	+ 1.30754E-04 /T	+ 1.63760E+00 /T^2
S3	2.34923E-04	+ 2.80434E-07 T	+ 1.07500E-02 /T	+ 1.27930E-01 /T^2
S4	2.34923E-04	+ 2.80434E-07 T	+ 1.07500E-02 /T	+ 1.27930E-01 /T^2
S5	4.54450E-05	+ 8.15079E-08 T	+ 4.46200E-03 /T	+ 0.00000E+00 /T^2
S6	4.54450E-05	+ 8.15079E-08 T	+ 4.46200E-03 /T	+ 0.00000E+00 /T^2
S7	5.43000E-06	+ 5.00000E-09 T	+ 0.00000E+00 /T	+ 0.00000E+00 /T^2
S8	2.30000E-06	+ 1.20000E-08 T	+ 6.20000E-03 /T	+ 1.13000E+00 /T^2

Using the Menu bar to generate thermodynamic property values

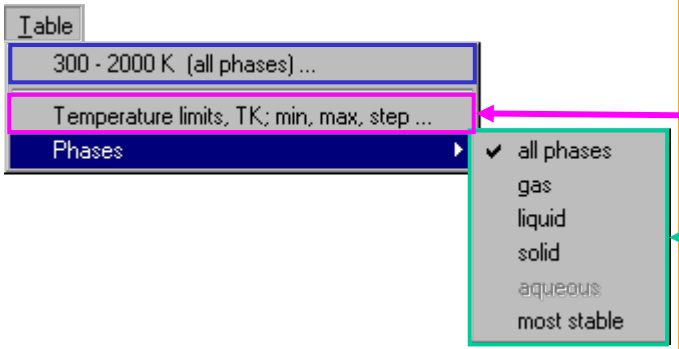
The following slides show how the View Data module can also be used to calculate the thermodynamic properties of a compound.

The properties values can be displayed in tables and also in graphs.

The Menu bar contains the appropriate option buttons.

The Menu Bar

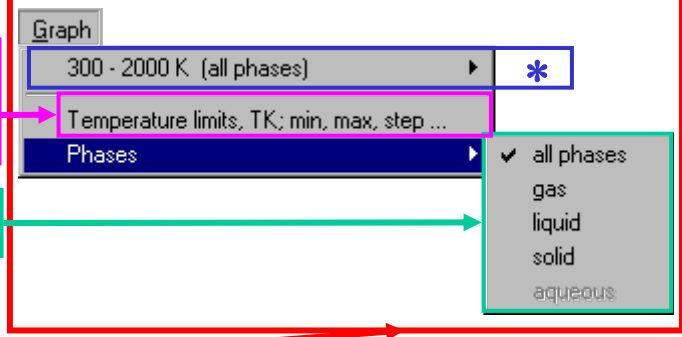
Table Menu:

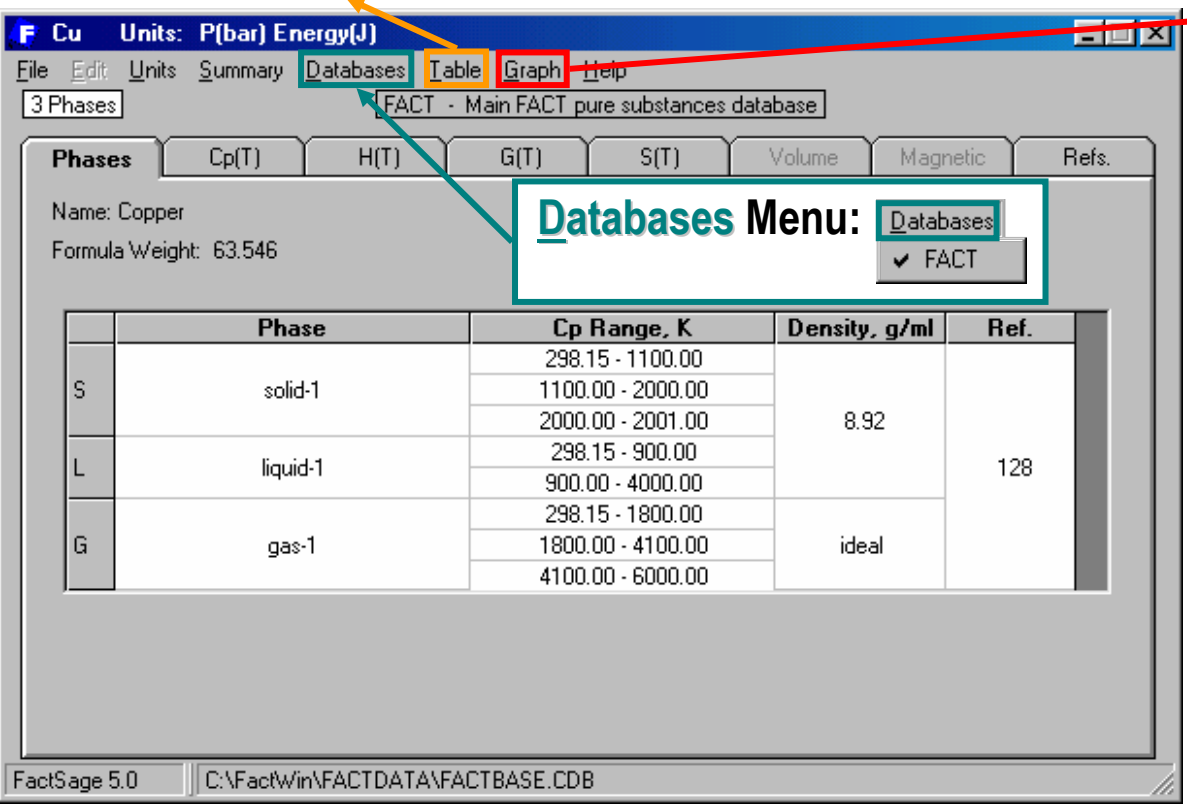


Selection of the temperature range and step.

Selection of the phase(s).

Graph Menu:

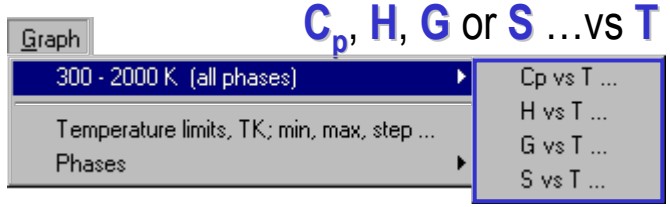




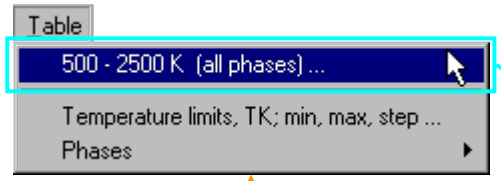
Databases Menu:

* Selection of thermodynamic data:

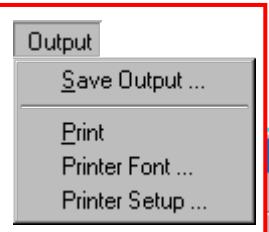
C_p, H, G or S …vs T



Thermodynamic Data for Cu: Tabular Output



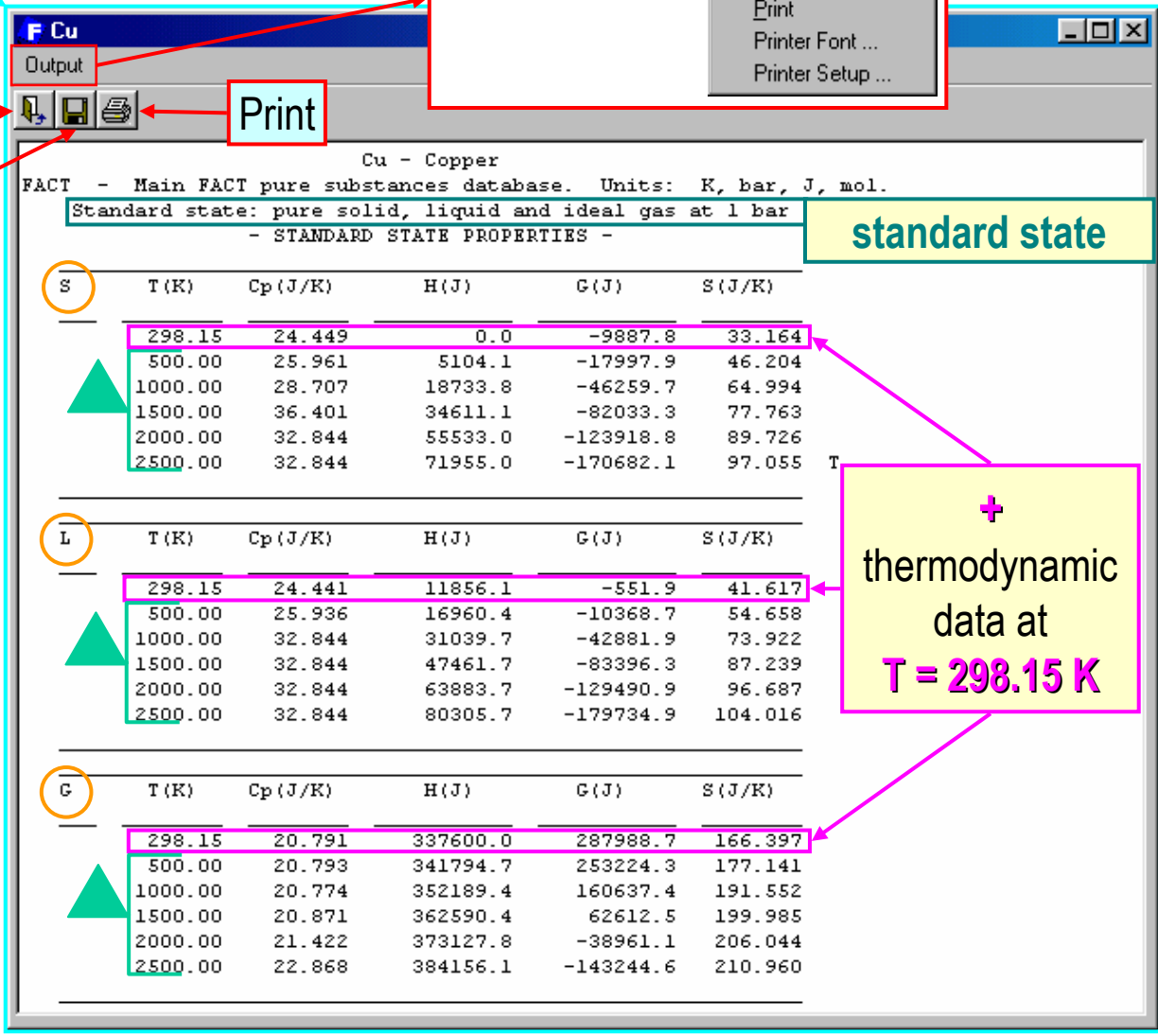
Output Menu:



Close

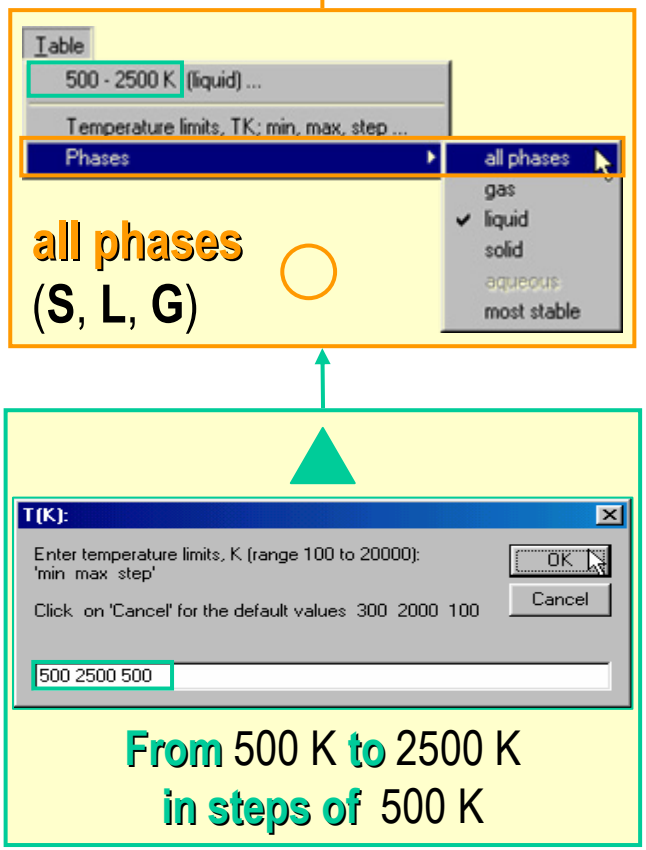
Save

Print

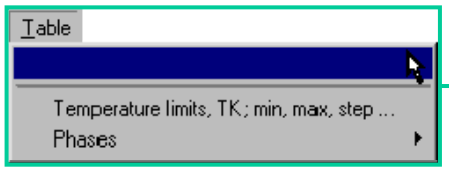


standard state

+ thermodynamic data at T = 298.15 K



Tabular output for **Fe**



Fe - Iron

FACT - Main FACT pure substances database. Units: K, bar, J, mol.
Standard state: pure solid, liquid and ideal gas at 1 bar
- STANDARD STATE PROPERTIES -

	T(K)	Cp(J/K)	H(J)	G(J)	S(J/K)
S1	298.15	24.845	0.0	-8133.5	27.280
	300.00	24.890	46.0	-8184.1	27.433
	500.00	29.356	5472.1	-15126.5	41.197
	700.00	35.098	11877.7	-24466.5	51.920
	900.00	44.964	19772.6	-35838.4	61.790
	1100.00	45.585	29902.5	-49232.4	71.941
	1184.81	41.635	33574.4	-55474.2	75.158
S1->S2	1184.81	Delta(H) =	1012.9	Delta(S) =	0.855
S2	1184.81	33.954	34587.3	-55474.2	76.013
	1300.00	34.940	38555.0	-64415.8	79.208
	1500.00	36.664	45715.1	-80777.6	84.328
	1667.47	38.123	51977.0	-95235.0	88.285
S2->S1	1667.47	Delta(H) =	825.8	Delta(S) =	0.495
S1	1667.47	40.306	52802.8	-95235.0	88.780
	1700.00	40.522	54117.5	-98135.8	89.561
	1810.95	41.346	58658.2	-108217.6	92.148
S1->L	1810.95	Delta(H) =	13806.9	Delta(S) =	7.624
L	1810.95	45.999	72465.1	-108217.6	99.772
	1900.00	46.000	76561.2	-117200.9	101.980
	2100.00	46.000	85761.2	-138065.0	106.584
	2300.00	46.000	94961.2	-159806.5	110.769
	2500.00	46.000	104161.2	-182349.1	114.604
	2700.00	46.000	113361.2	-205628.5	118.144
	2900.00	46.000	122561.2	-229590.0	121.431
	3100.00	46.000	131761.2	-254186.5	124.499
	3131.93	46.000	133229.8	-258168.8	124.971
L->G	3131.93	Delta(H) =	349631.2	Delta(S) =	111.635
G	3131.93	27.062	482861.0	-258168.8	236.605
(1 bar)	3300.00	27.062	487409.4	-298055.8	238.020

The allotropic transformation S1 → S2 (alpha → gamma) at 1184.81 K

The allotropic transition reverses at 1667.47 K where S2 → S1 (gamma → delta).

Phase transitions **S1→S2→S1→L→G** as **T** increases.

…with an associated enthalpy of transformation of (34587.3 - 33574.4) = 1012.9 J

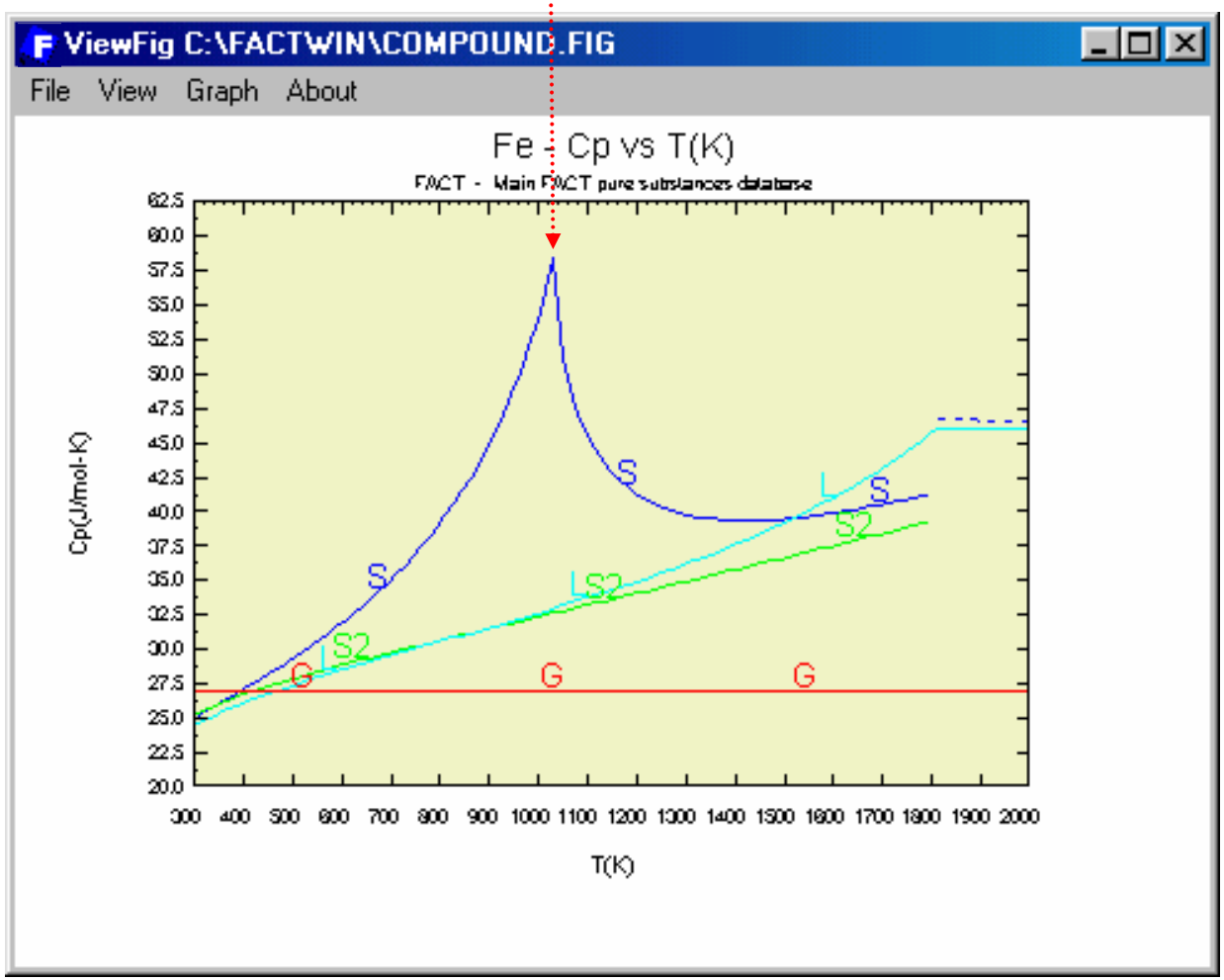
At this temperature G(S1) = G(S2) (two phases in equilibrium).

The enthalpy of fusion is 13806.9 J at 1810.95 K.

The enthalpy of vaporization to form monatomic Fe(g) at 1 atm is (482861.0 - 133229.8) = 349631.2 J at 3131.93 K.

Plotted C_p data for **Fe**

Curie temperature = **1043 K**



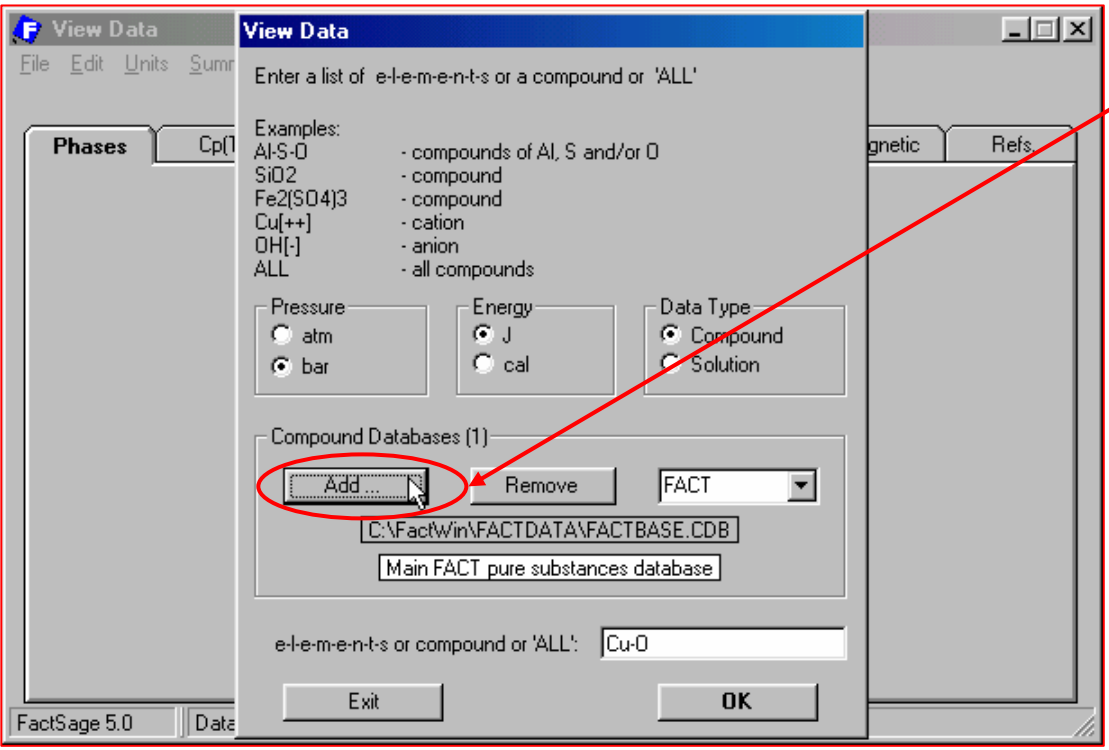
The View Data module links Databases with the FactSage program, I

The following slides show how the View Data module is used in order to link additional Compound databases with the FactSage program.

Once several databases are linked with FactSage it is possible to use them in combined searches for compounds. The result of such a combined search is shown.

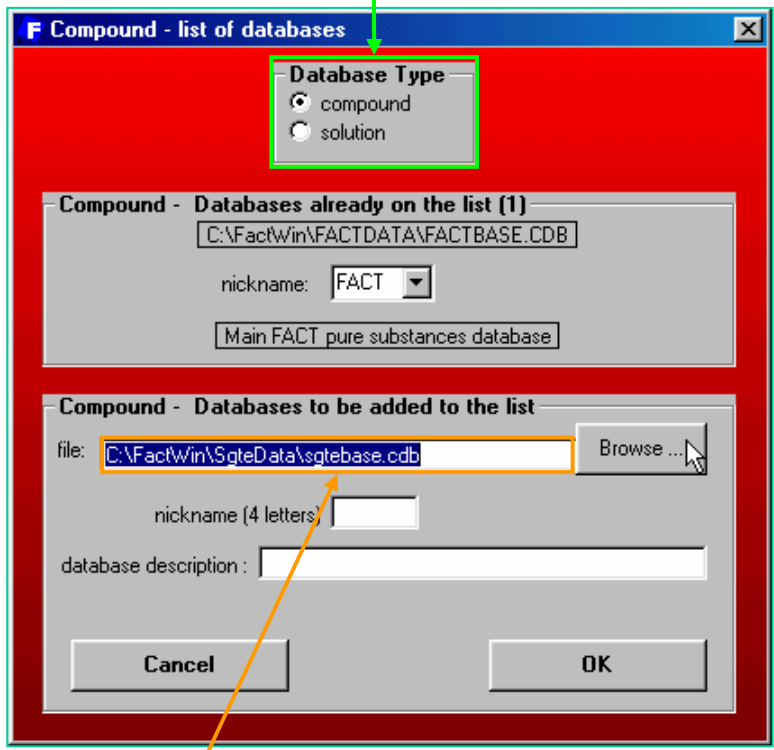
NOTE: The additionally linked databases are also available for use in other modules. Thus View Data can be considered a general entry point for databases.

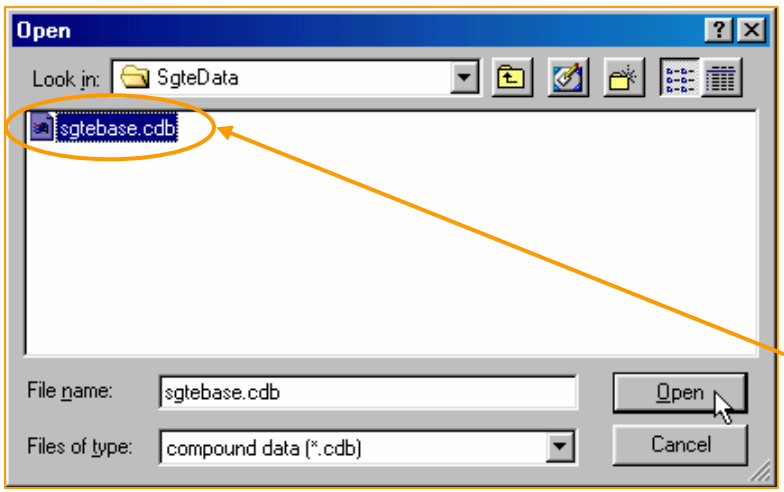
Adding a compound database to the list



1. Press the « Add… » button in the Compound Databases (1) frame.

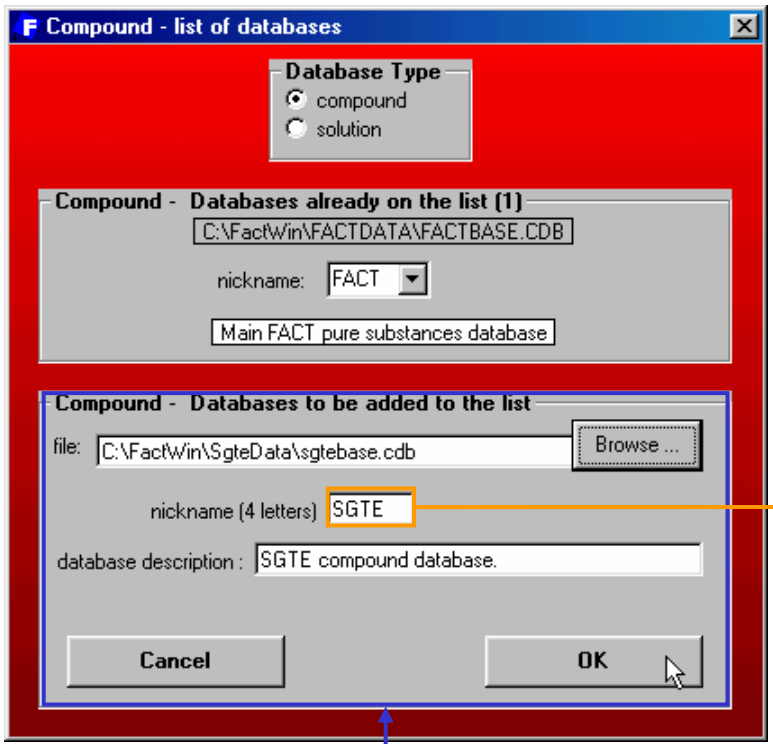
2. Select «compound»

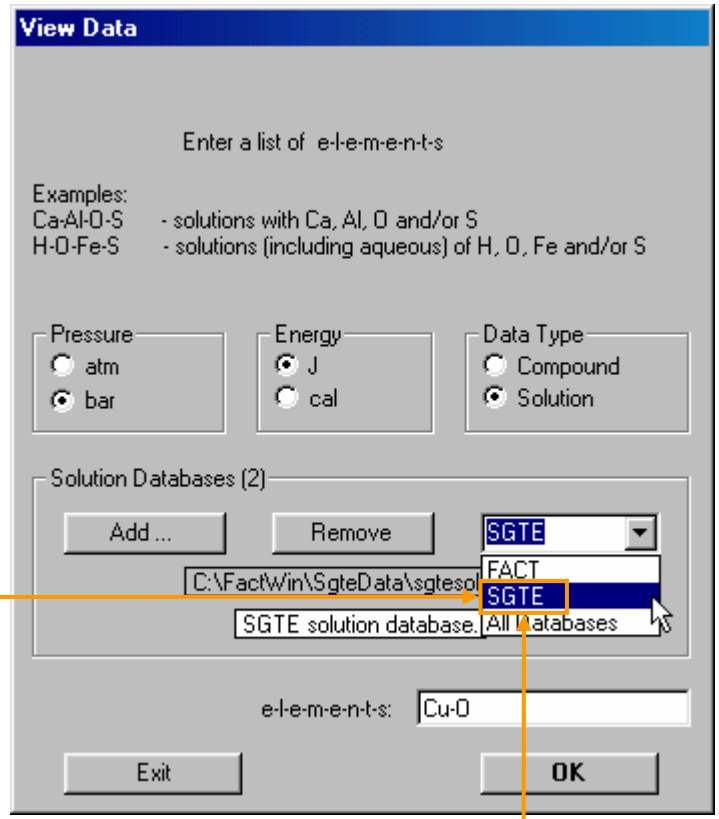




3. This opens the dialog box “Compound - list of databases”. Type in the full name or browse to locate.

Adding a compound database to the list (continued)

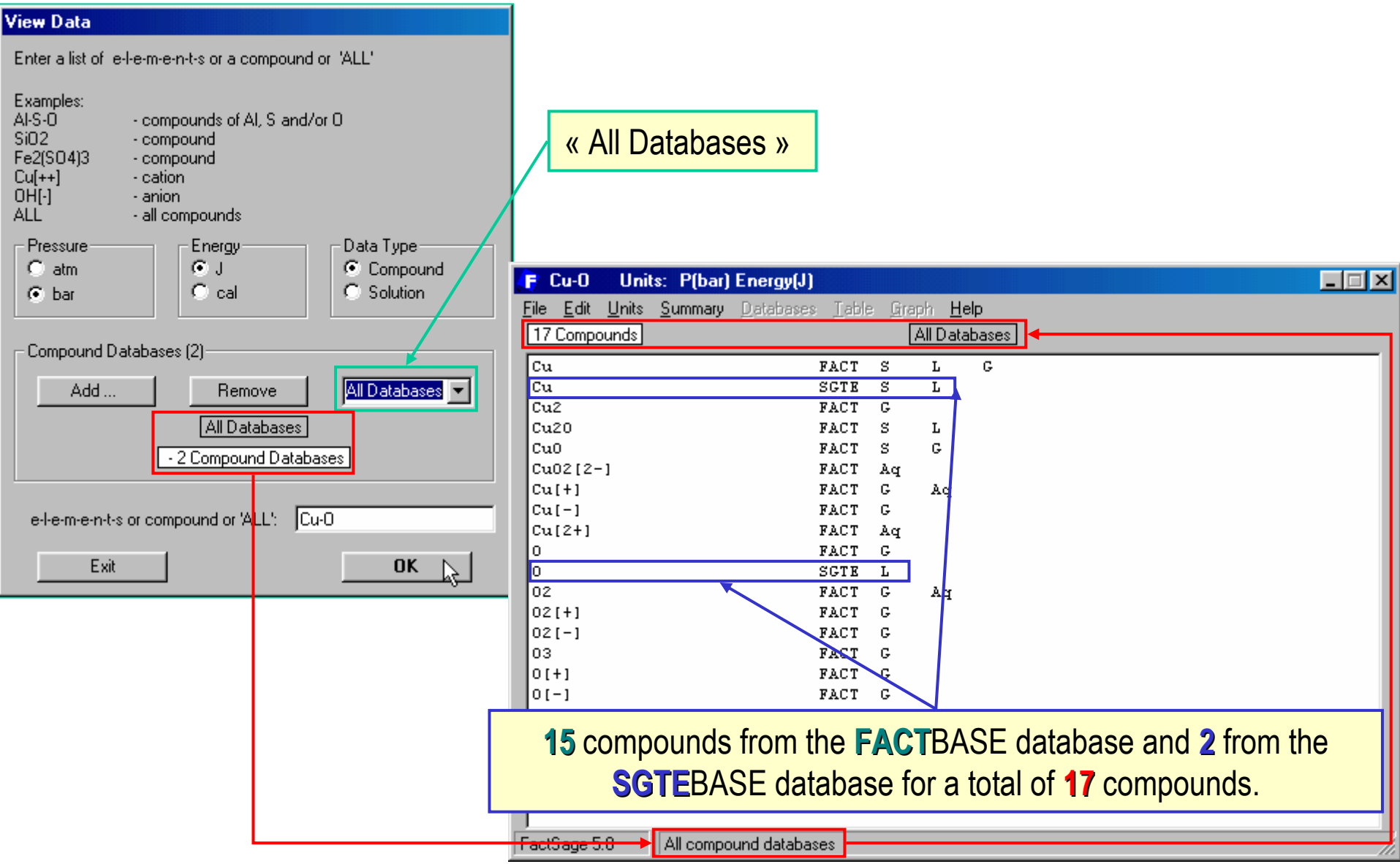




4. Enter a nickname (4 characters).
   Enter a description (one line).
   Click on «OK».

5. The SGTE database is now included in the list of compound databases.

Data in 2 or more compound databases

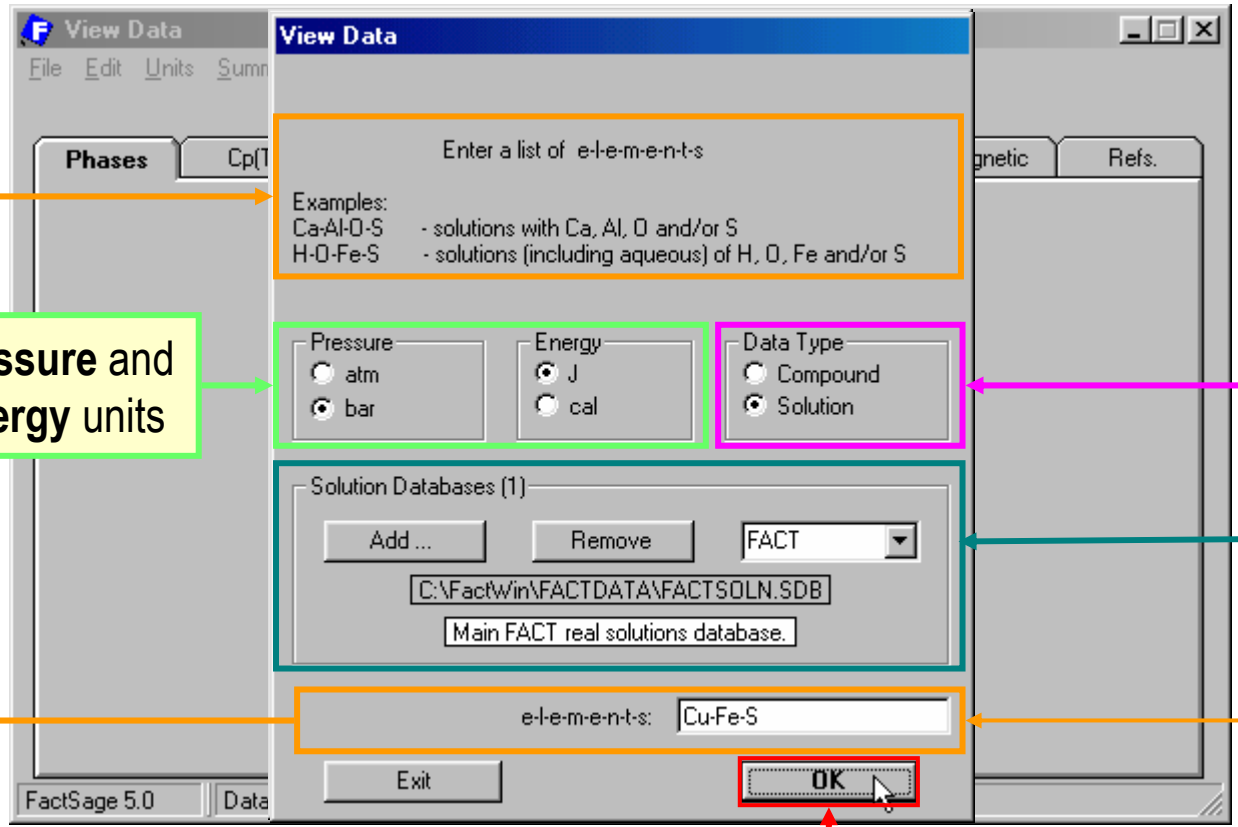


Using View Data with Solution databases

In addition to the use of View Data for the inspection of Compound databases it is also possible to apply this module for the search in Solution databases.

The following slides will give an overview of this application.

View Data of a Solution Database



Pressure and **Energy** units

Solution Database

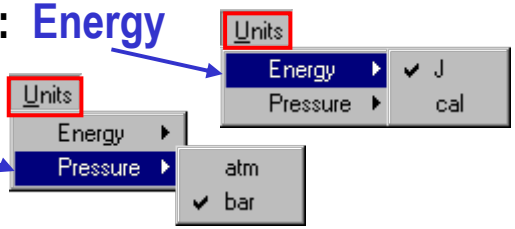
Possibility to add other databases in the data search – see slide 23.

For example, the elements **Cu**, **Fe** and **S**

Click on «OK» to scan the **Main *FACT* real solutions database** for all solutions containing **Cu**, **Fe** and **S**.

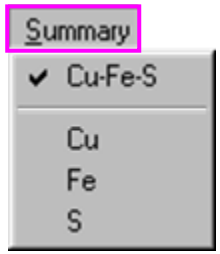
The solution datasets window

Units Menu: Energy



Pressure

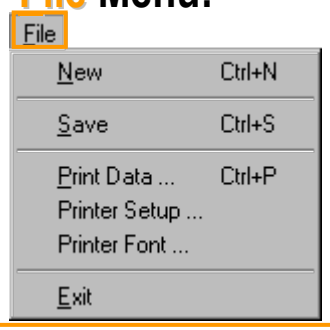
Summary Menu:

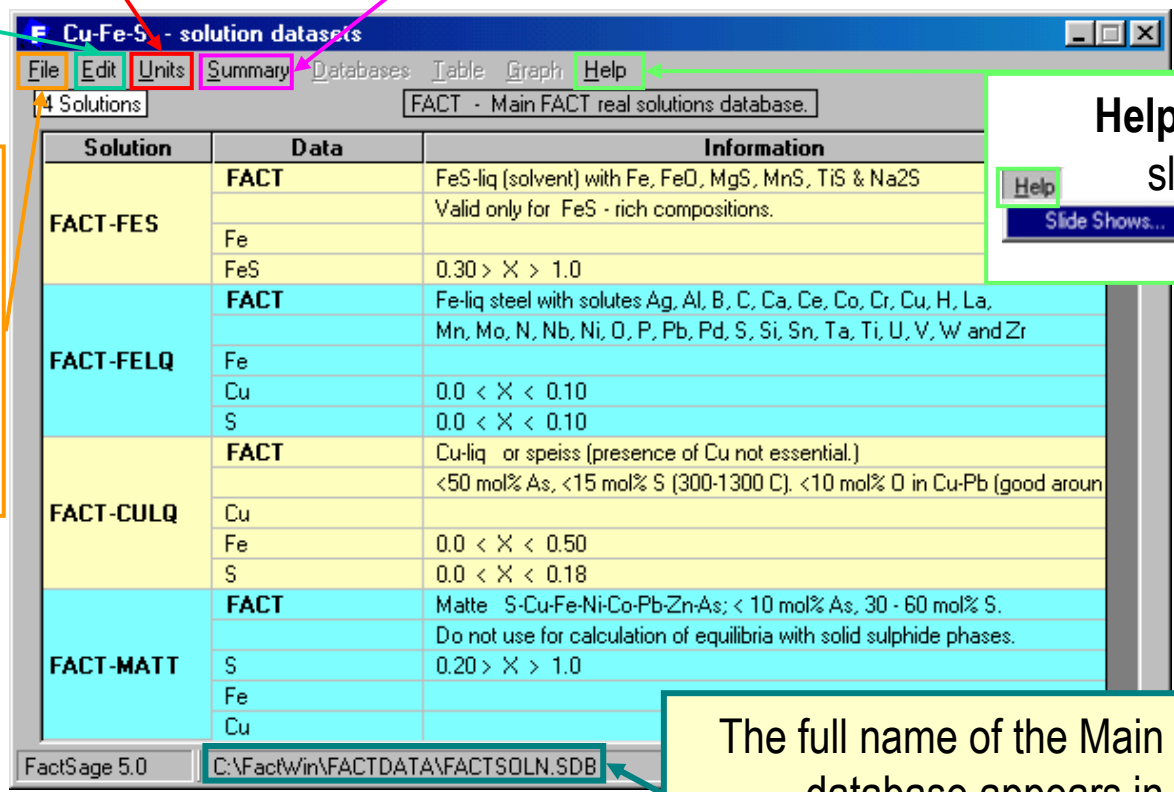


- **All solutions containing Cu, Fe or O**
- **All solutions containing Cu**
- **All solutions containing Fe**
- **All solutions containing O**

Edit Menu:

File Menu:





Help is provided through a slide show presentation

The full name of the Main ***FACT*** real solutions database appears in the Status Bar: [**C:\FactWin\FACTDATA\FACTSOLN.SDB**].

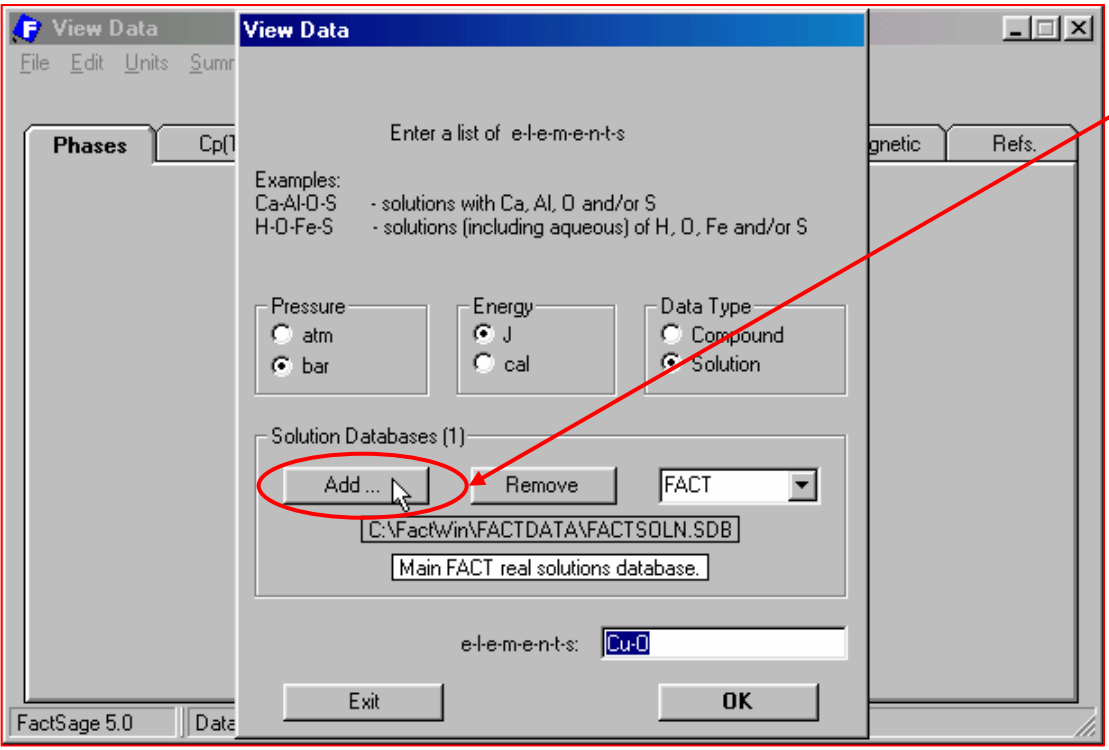
The View Data module links Databases with the FactSage program, II

The following slides show how the View Data module is used in order to link additional Solution databases with the FactSage program.

Once several databases are linked with FactSage it is possible to use them in combined searches for compounds. The result of such a combined search is shown.

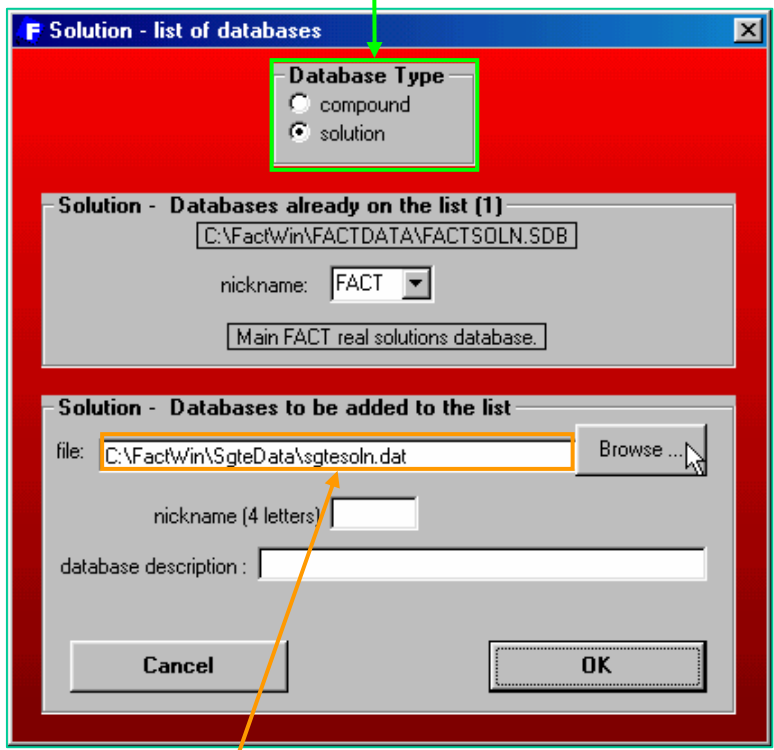
NOTE: The additionally linked databases are also available for use in other modules. Thus View Data can be considered a general entry point for databases.

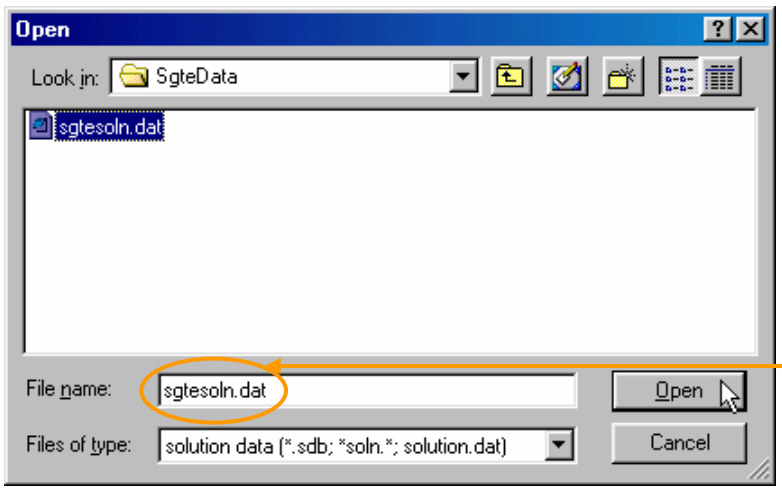
Adding a solution database to the list



1. Press « Add… » button in the Solution Databases (1) frame.

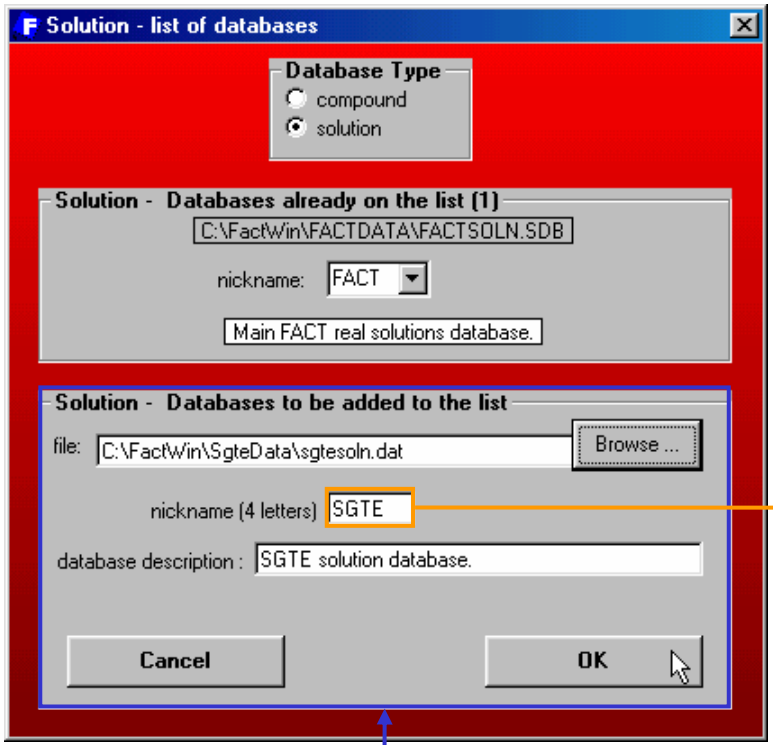
2. Select «solution»

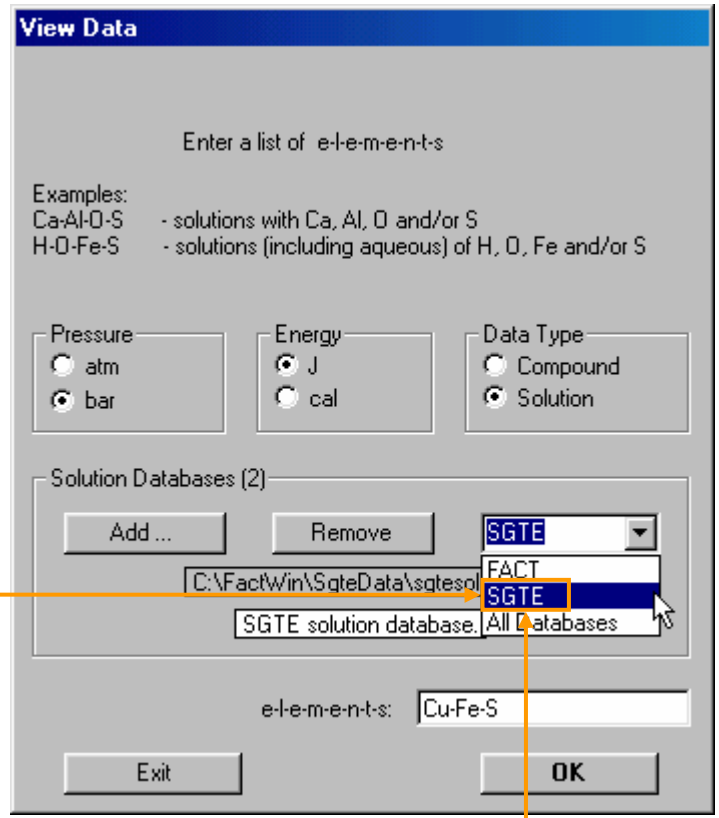




3. This opens the dialog box “Solution - list of databases”. Type in the full name or browse to locate.

Adding a solution database to the list (continued)



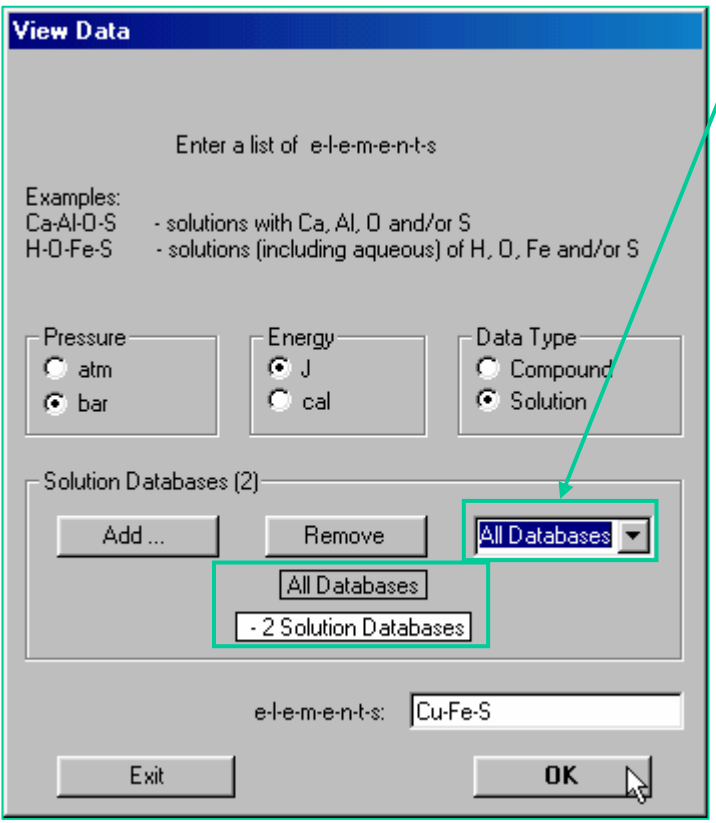


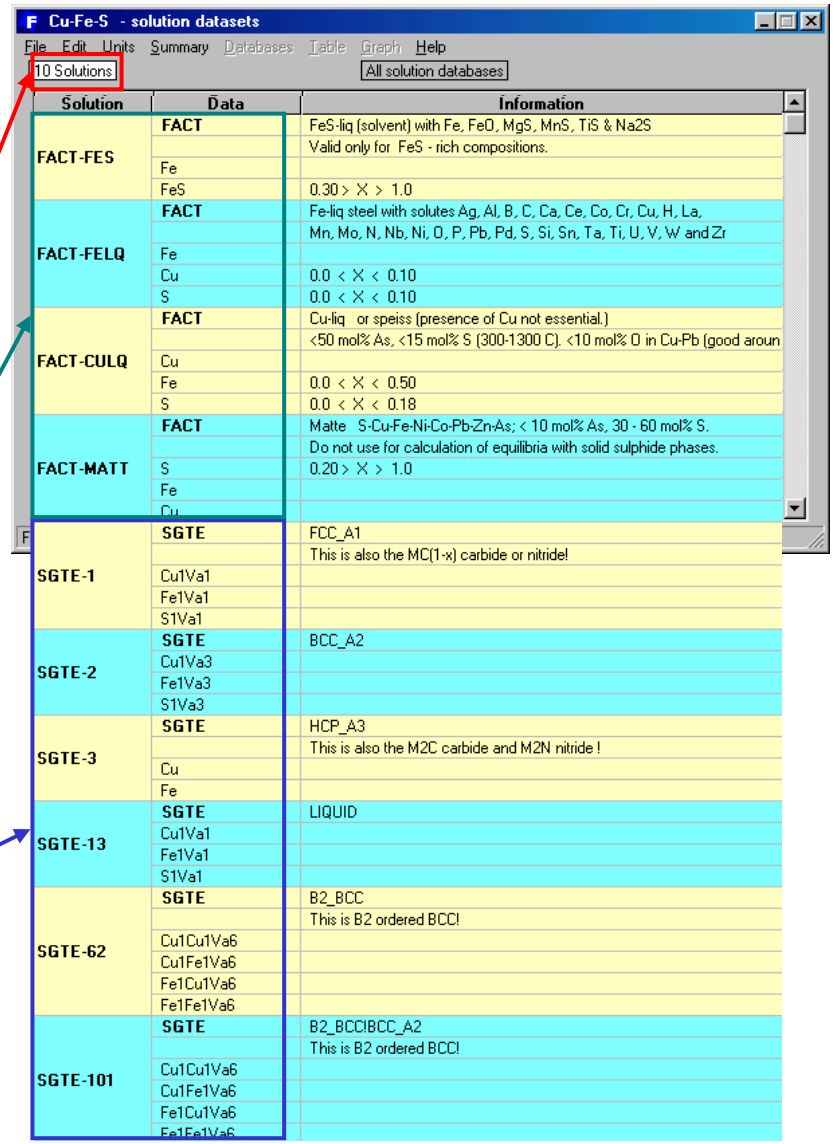
4. Enter a nickname (4 characters).
   Enter a description (one line).
   Click on «OK».

5. The SGTE database is now included in the database list.

Data in 2 or more solution databases

« All Databases »





A total of **10** Solutions:
4 solutions from the **FACT** database
and **6** from the **SGTE** database.