Use ***View Data*** to examine stored compound data (C_p(T),H, G, S, etc.) in ***Compound*** databases and list solution phases in ***Solution*** databases.

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Volume data - expansivities, compressivities and derivative of bulk modulus, Data for SiO_2

NOTE: Use the HOME/Pos1 button to return to the table of contents.

(continued)

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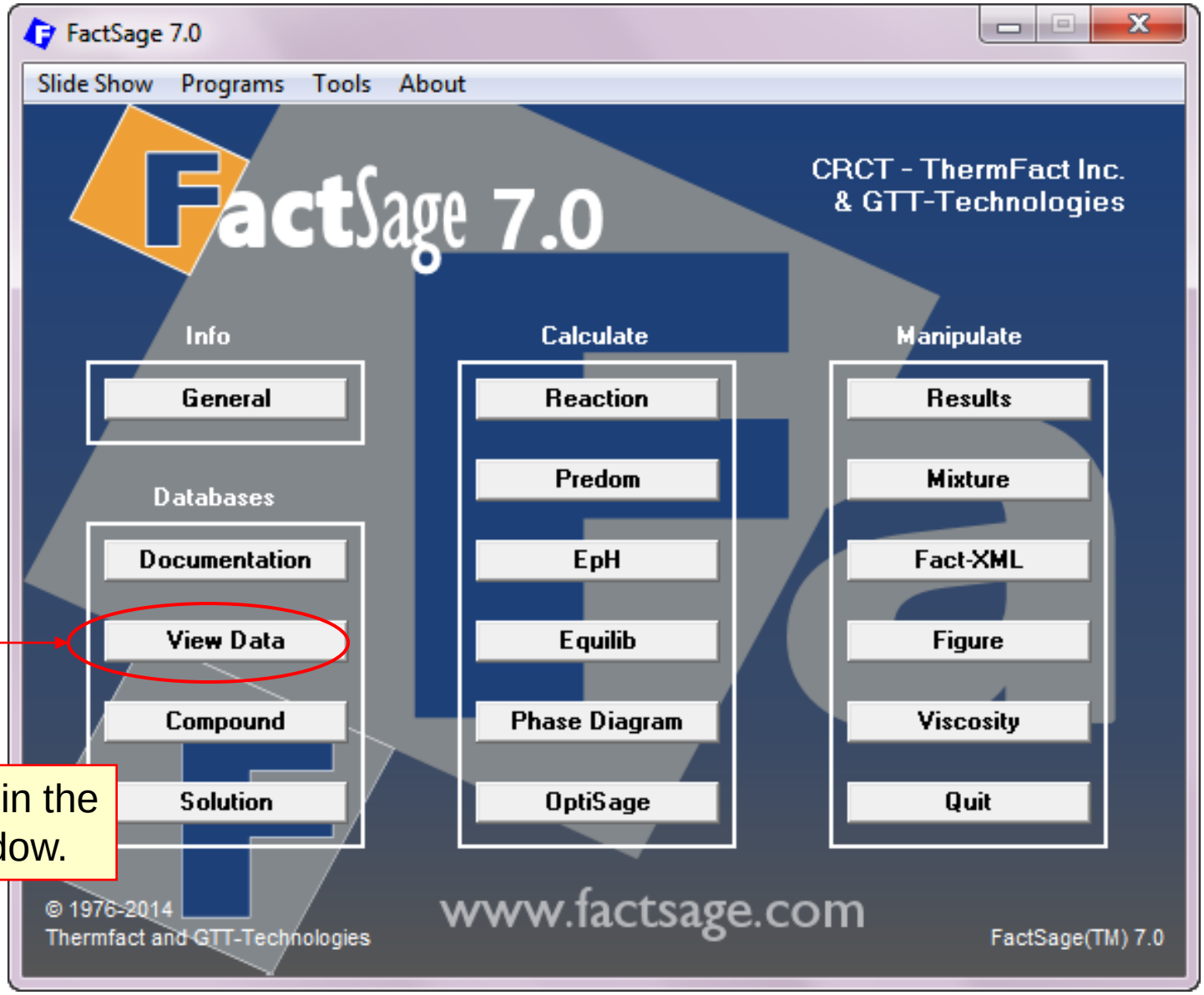
NOTE: Use the HOME/Pos1 button to return to the table of contents.

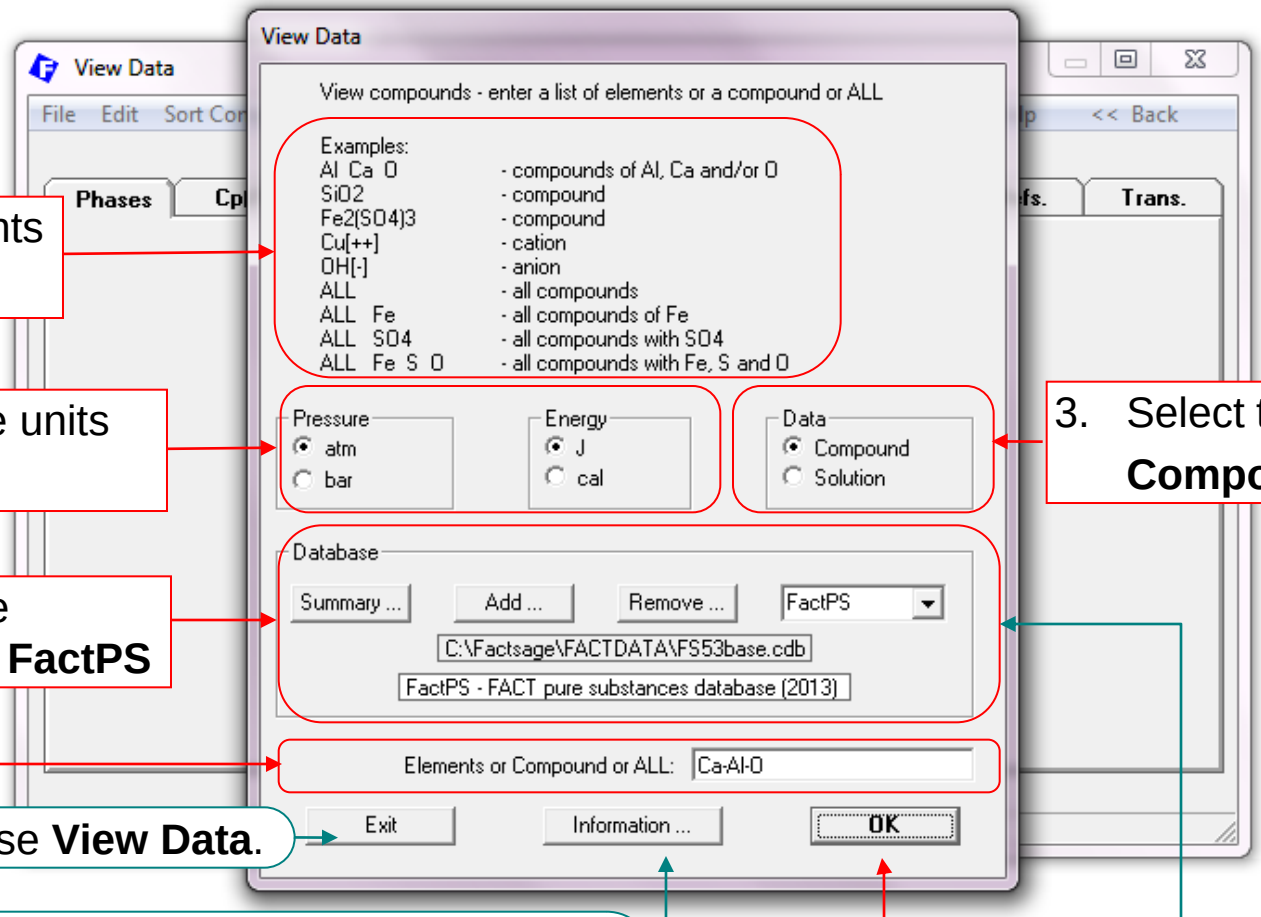
The *View Data* module



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

View Data of a Compound Database

In this example we scan **FactPS –** the FACT pure substances compound database **–** for all species with **Ca**, **Al** and/or **O**.



1. Enter the elements **Ca Al O**

2. Select the units **atm J**

3. Select the data **Compound**

4. Select the database **FactPS**

5. Click on «OK» to scan the database.

Click on «Exit» to close **View Data**.

Click on «Information …» to open **FactSage Browser** (when available).

For database management see section 10.

List of Compounds

List of compounds with **Ca**, **Al** and/or **O** stored in **FactPS –** the FACT pure substances database

Elements specified

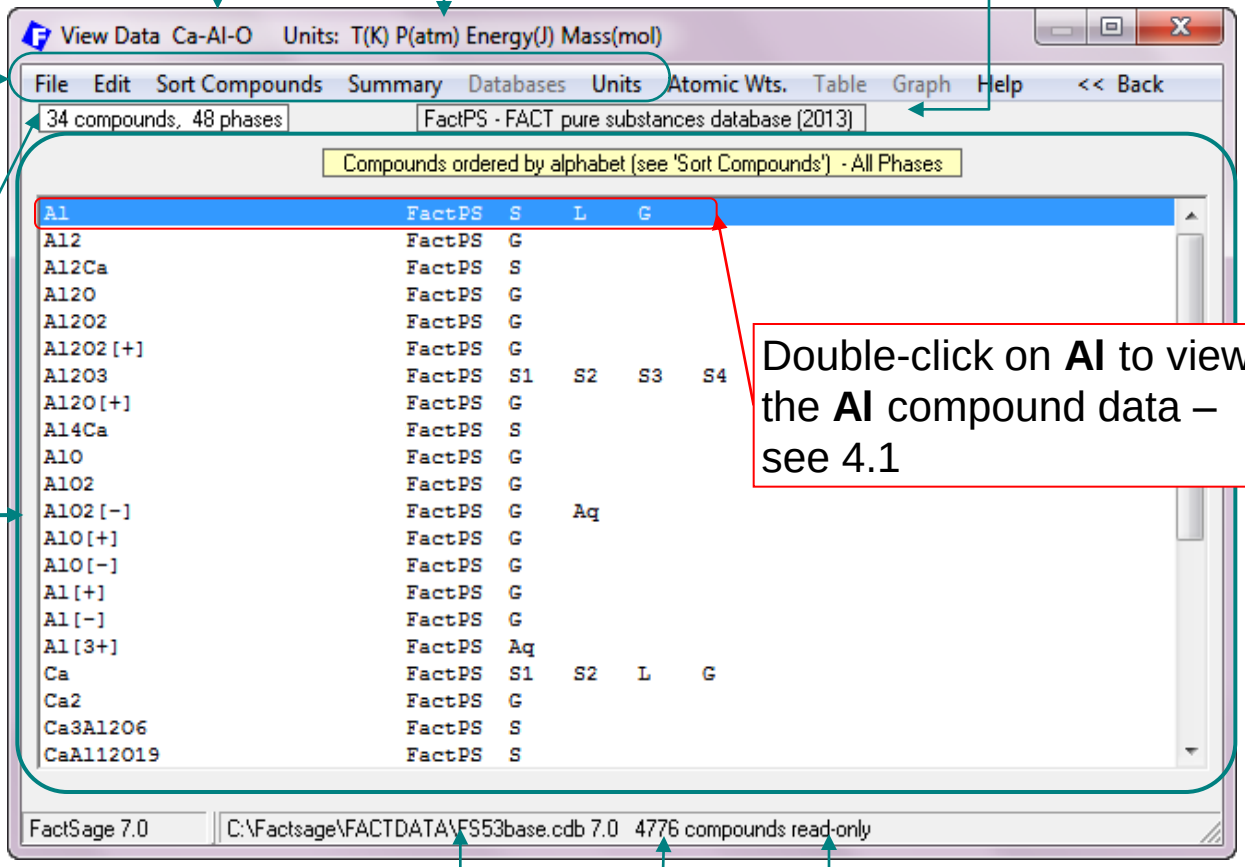
Units selected

Name of the database

Menu Bar - for more details see the next slide

Number of compounds and phases in the database

List of Ca-Al-O compounds and their phases: G, S1, S2 .., L, Aq



Double-click on **Al** to view the **Al** compound data – see 4.1

Location of the database

Total number of compounds in the database

Status of the database

Menu Bar – List of Compounds

Menus available with the List of Compounds window:

File

New	Ctrl+N
Save As …	Ctrl+S
Print …	Ctrl+P
Print Setup …	
Print Font …	
Exit	

Initiate a new search in View Data.

Open the «Save As …» dialog box (you can save your data in a text file [*.txt]).

Open the «Print…», «Print Setup…» or «Print Font…» dialog boxes (Windows features).

Exit the View Data program.

Edit

Find	Ctrl+F
Find Next	F3

Open the «Find…» dialog box.

Units

- Energy ▸ ✔ J, cal
- Pressure ▸ ✔ atm, bar
- Mass ▸ ✔ mol, gram, lb

Click to select your units.

Summary

- ✔ Ca-Al-O
- Ca
- Al
- O

Click to list all species containing :

- Ca, Al and/or O;
- Ca;
- Al;
- O.

Help

- Explanation of absolute H, G and S …
- Slide Show … ▸ View Data …
- About View Data …

Open this slide show.

The Chemical Species Window: Phases Tab

This window appears after you select a particular compound in the **List of compounds frame** or after entering a particular compound in the **View Data New Search window**.

Chemical species specified

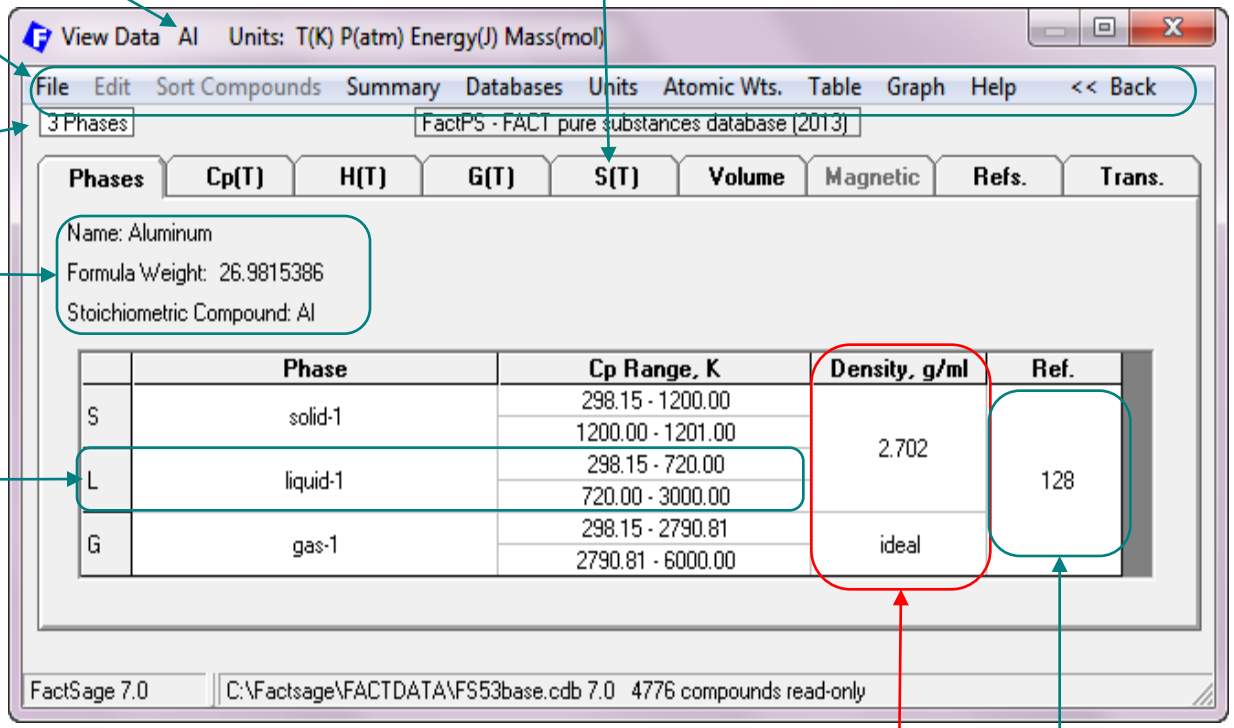
Menu Bar - see more details in the next slides

Number of phases in the database for the specified chemical species

Species name, formula weight and composition

There are 2 temperature ranges for Al (liquid-1) – each has its own C_P expression.

Click on the Cp(T), H(T), etc. tabs for additional data



References

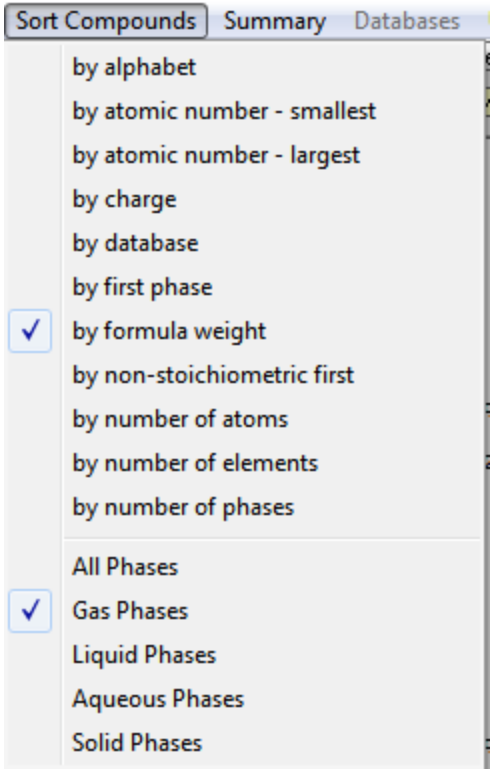
Density

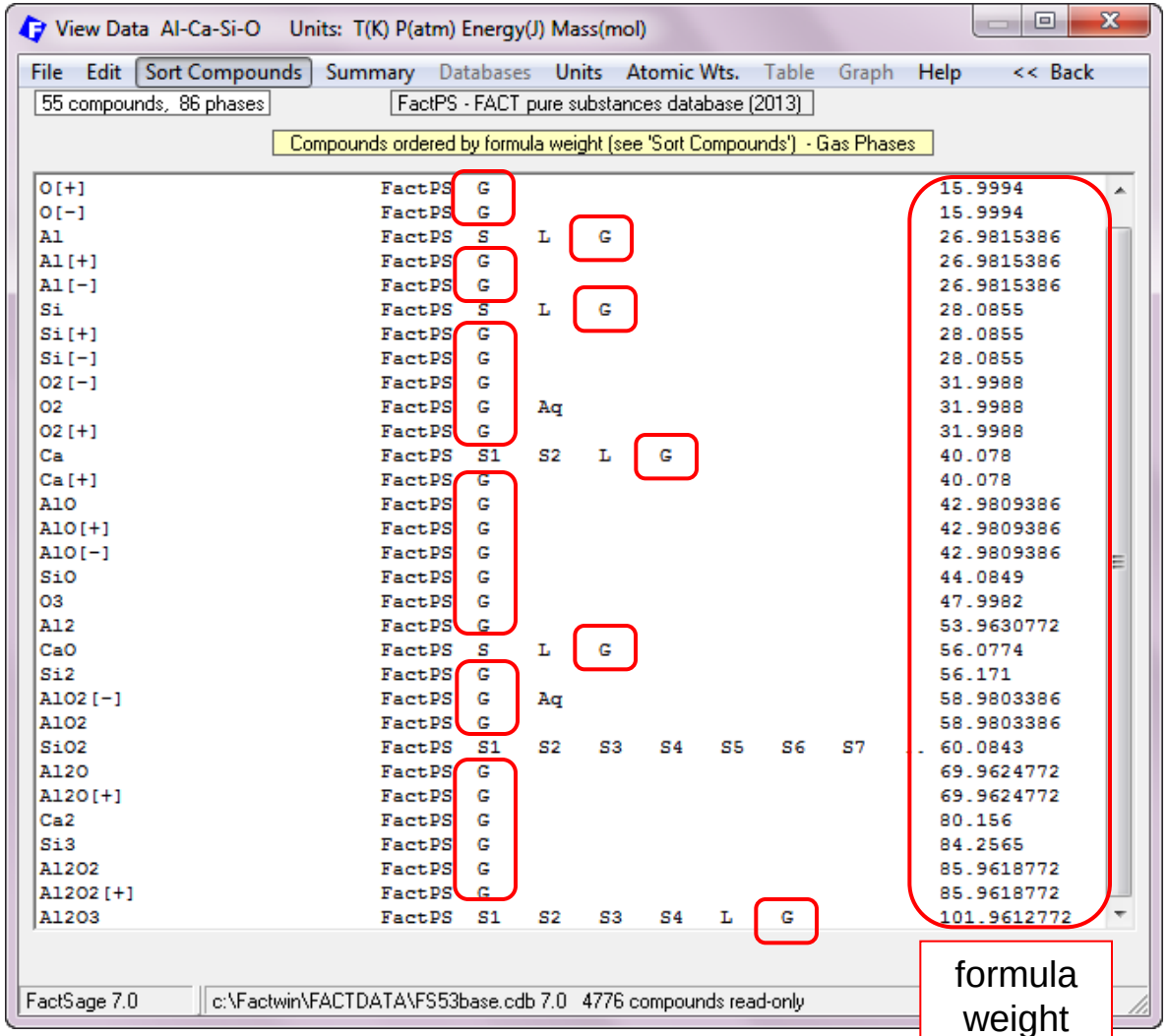
Data retrieved from the database include :

- **Phases**;
- **Cp(T)** polynomial expressions and the derived values of **H(T)**, **G(T)** and **S(T)**;
- Bibliographic **references** and the standard state **transitions** at 1 atm or bar.

Menu Bar: Sort Compounds

Use the **Sort Compounds** drop-down menu to sort the compounds by alphabet, atomic number, etc. and limit the list to gases, liquids, solids or aqueous species.





formula weight

Here the display of **FactPS** Ca-Al-O compounds is ordered by **formula weight** and limited to compounds that have a **gas** phase, G.

Menu Bar: Menus available with the Chemical Species window

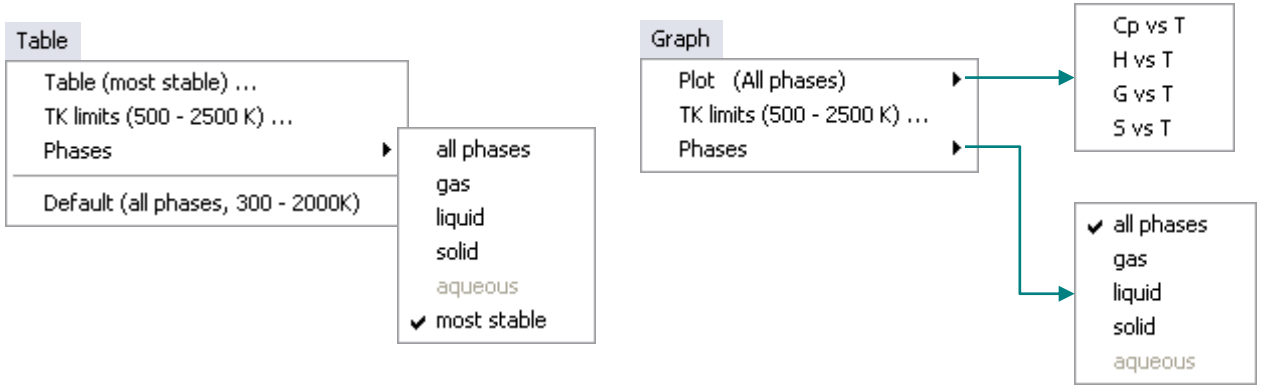
In the **Menu Bar** you can access the **Databases**, **Table** and **Graph** menus.

Databases menu lists all the available databases.

Data for the current chemical species (Al) is retrieved from the selected database (FactPS) but data on this chemical species (Al) is also found in other databases.

To view the data in another database, click on the database name.

The **Table** and **Graph** menus enable you to calculate thermodynamic properties and display the values in a tabular or graphical output.
See section 8 for an example.



References and Transitions Tabs

Refs. Tab:
Complete references

Trans. Tab:
Standard state transitions at 1 atm (or bar, in accordance with your choice of pressure units).

Phases | Cp(T) | H(T) | G(T) | S(T) | Volume | Magnetic | Refs. | Trans.

Name: Aluminum

References

Ref. 128
"JANAF Thermochemical Tables",
D.R. Stull and H. Prophet,
U.S. Department of Commerce, Washington, 1985.
Cp Fitted by CRCT, Montreal.

Phases | Cp(T) | H(T) | G(T) | S(T) | Volume | Magnetic | Refs. | Trans.

Name: Aluminum

Standard state transitions at 1 atm

Transition	T(K)	T(C)	Delta H	Delta S	Delta Cp
			J/mol	J/mol-K	J/mol-K
S --> L	933.45	660.30	10711.0	11.475	-1.206
L --> G (1 atm)	2793.71	2520.56	293969.2	105.225	-10.958

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 increasing temperature, each new phase will have at least one new C_p-polynomial expression.

Heat capacity expressions – $C_p(T)$

$C_p(T)$ expressions are stored as polynomials in the C_p range [T_{min}, T_{max}]

:

Outside the C_p range:

- When $T < T_{min}$, $C_p(T)$ is extrapolated;
- When $T > T_{max}$, $C_p(T)$ at T_{max} is used.

$$C_p = \sum_{i=1}^{8} C_{(i)} T^{P(i)}$$

The heat capacity expression of solid aluminum between 298K and 1200K is:

$\mathbf{C_p(T)}$ = (45.924818 + 1.56972870 × 10^{-5} $\mathbf{T}^2$ – 2850.4189 $\mathbf{T}^{-1}$ – 0.77191758 $\mathbf{T}^{0.5}$ - 5945470.3 $\mathbf{T}^{-3}$) [J/mol·K]

Phases | Cp(T) | H(T) | G(T) | S(T) | Volume | Magnetic | Refs. | Trans.

Name: Aluminum

$$C_P = \sum_{i=1}^{8} C_{(i)} T^{P(i)}$$

Cp range: T(min) - T(max).
When T < T(min), Cp(T) is extrapolated.
When T > T(max), Cp(T) at T(max) is used.

	DH(298.15) (J/mol)	S(298.15) (J/mol-K)	C(i)	P(i)	C(i)	P(i)	Cp (K)
S	0.00	28.275000	45.924818	0	1.56972870E-05	2	
			-2850.4189	-1	-0.77191758	0.5	298 - 1200
			-5945470.3	-3			
S			31.751000	0			1200 - 1201
L	10563.36	39.550829	-117.83044	0	4.89839843E-02	1	
			1905633.6	-2	-52047.426	-1	298 - 720
			4844.5352	-0.5			
L			31.751000	0	-8.78407673E-12	-2	720 - 3000
G	329699.97	164.445504	20.791863	0	53510.965	-2	298 - 2791
			-0.30007285	-0.5	365227.17	-3	

Note that the 2nd C_p expression for the liquid is constant at temperatures above 1200 K.

Derived thermodynamic functions: H(T), S(T) and G(T)

The basic data for 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 importantly, the Gibbs energy, G(T).

Absolute S(T) is calculated from the 3rd law :

$$S(T) = \int_0^T \frac{C_p(T)}{T}\,dT \quad or \quad S(T) = S_{298} + \int_{298}^T \frac{C_p(T)}{T}\,dT$$

Absolute H(T) is given by :

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

Absolute G(T) is given in the Gibbs-Helmholtz equation:

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

Enthalpy **H(T)**, Entropy **S(T)** and Gibbs Energy **G(T)** Expressions

Phases | Cp(T) | H(T) | G(T) | S(T) | Volume | Magnetic | Refs. | Trans.

Name: Aluminum

H(T) J/mol

These values are absolute H (not Delta H) - click on 'Help' for an explanation.

	H(T)			T(K)
S	5025.23805	+ 45.9248180 T	+ 5.232429015E-06 T^3	298 - 1200
	- 2850.41894 ln(T)	- 0.514611719 T^1.5	+ 2972735.17 T^-2	
S	- 10524.1753	+ 31.7510000 T		1200 - 1201
L	179152.718	- 117.830437 T	+ 2.449199213E-02 T^2	298 - 720
	- 1905633.58 T^-1	- 52047.4259 ln(T)	+ 9689.07046 T^0.5	
L	- 944.029090	+ 31.7510000 T	+ 8.784076731E-12 T^-1	720 - 3000
G	323692.765	+ 20.7918626 T	- 53510.9653 T^-1	298 - 2791
	- 0.600145710 T^0.5	- 182613.586 T^-2		
G	11247118.8	- 893.860737 T	- 664787396. T^-1	2791 - 6000
	- 2009411.03 ln(T)	+ 2.84015836 T^1.5	+ 139915.245 T^0.5	

Phases | Cp(T) | H(T) | G(T) | S(T) | Volume | Magnetic | Refs. | Trans.

Name: Aluminum

S(T) J/mol-K - 1 atm

These values are absolute S (not Delta S) - click on 'Help' for an explanation.

	S(T)			T(K)
S	- 217.061479	+ 45.9248180 ln(T)	+ 7.848643522E-06 T^2	298 - 1200
	+ 2850.41894 T^-1	- 1.54383516 T^0.5	+ 1981823.45 T^-3	
S	- 156.369496	+ 31.7510000 ln(T)		1200 - 1201
L	1093.57886	- 117.830437 ln(T)	+ 4.898398426E-02 T	298 - 720
	- 952816.788 T^-2	+ 52047.4259 T^-1	- 9689.07046 T^-0.5	
L	- 145.926762	+ 31.7510000 ln(T)	+ 4.392038366E-12 T^-2	720 - 3000
G	46.2526763	+ 20.7918626 ln(T)	- 26755.4827 T^-2	298 - 2791
	+ 0.600145710 T^-0.5	- 121742.391 T^-3		
G	8824.23979	- 893.860737 ln(T)	- 332393698. T^-2	2791 - 6000
	+ 2009411.03 T^-1	+ 8.52047508 T^0.5	- 139915.245 T^-0.5	

The enthalpy expression of solid aluminum between 298K and 1200K is:

$$\mathbf{H(T)} = (5025.23805 + 45.9248180\ T + 5.232429015 \times 10^{-6}\ \mathbf{T}^{3} - 2850.41894\ \ln(\mathbf{T}) - 0.514611719\ \mathbf{T}^{1.5} + 2972735.17\ \mathbf{T}^{-2})\ [\text{J/mol}]$$

Phases | Cp(T) | H(T) | G(T) | S(T) | Volume | Magnetic | Refs. | Trans.

Name: Aluminum

G(T) J/mol - 1 atm

These values are absolute G (not Delta G) - click on 'Help' for an explanation.

	G(T)			T(K)
S	2174.81911	+ 262.986297 T	- 2.616214507E-06 T^3	298 - 1200
	- 2850.41894 ln(T)	+ 1.02922344 T^1.5	+ 990911.725 T^-2	
	- 45.9248180 T ln(T)			
S	- 10524.1753	+ 188.120496 T	- 31.7510000 T ln(T)	1200 - 1201
L	127105.292	- 1211.40930 T	- 2.449199213E-02 T^2	298 - 720
	- 952816.788 T^-1	- 52047.4259 ln(T)	+ 19378.1409 T^0.5	
	+ 117.830437 T ln(T)			
L	- 944.029090	+ 177.677762 T	+ 4.392038366E-12 T^-1	720 - 3000
	- 31.7510000 T ln(T)			
G	323692.765	- 25.4608137 T	- 26755.4827 T^-1	298 - 2791
	- 1.20029142 T^0.5	- 60871.1953 T^-2	- 20.7918626 T ln(T)	

H(T), G(T) and S(T) are **absolute values** - not the delta values.

For tabular values of Delta H, Delta G and Delta S, use the Reaction module.

Additional basic data of a compound

With the compound database it is also possible to store :

- data for the magnetic Gibbs energy of a solid compound;
- basic data to enable the calculation of virial coefficients of gaseous compounds;
- 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

View Data Fe Units: T(K) P(atm) Energy(J) Mass(mol)

File Edit Sort Compounds Summary Databases Units Atomic Wts. Table Graph Help << Back

4 Phases FactPS - FACT pure substances database (2013)

Phases | Cp(T) | H(T) | G(T) | S(T) | Volume | Magnetic | Refs. | Trans.

Name: Iron

Formula Weight: 55.845

Stoichiometric Compound: Fe

	Phase	Cp Range, K	Density, g/ml	Ref.
S1	bcc	298.15 - 1811.00	7.86	143
		1811.00 - 1812.00		
S2	fcc	298.15 - 1811.00		
		1811.00 - 1812.00		
L	liquid	298.15 - 1811.00		
		1811.00 - 6000.00		
G	gas	298.15 - 6000.00	ideal	1

Phases | Cp(T) | H(T) | G(T) | S(T) | Volume | Magnetic | Refs. | Trans.

Name: Iron

Standard state transitions at 1 atm

Transition	T(K)	T(C)	Delta H	Delta S	Delta Cp
			J/mol	J/mol-K	J/mol-K
S1 --> S2	1184.81	911.66	1012.9	0.855	-7.681
S2 --> S1	1667.47	1394.32	825.8	0.495	2.183
S1 --> L	1810.95	1537.80	13806.9	7.624	4.653
L --> G (1 atm)	3135.00	2861.85	349573.0	111.507	-18.938

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

Phases | Cp(T) | H(T) | G(T) | S(T) | Volume | Magnetic | Refs. | Trans.

Name: Iron

$$C_P = \sum_{i=1}^{8} C_{(i)} T^{P(i)}$$

Cp range: T(min) - T(max).
When T < T(min), Cp(T) is extrapolated.
When T > T(max), Cp(T) at T(max) is used.

	DH(298.15)	S(298.15)	C(i)	P(i)	C(i)	P(i)	Cp
	(J/mol)	(J/mol-K)					(K)
S1	9149.45	36.863493	23.514300	0	8.79504000E-03	1	298 - 1811
			-154717.00	-2	3.53561400E-07	2	
	+ H(magnetic)	+ S(magnetic)	+ Cp(magnetic)				
S1			46.000000	0			1811 - 1812
			+ Cp(magnetic)				
S2	7973.03	35.902097	24.664300	0	7.51504000E-03	1	298 - 1811
			-154717.00	-2	3.53561400E-07	2	
	+ H(magnetic)	+ S(magnetic)	+ Cp(magnetic)				
S2			46.000000	0			1811 - 1812
			+ Cp(magnetic)				

Phases | Cp(T) | H(T) | G(T) | S(T) | Volume | Magnetic | Refs. | Trans.

Name: Iron

Magnetic Properties

$$G_{mag} = RT\ln(\beta+1)g(\tau) \qquad \text{where } \tau = \frac{T}{T_c}$$

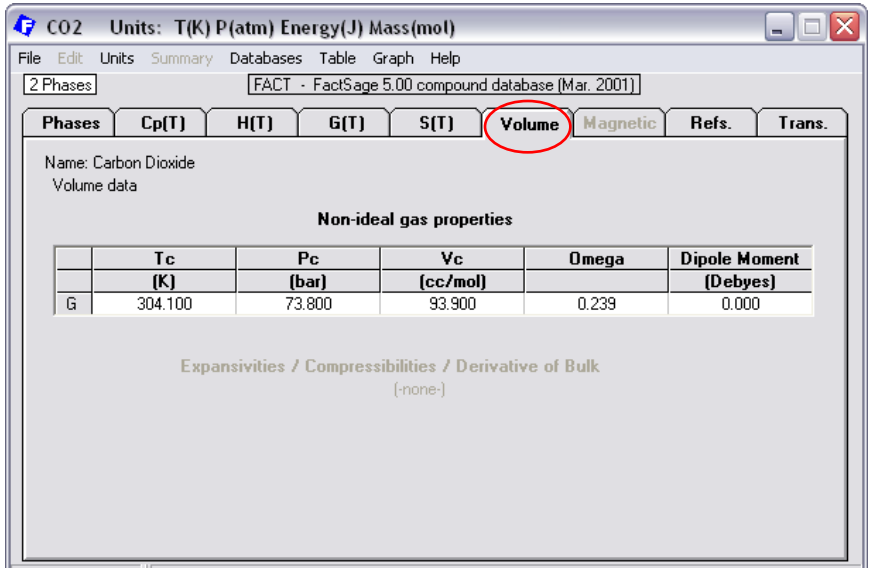
$$g(\tau) = \frac{1}{D}\left(1 - \left[\frac{79\tau^{-1}}{140p} + \frac{474}{497}\left(p^{-1}-1\right)\left(\frac{\tau^3}{6} + \frac{\tau^9}{135} + \frac{\tau^{15}}{600}\right)\right]\right) \qquad \text{when } \tau \le 1$$

$$g(\tau) = -\frac{1}{D}\left[\frac{\tau^{-5}}{10} + \frac{\tau^{-15}}{315} + \frac{\tau^{-25}}{1500}\right] \qquad \text{when } \tau > 1$$

$$\text{where } D = \frac{518}{1125} + \frac{11692}{15975}\left(p^{-1}-1\right)$$

	Critical Temp. Tc (K)	Magnetic Moment B	P Factor	Structure Factor
S1	1043.00 (Curie)	2.2200	0.40000	1.0000
S2	67.00 (Neel)	0.7000	0.28000	0.3333

Real gas coefficients for carbon dioxide 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.

Pressure dependence of SiO_2

9 phases including **8 solid phases** with **volume** data.

View Data SiO2 Units: T(K) P(bar) Energy(cal) Mass(mol)

File Edit Sort Compounds Summary Databases Units Atomic Wts. Table Graph Help << Back

10 Phases | FactPS - FACT pure substances database (2013)

Phases | Cp(T) | H(T) | G(T) | S(T) | Volume | Magnetic | Refs. | Trans.

Name: silicon dioxide

$$C_P = \sum_{i=1}^{8} C_{(i)} T^{P(i)}$$

Cp range: T(min) - T(max).
When T < T(min), Cp(T) is extrapolated.
When T > T(max), Cp(T) at T(max) is used.

	DH(298.15) (cal/mol)	S(298.15) (cal/mol-K)	C(i)	P(i)	C(i)	P(i)	Cp (K)
S1	-217662.51	9.909178	19.123325	0	-847677.82	-2	298 - 373
			-57.427342	-0.5	1.17487660E+08	-3	
S1			19.123325	0	2.01721360E-03	1	373 - 848
			-847677.82	-2	-1.08060950E-05	2	
			1.44719040E-08	3	-57.427342	-0.5	
			1.17487660E+08	-3			
S1			1.00000000E-02	0			848 - 850
S2	-217167.01	10.565679	19.123325	0	-847677.82	-2	298 - 1996
			-57.427342	-0.5	1.17487660E+08	-3	
S2			20.500000	0			1996 - 3000
S3	-216922.84	10.461329	18.014500	0	4.35174640E-02	1	298 - 390
			-1424018.9	-2	-2.94889390E-04	2	
			4.99568120E-07	3	2.29026320E+08	-3	
S3			1.00000000E-02	0			390 - 392
S4	-216788.99	10.880425	18.014500	0	-1424018.9	-2	298 - 1991
			2.29026320E+08	-3			
S4			20.500000	0			1991 - 3000
S5	-216958.26	10.371487	19.960229	0	4.83030500E-03	1	298 - 535
			-586845.12	-2	-2.99966990E-05	2	
			4.65706550E-08	3	-89.553776	-0.5	
			66938861.	-3			
S5			1.00000000E-02	0			535 - 537
S6	-216629.36	11.001147	19.960229	0	-586845.12	-2	298 - 1996
			-89.553776	-0.5	66938861.	-3	
S6			20.500000	0			1996 - 3000
S7	-216754.00	9.679732	18.642450	0	-740918.00	-2	298 - 3000
			1.40009600E+08	-3	-1598.7090	-1	
S8	-206501.00	7.050669	13.891010	0	1.67351800E-03	1	
			-3008840.0	-2	4.28489000E+08	-3	
			4065.4900	-1			
L 1	-214339.36	12.148447	19.960229	0	-586845.12	-2	298 - 1996
			-89.553776	-0.5	66938861.	-3	

View Data SiO2 Units: T(K) P(bar) Energy(cal) Mass(mol)

File Edit Sort Compounds Summary Databases Units Atomic Wts. Table Graph Help << Back

10 Phases | FactPS - FACT pure substances database (2013)

Phases | Cp(T) | H(T) | G(T) | S(T) | Volume | Magnetic | Refs. | Trans.

Name: silicon dioxide

Formula Weight: 60.0843

Stoichiometric Compound: SiO2

	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		
G	gas	298.15 - 1000.00	ideal	56
		1000.00 - 2400.00		
		2400.00 - 6000.00		

SiO_2 volume data - expansivities, compressibilities, bulk modulus

Phases | Cp(T) | H(T) | G(T) | S(T) | Volume | Magnetic | Refs. | Trans.

Name: silicon dioxide
Volume data

Non-ideal gas properties
[-none-]

Expansivities / Compressibilities / Derivative of Bulk

	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

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

Compressibility expression (compressibilities) :

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

	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

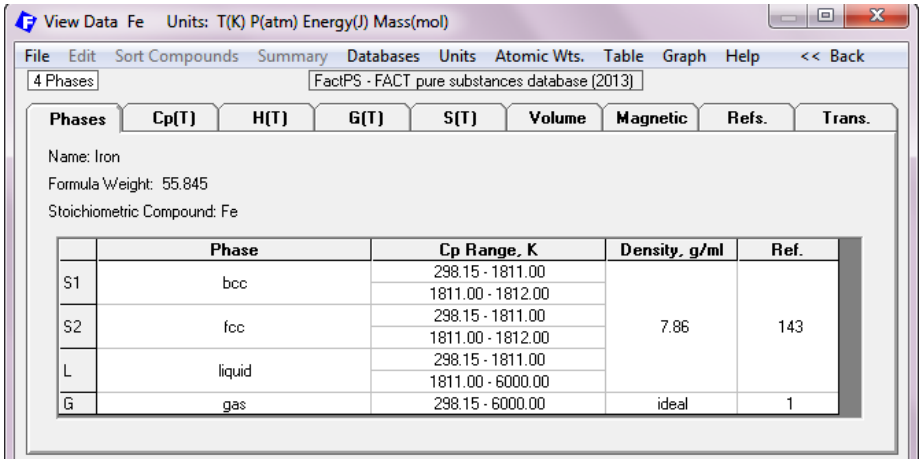
Derivative of the bulk modulus :

$$a + bT \ln T$$

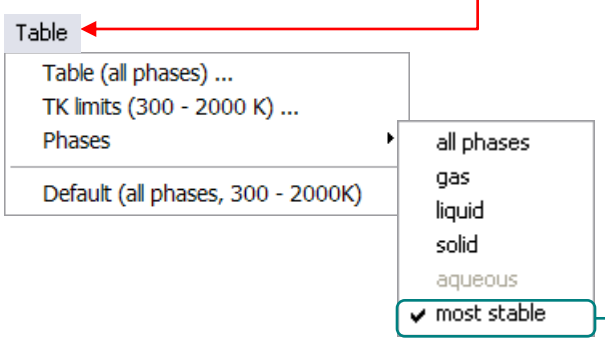
	Derivative of Bulk Modulus = a + bT ln(T)	
S1	6.40000E+00	+ 0.00000E+00 T ln(T)
S2	5.34600E+00	+ 0.00000E+00 T ln(T)
S3	6.00000E+00	+ 1.00000E-03 T ln(T)
S4	6.00000E+00	+ 1.00000E-03 T ln(T)
S5	6.00000E+00	+ 0.00000E+00 T ln(T)
S6	6.00000E+00	+ 0.00000E+00 T ln(T)
S7	8.40000E+00	+ 0.00000E+00 T ln(T)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

Generation of tabular output

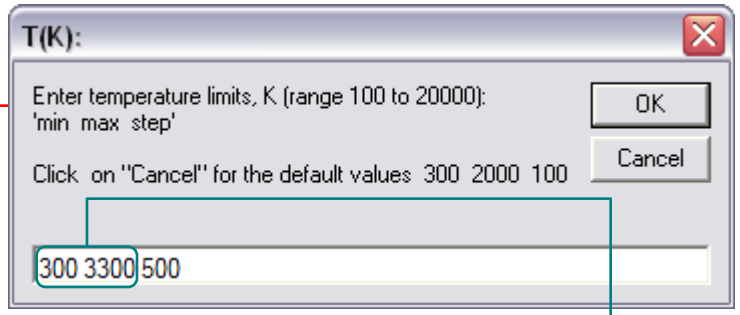
In this example we calculate the thermodynamic properties of **Fe**.



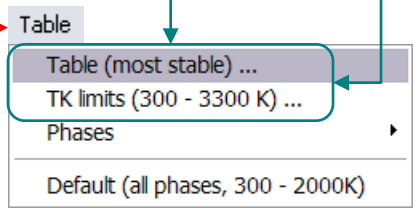
1. Click on the Table menu, and then select the type of phase(s).



2. Click again on the Table menu, select «TK limits (default values) …» and enter the limits of temperature.



3. Click again on the Table menu and select the command «Table (your selection of phases) …» to generate the table.



Tabular output for **Fe**

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

The allotropic transformation S1 → S2 (alpha → gamma) at 1184.81 K with an enthalpy of transformation of (34587.3 - 33574.4) = 1012.9 J

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

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

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 (482944.2 – 133371.2) = 349573.0 J at 3135.00 K.

Fe

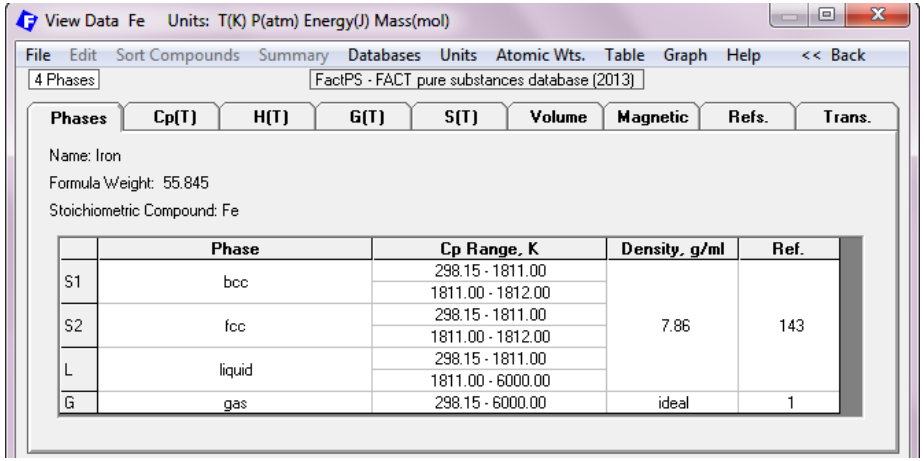
File Edit

Fe - most stable phases
FactPS - FACT pure substances database (2013).
Units: K, atm, J, mol
Standard state: pure solid, liquid and ideal gas at 1 atm
- STANDARD STATE PROPERTIES / MOLE -

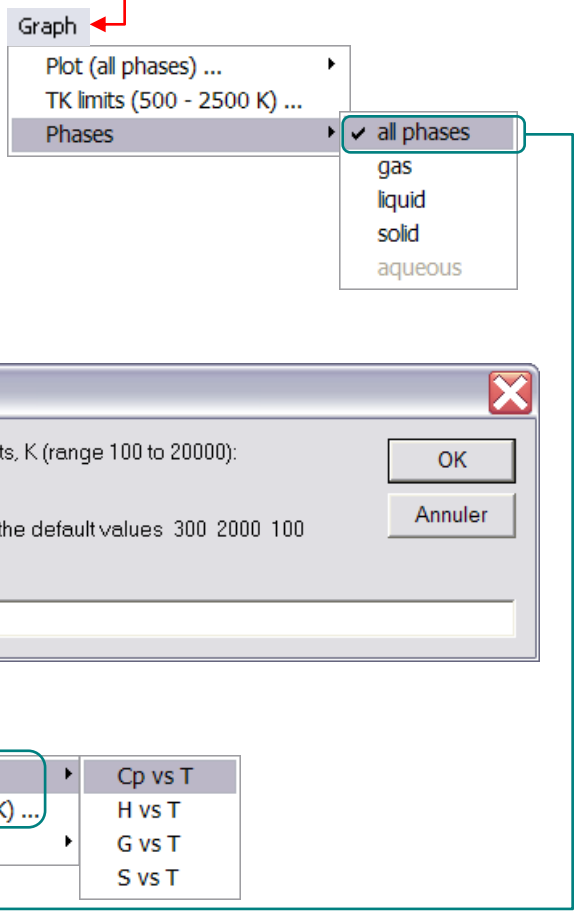
	T(K)	Cp(J/K)	H(J)	G(J)	S(J/K)
S1	298.15	24.845	0.0	-8133.5	27.280
	300.00	24.890	46.0	-8184.1	27.433
	800.00	39.204	15583.0	-29906.6	56.862
	1184.81	41.636	33574.4	-55474.2	75.158
S1->S2	1184.81	Delta(H) =	1012.9	Delta(S) =	0.855
S2	1184.81	33.954	34587.3	-55474.2	76.013
	1300.00	34.940	38555.0	-64415.8	79.208
	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
	1800.00	41.259	58205.7	-107209.5	91.897
	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
	2300.00	46.000	94961.2	-159806.5	110.769
	2800.00	46.000	117961.2	-217527.1	119.817
	3135.00	46.000	133371.2	-258553.0	125.016
L->G	3135.00	Delta(H) =	349573.0	Delta(S) =	111.507
G	3135.00	27.062	482944.2	-258553.0	236.522
(1 atm)	3300.00	27.062	487409.4	-297694.7	237.910

Generation of graphical output

In this example we plot the C_p data of **Fe**.



1. Click on the Graph menu and select the type of phase(s).



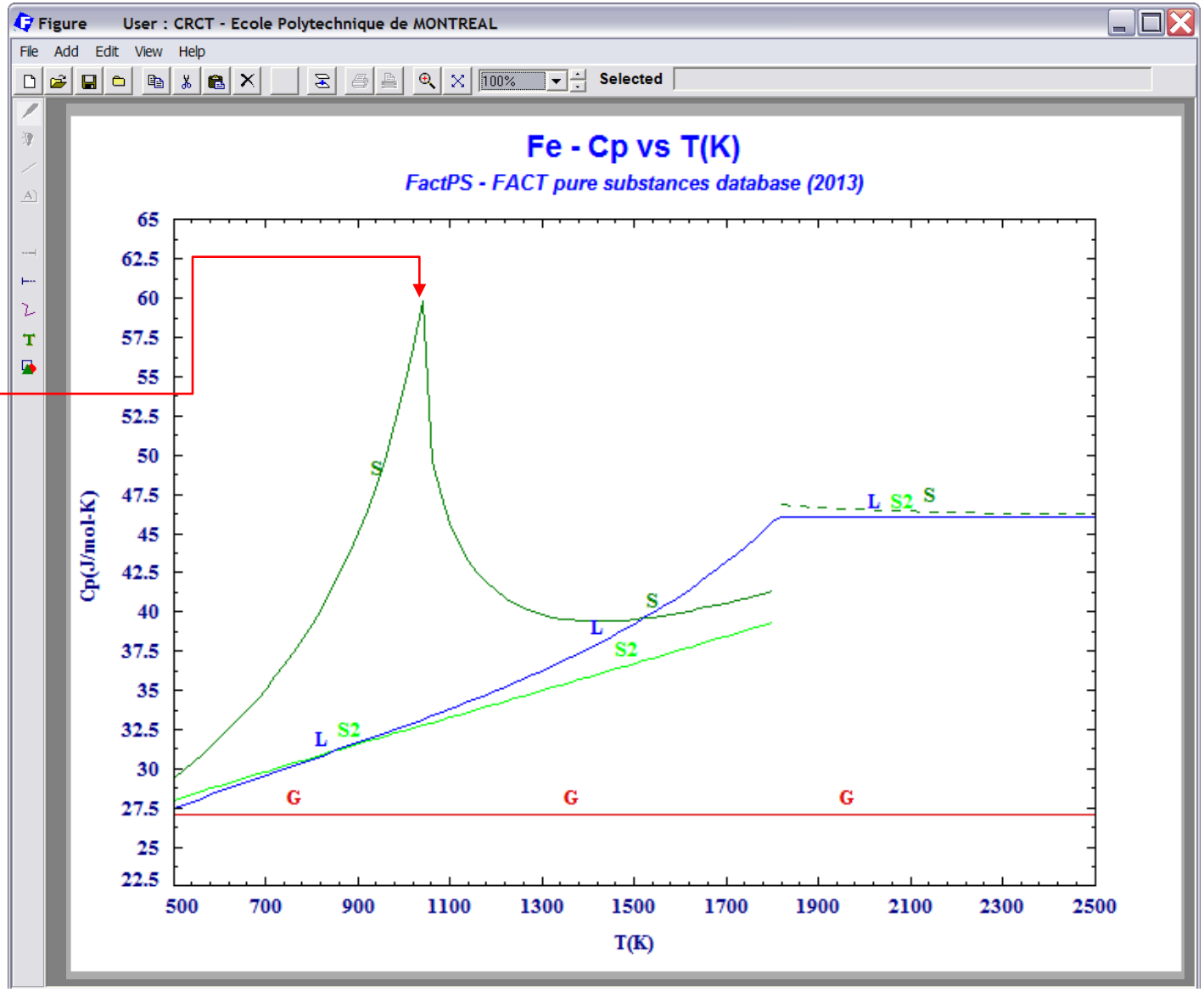
2. Click again on the Table menu, select «TK limits (default values) …» and enter the limits of temperature.

3. Click again on the Table menu and select the command «Table (your selection of phases) …» to generate the graph.

Plotted C_p data for **Fe**

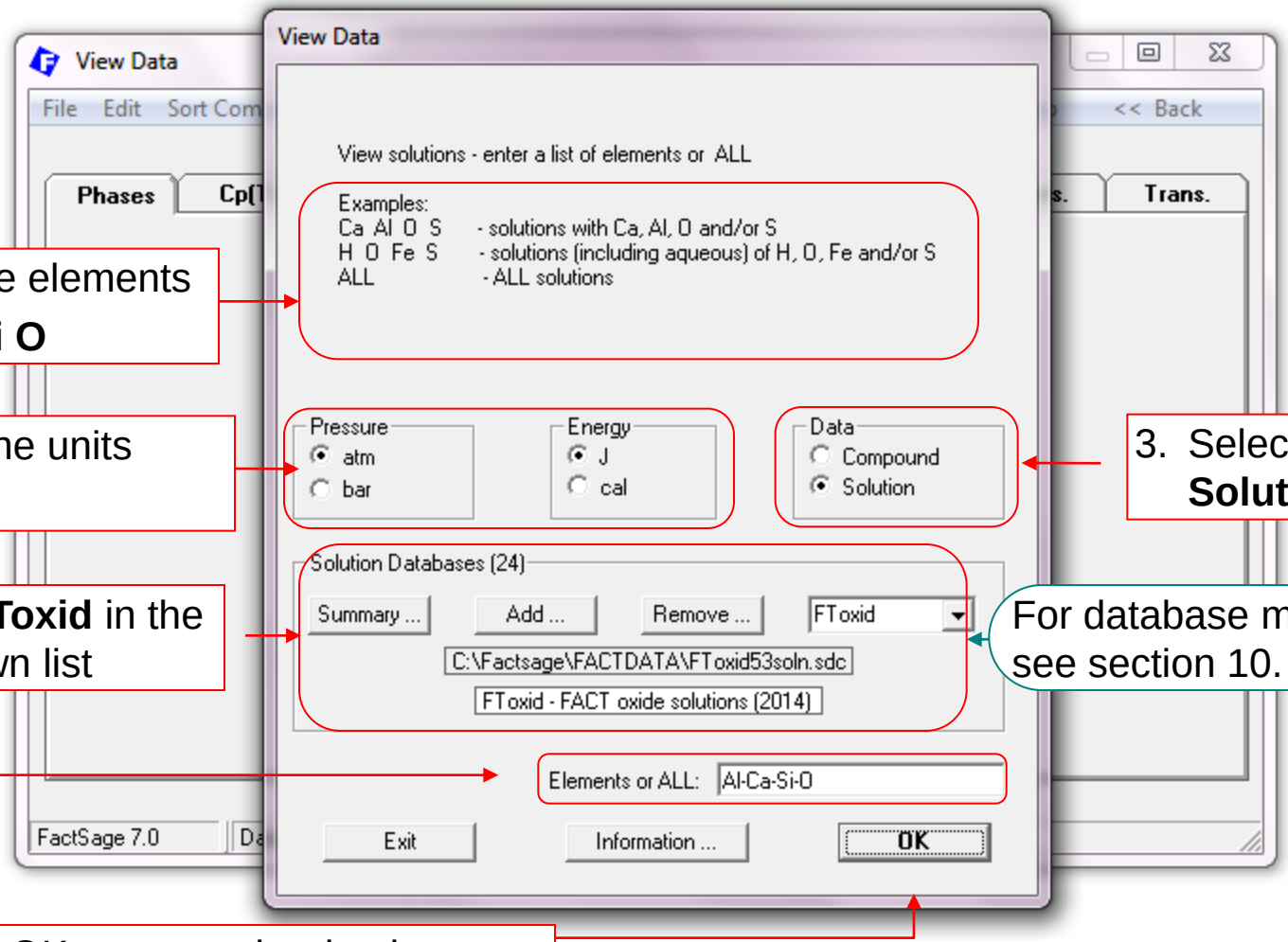
View Data uses the **Figure** Module to generate the graphical output.

Curie temperature = **1043 K**



View Data of a Solution Database

In this example we scan **FToxid -** the FACT oxides solution database - for all solution phases containing **Al**, **Ca, Si** and/or **O**



1. Enter the elements **Al Ca Si O**

2. Select the units **atm J**

3. Select the data **Solution**

4. Select **FToxid** in the drop-down list

For database management, see section 10.

5. Click on «OK» to scan the database.

The solution datasets window

List of all solution phases in **FToxid** containing **Al**, **Ca, Si** and/or **O**

Elements specified

Name of the database

Phase information

Menu Bar - more details on the next slide

Number of solutions in the database

List of solutions frame

In **FToxid-Mel_** the species Al2SiO5 must be selected

In **FToxid-Mull** the species Al2SiO5 must be selected

View Data Al-Ca-Si-O - FToxid datasets

File Edit Sort Solutions Summary Databases Units Atomic Wts. Table Graph Help << Back

4 Solutions

FToxid - FACT oxide solutions (2014)

Solutions sorted by phase number (see 'Sort Solutions')

Phase	Name and Species	Information
1. FToxid-SLAGA	ASlag-liq	oxide Al,As,B,Ca,Co,Cr,Cu,Fe,Ge,K,Mg,Mn,Na,Ni,Pb,Si,Sn,Ti,Zn,Z
	3 species 4 elements #99	dilute S (Mis.gap at high SiO2,use [I] option).
	Al2O3	
	SiO2	
	CaO	
2. FToxid-MeO_A	AMonoxide	Rocksalt-str. Fe(2),Ca,Mg,Ni,Co,Mn(2);dilute Zn,Al,Cr,Fe(3),Mn(3),
	2 species 3 elements #1	Cu,Zr. Mis. gap if CaO is present (use I option). Replaces MONO.
	CaO #	- at least one species # must be present
	Al2O3	
3. FToxid-Mel_	Melilite	(Ca,Pb)2[Zn,Mg,Fe2+,Fe3+,Al]{Fe3+,Al,Si}2O7
	2 species 4 elements #12	(Do not select simultaneously with FToxid-Gehl)
	Ca2Al3O7[1-]	
	Ca2Al1Si2O7[1+] #	- at least one species # must be present
4. FToxid-Mull	Mullite	[Al]2[Al,Si,B][O,Va]5, accounts for non-stoichiometry.
	4 species 3 elements #12	Replaces MULL and MulB. Do not select simultaneously with Mulf
	Al2Al1O5	
	Al2Al1Va5	
	Al2Si1O5 !	- this species must be present !
	Al2Si1Va5	

Solution model # 99 - Quasichemical (quadruplets)

FactSage 7.0 C:\Factsage\FACTDATA\FToxid53soln.sdc 7.0 read-only

Location of the database

Status of the database

Menu Bar – Solution Datasets Window

Menus available with the solution datasets window:

File

New	Ctrl+N
Save As …	Ctrl+S
Print …	Ctrl+P
Print Setup …	
Print Font …	
Exit	

Initiate a new search in View Data.

Open the «Save As …» dialog box (you can save your data in a text file [*.txt]).

Open the «Print…», «Print Setup…» or «Print Font…» dialog boxes (Windows features).

Exit the View Data program.

Edit

Find	Ctrl+F
Find Next	F3

Open the «Find…» dialog box (Windows features).

Units

- Energy ▸ ✔ J, cal
- Pressure ▸ ✔ atm, bar
- Mass ▸ ✔ mol, gram, lb

Click to select your units.

Summary

- ✓ Al-Ca-Si-O
- Al
- Ca
- Si
- O

Click to view a list of all solutions containing :

- Al. Ca, Si and/or O;
- Al;
- Ca;
- …

Use the Summary Menu to narrow your search (for example, all solutions containing Ca).

Help

- Explanation of absolute H, G and S …
- Slide Show … ▸ View Data …
- About View Data …

Open this slide show.

Note:
You can not access the **Databases**, **Table** and **Graph** menus in the Solution Datasets window.

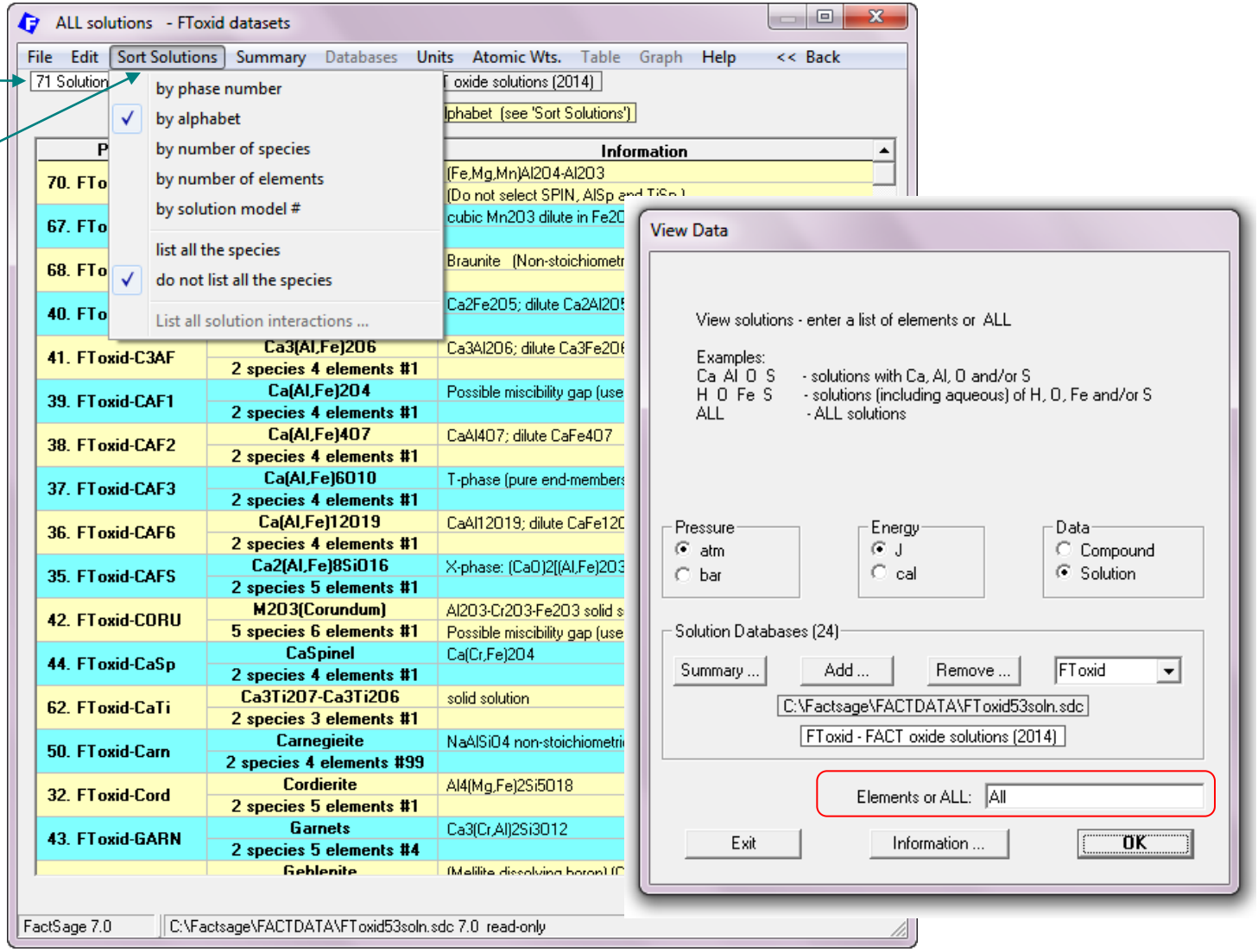
View Data of All Phases in a Solution Database

Here we scan **FToxid** for **ALL** solution phases

71 solution phases

Use the **Sort Solutions** drop-down menu to sort the solutions by phase number, alphabet, etc. and to limit the list of species.

Here the display of **FToxid** solutions is ordered by alphabet and the species are not listed.



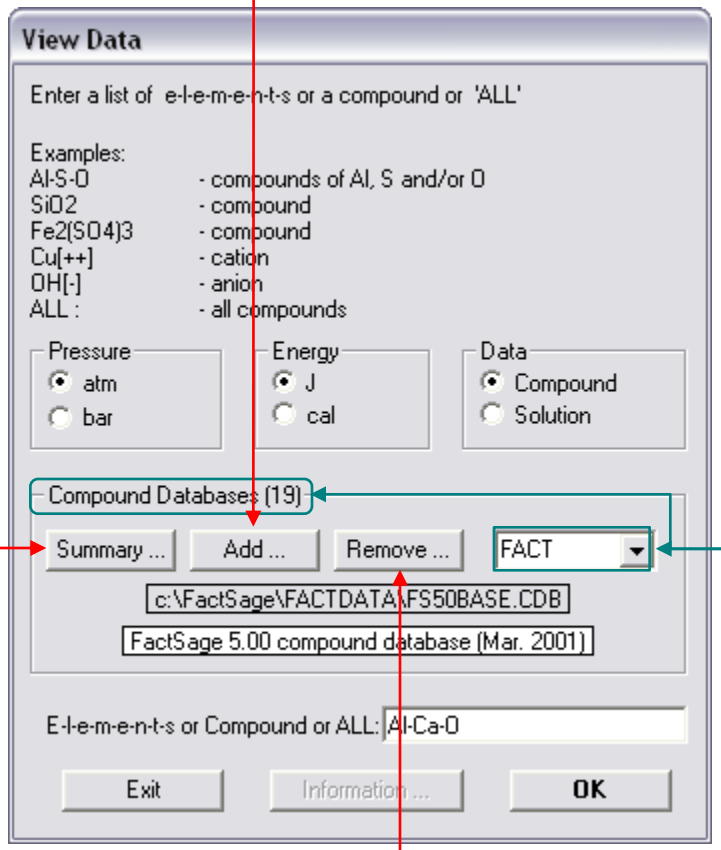
The following slides show how the View Data module can be used to add private Compound and Solution files to the list of databases accessible to FactSage.

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

View Data New Search window Databases Frame

Click on «Summary…» to open the **Summary of Databases** window – see the next slide.

Click on «Add…» to open the **List of Databases** window.



Here there are **19** compound databases on the search list. Your PC will not have all of them. Scroll down to view a **list** of their **nicknames**.

ELEM
FACT53
FACT
FScopp
FSlead
FSlite
FSnobl
FSstel
FSupsi
FThall
FThelg
FTlite
FTmisc
FToxid
FTpulp
FTsalt
SGPS
SGSL
SGTE*
SGTE
SGnobl
SGnucl
SGsold
All Database

Click on «Remove…» to remove a database from the list.
(The database is not erased from your computer, it is only removed from the list)

Summary of Databases Window

The summary of databases gives the current status of the databases on your computer

Summary of Databases in c:\FactSage\FACTDATA\

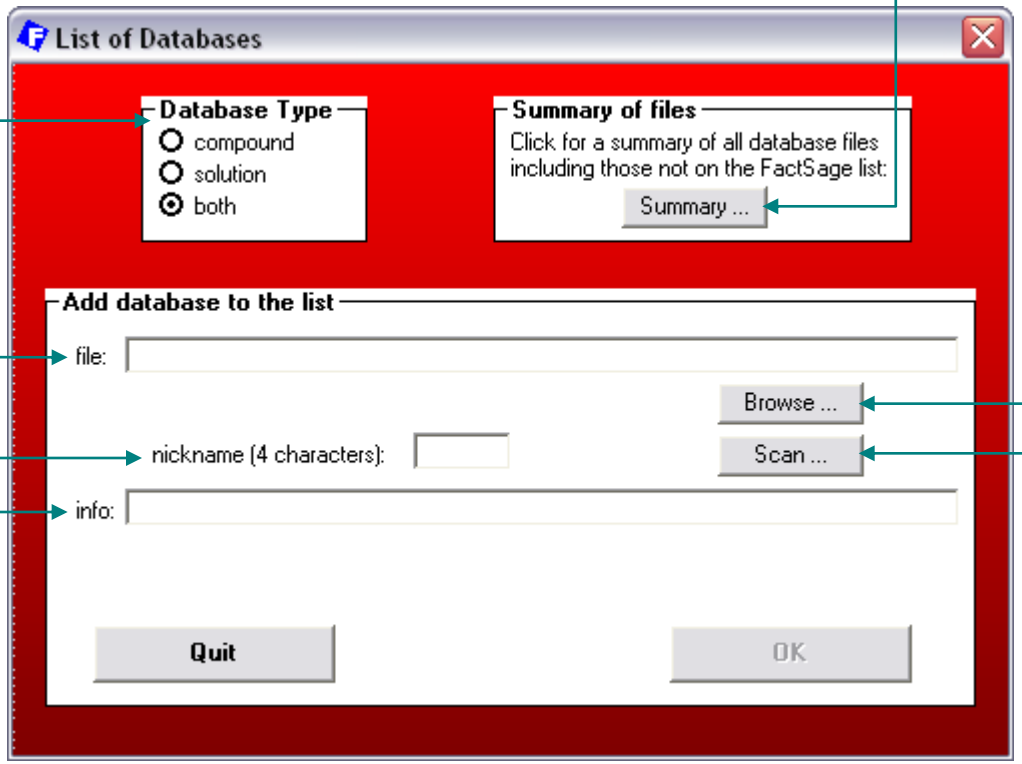
File Edit

```
==========================================================================================
 FactSage 6.0 - Summary of All Databases in c:\FactSage\FACTDATA\   27Nov08  3:29:24 PM
==========================================================================================

 Name     : 4-6 letter nickname
 ----

 Type     : R = Read-only (public) or W = Read/Write (private)
 ----       C = compound or S = solution.

 Database : file name
 --------

 Status   : 'OK' = file is accessible to you (client 0010), or 'X' = not accessible.
 ------     mmm-yy = expiration date (when applicable),
            1 (2.. 9) = database accessibility expires within 1 (2.. 9) months,
            '!' denotes database recently expired and will become non-accessible.

 List     : 'Yes' = the file is already on your List.
 ----       'No' = the file is accessible but not yet on your List of databases
                 - you may wish to add this database to the List (click on 'Add ...').

==========================================================================================

 ------ ---- ------------------  --------  ----  ----------------------------------------------
  Name  Type      Database        Status   List     Database Description
 ------ ---- ------------------  --------  ----  ----------------------------------------------
 BINS   R-C     BINSbase.cdb        OK     >No<  BINS - binary (SGTE) intermetallic alloy compounds Jan. 2007)
        W-S     BINSsoln.sdb        OK     >No<  BINS database

 ELEM   R-C     ELEMBASE.CDB        OK      Yes  FactSage 5.00 elements database (revised Jan. 2006)

 EXAM   W-S     Examsoln.dat        OK     >No<  EXAM database

 FACT   R-C     FS50BASE.CDB        OK      Yes  FactSage 5.00 compound database (Mar. 2001)
        R-S     FS50SOLN.SDA        OK      Yes  FactSage 5.00 solution database (Mar. 2001)

 FACT53 R-C     FS53base.cdb        OK      Yes  FACT53 - FactSage 5.3 compound database (Jan. 2007)

 FScopp R-C   FScopp54base.cdb   Dec-08 1   Yes  FScopp - FactSage Cu-rich alloy database - compounds (Jan. 2007)
        R-S   FScopp54soln.sda   Dec-08 1   Yes  FScopp - FactSage Cu-rich alloy database - solutions (Jan. 2007)

 FSlead R-C   FSlead54base.cdb   Dec-08 1   Yes  FSlead - FactSage lead intermetallic compounds (Jan. 2007)
        R-S   FSlead54soln.sda   Dec-08 1   Yes  FSlead - FactSage lead alloy solutions (Jan. 2007)

 FSlite R-C   FSlite53base.cdb   Dec-08 1   Yes  FSlite - FactSage light metal intermetallic compounds (Jan. 2007)
        R-S   FSlite53soln.sda   Dec-08 1   Yes  FSlite - FactSage light metal alloy solutions (Jan. 2007)
```

List of Databases Window

Select the Database Type to add.

Click on «Summary…» to open the **Summary of Databases** window.



Filename including the path.

Description (one line) of the selected database.

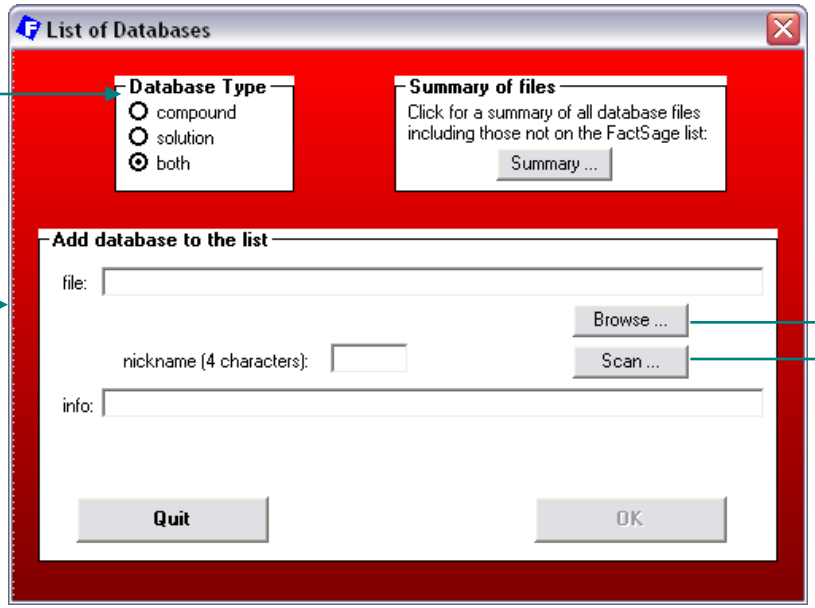
Nickname (4 characters) of the selected database.

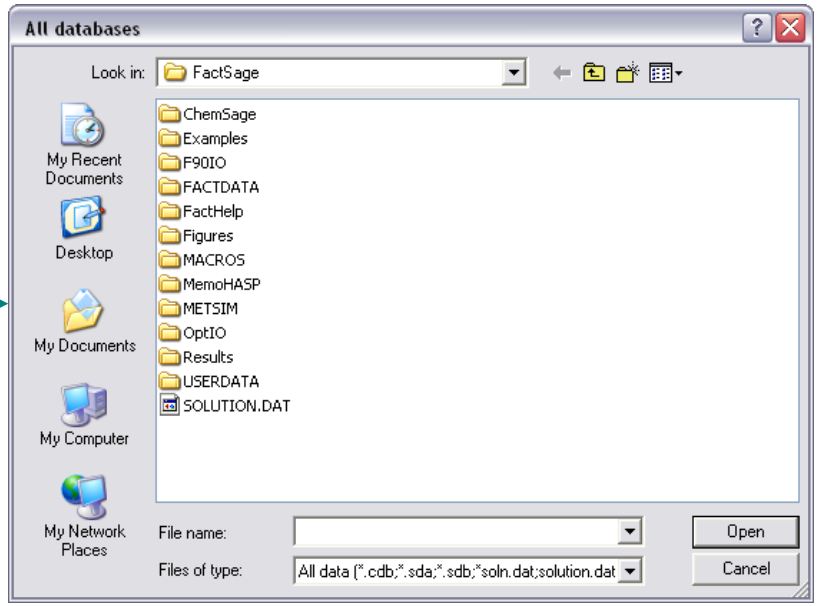
Click on «Scan …» to scan through the **/FACTDATA** directory and identify databases that are not already on the list.

Click on «Browse…» to open the **All databases** dialog box.

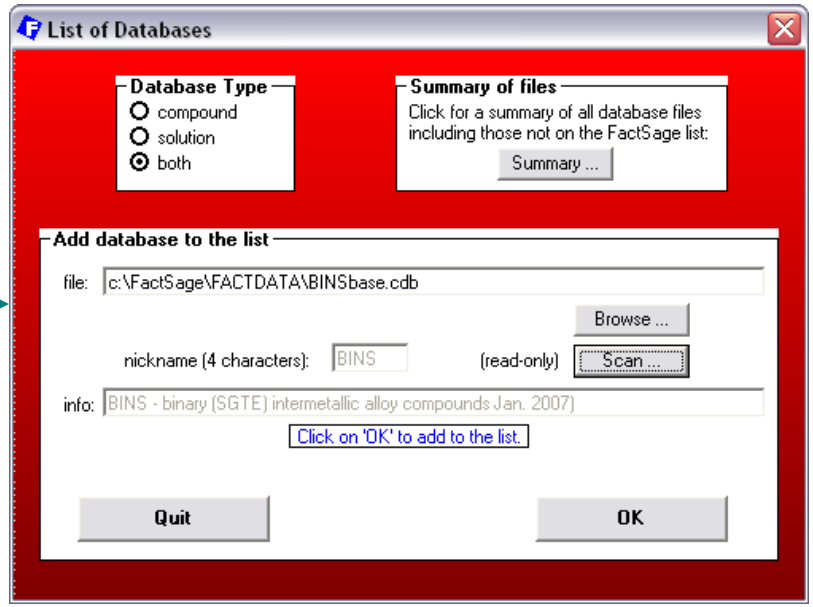
Add database to the list

1. Select the Database Type to add.



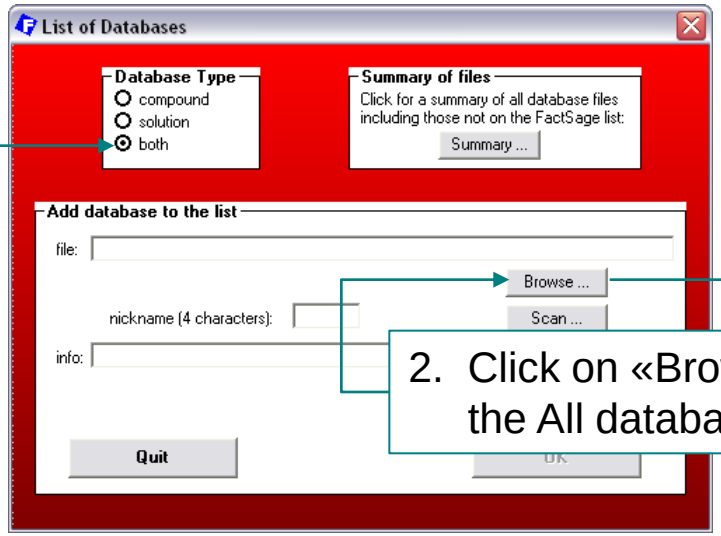


2. Enter the database to add by:
   a. Typing the complete **file**name (including the path); or,
   b. Click on «Browse…» to open the **All databases** dialog box; or,
   c. Click on «Scan …» to scan through the **/FACTDATA** directory and identify databases that are not already on the list.

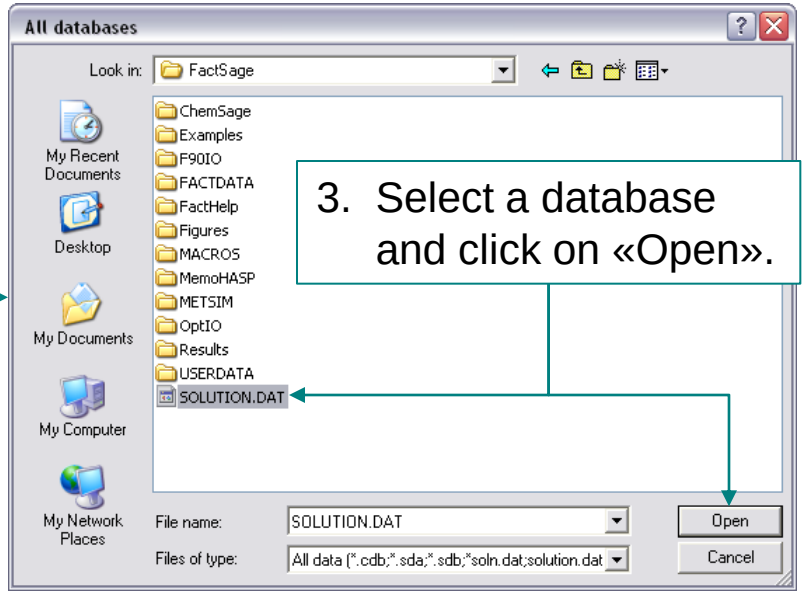


Add database to the list using the «Browse…» button

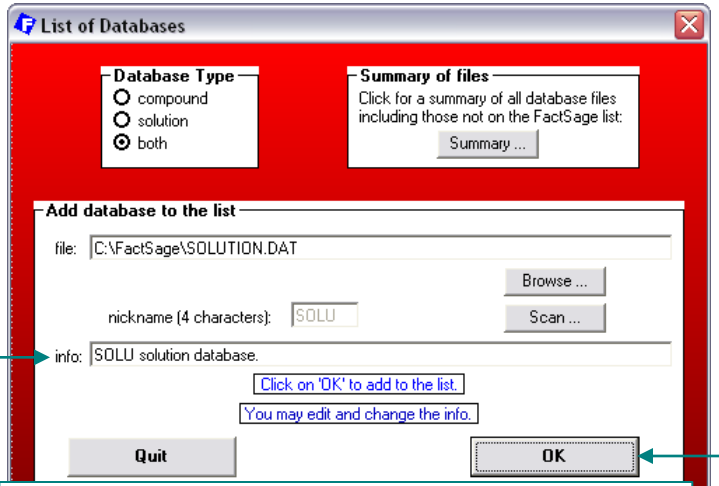
1. Select the Database Type to add.



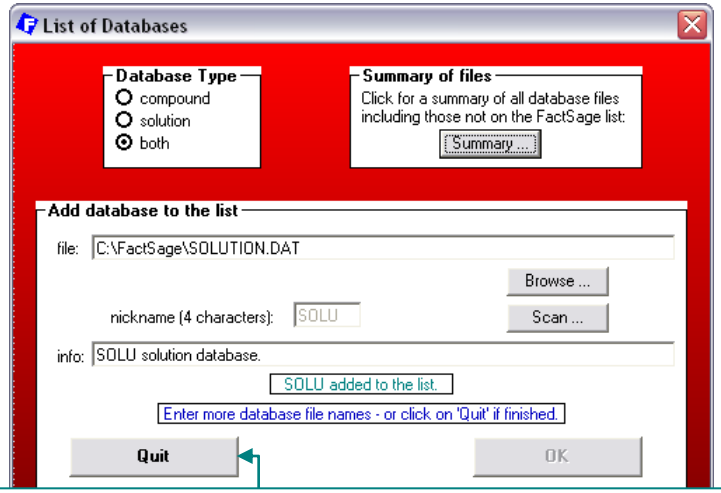
2. Click on «Browse…» to open the All databases dialog box.



3. Select a database and click on «Open».



4. Click on «OK» to add to the list. You may edit and change the info.

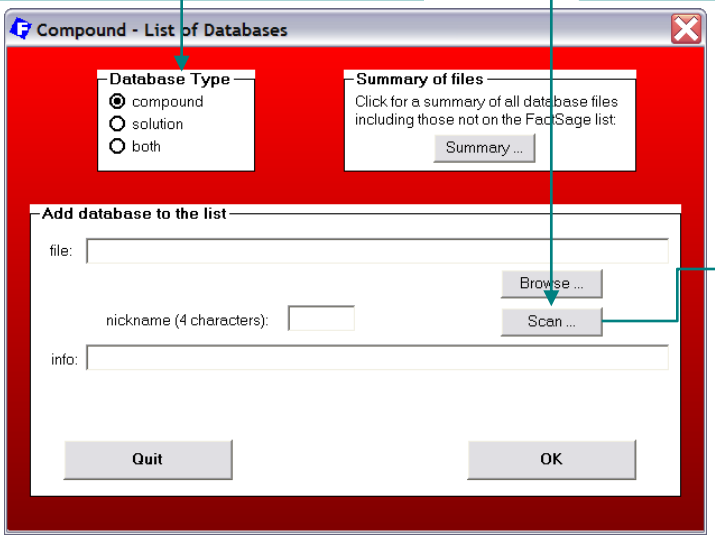


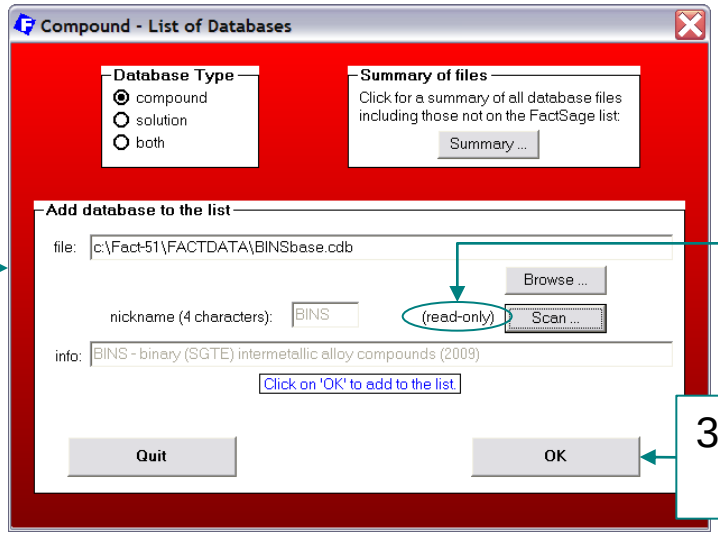
5. You can add more databases to the list (return to step 1) or click on «Quit» to finish adding databases.

Add database to the list using the «Scan…» button

1. Select the Database Type to add.

2. Click on «Scan…» to scan through the **/FACTDATA** directory and identify databases that are not already on the list.

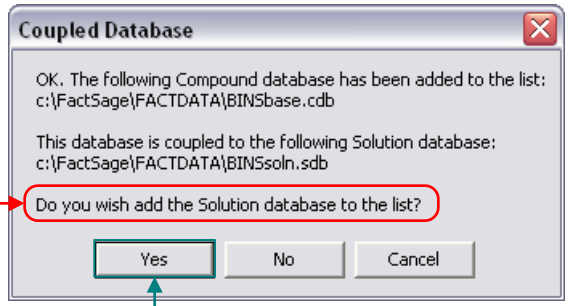




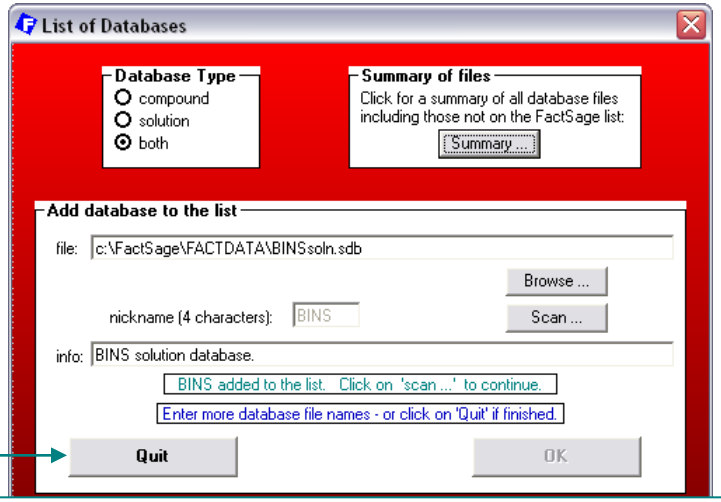
Note:
This is a **read-only** database.

3. Click on «OK» to add to the list.

If the selected database is coupled with another one, **View Data** will prompt you.

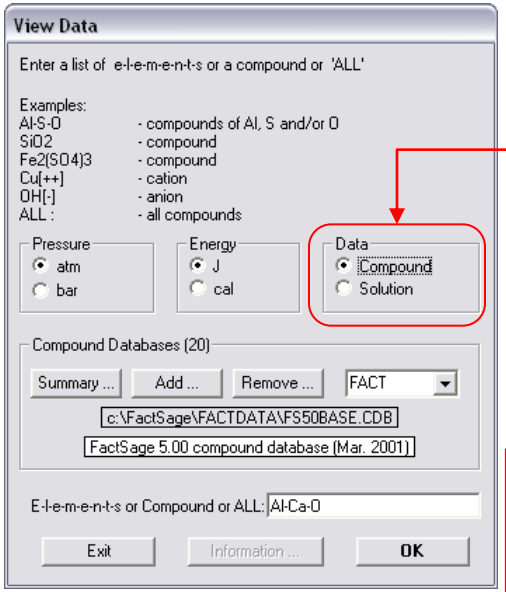


4. In the case of coupled databases, it is usually wise to answer «Yes».



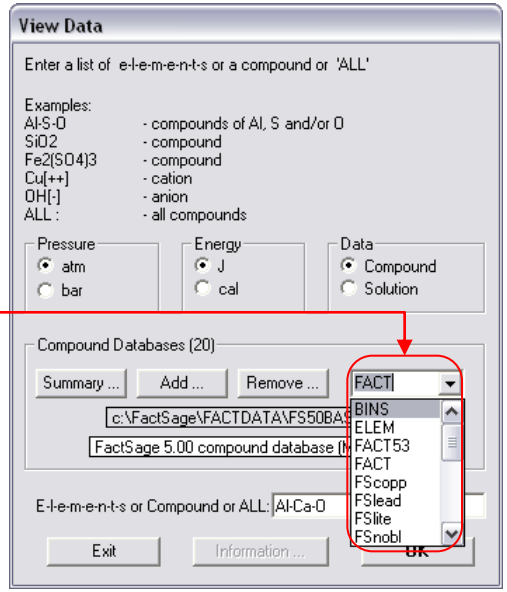
5. You can add more databases to the list (return to step 1) or click on «Quit» to finish.

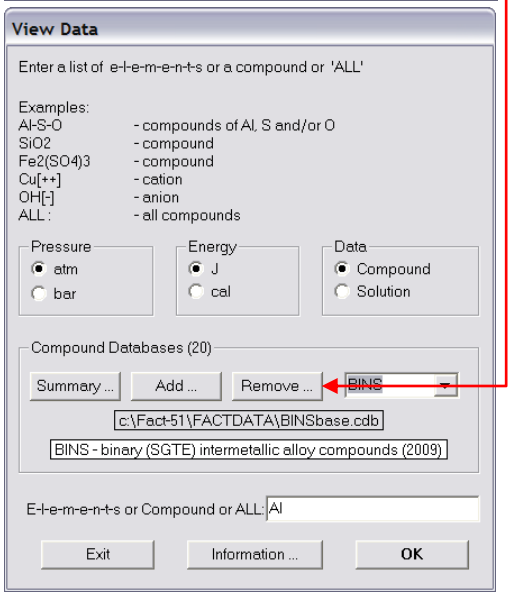
Removing a database from the list

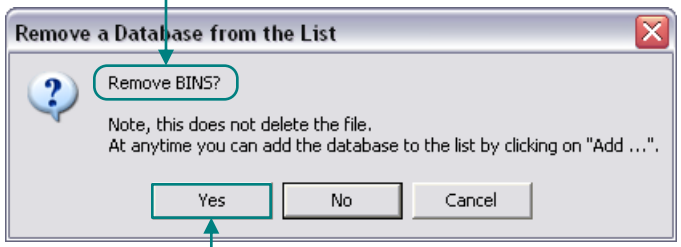


To remove a database:

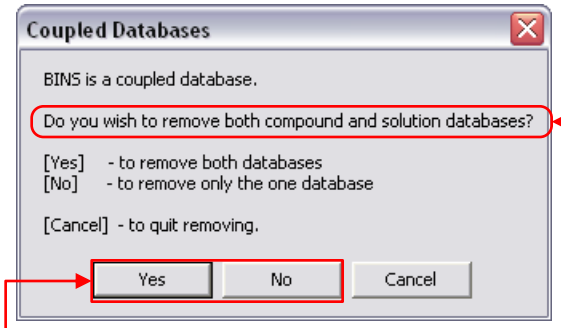
1. Select the type of database in the View Data window.
2. Select the database you wish to remove from the drop-down menu.
3. Click on «Remove…».
4. **View Data** will prompt you:
   a. If the selected database is **not** coupled with another one.
   b. If the selected database is coupled with another one.







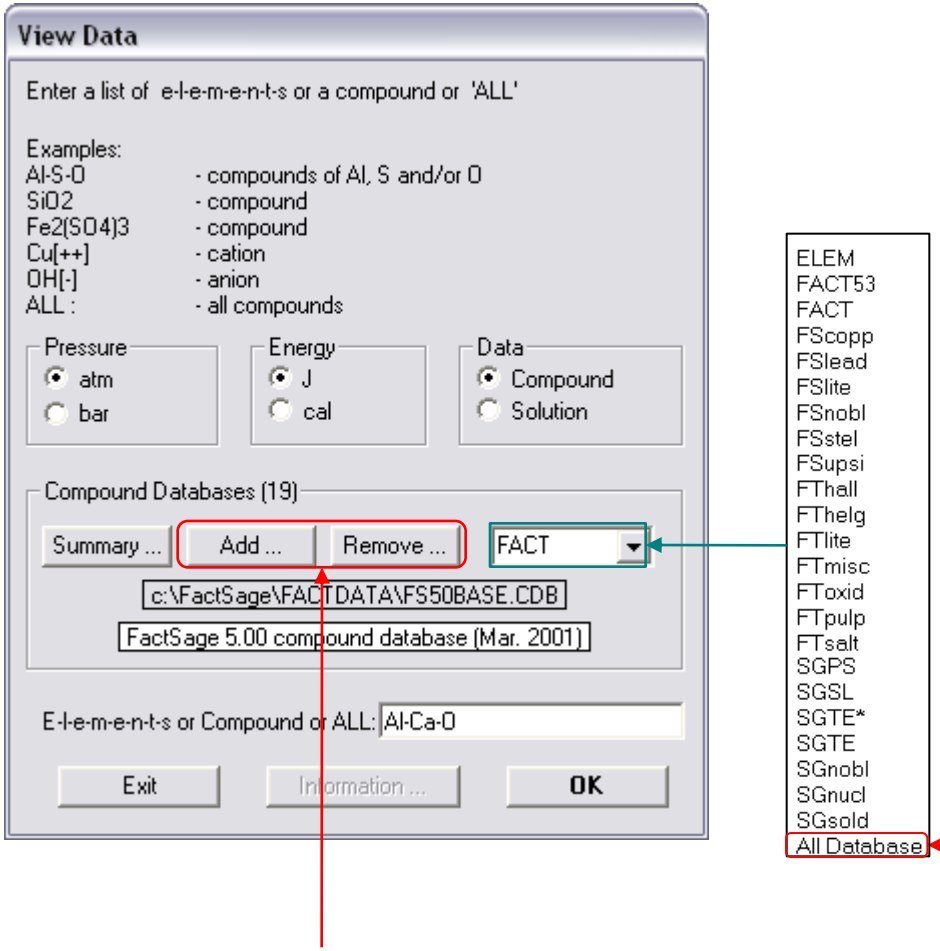
Yes will remove the BINS Compound database.



Yes will remove both (compound and solution) database.
No will remove your selection of the type of database made in step 1.

Search in more than one database

1. To search more than one database, select the option «All Databases» in the scroll down list.



Note: You can use the «Add…» and «Remove…» features to expand or narrow the number of databases included in your search.