

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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The *View Data* module



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

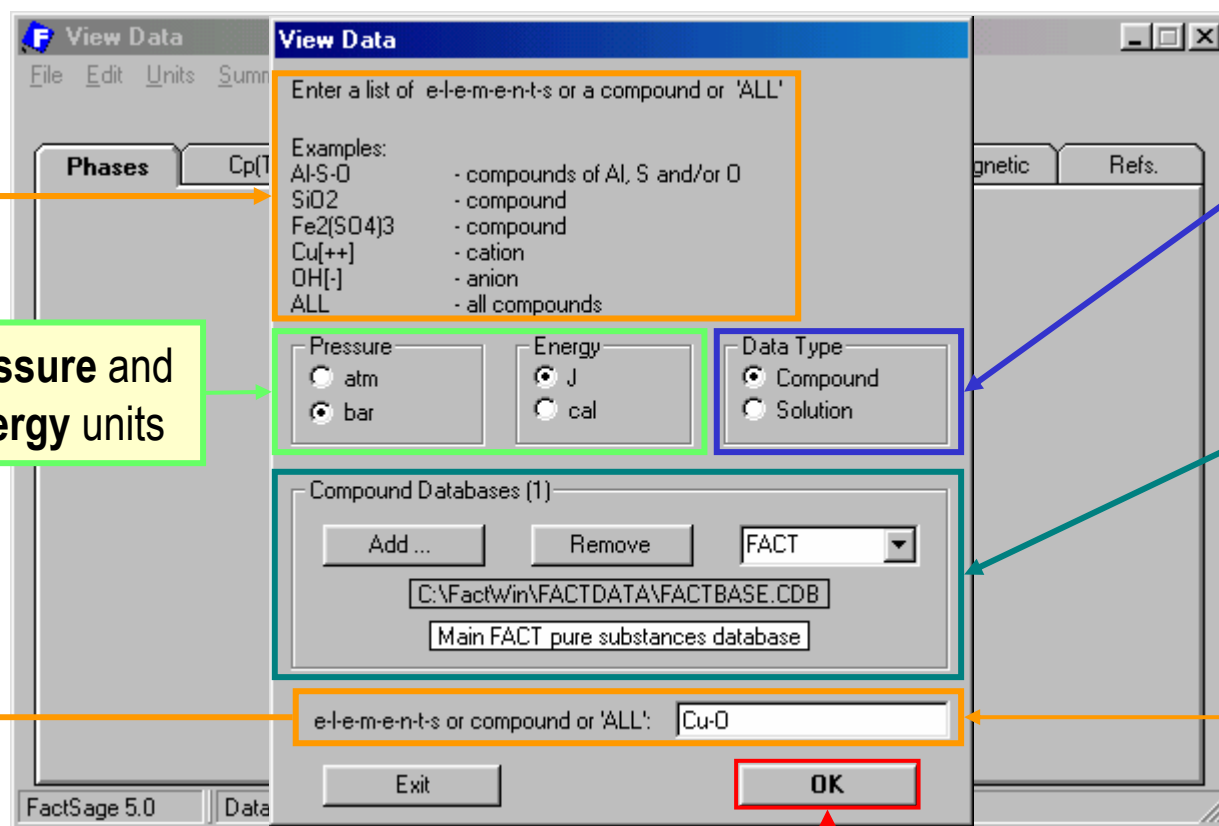
View Data of a **Compound** Database

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

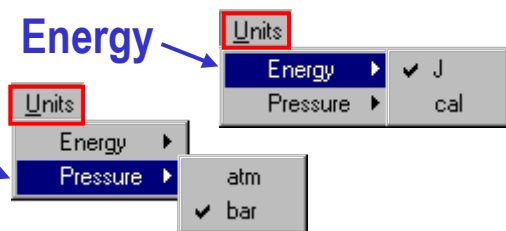
For example, the elements **Cu** and **O**

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

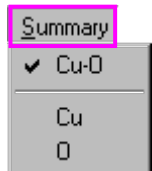
The Menu Bar

Units Menu: Energy

Pressure



Summary Menu:



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

Edit Menu:

Edit

Find Ctrl+F
Find Next F3

File Menu:

File

New Ctrl+N
Save Ctrl+S
Print Data ... Ctrl+P
Printer Setup ...
Printer Font ...
Exit

The screenshot shows the FactSage 5.0 interface. The menu bar includes File, Edit, Units, Summary, Databases, Table, Graph, and Help. The 'Units' menu is open, showing 'P(bar)' and 'Energy(J)'. The 'Summary' menu is also open, showing 'Cu-O', 'Cu', and 'O'. The 'Help' menu is open, showing 'Slide Shows...' and 'FACT-Demo slide show ...'. The main window displays a list of 15 compounds from the 'FACT - Main FACT pure substances database'. The 'Cu' compound is highlighted, and a red starburst indicates a double-click or 'Enter' action to view its data.

Compound	Phase	State	Charge
O [-]	FACT	G	
O	FACT	G	
O [+]	FACT	G	
O2 [-]	FACT	G	
O2	FACT	G	Aq
O2 [+]	FACT	G	
O3	FACT	G	
Cu [-]	FACT	G	
Cu	FACT	S	L G
Cu [+]	FACT	G	Aq
Cu [2+]	FACT	Aq	
Cu2	FACT	G	
Cu0	FACT	S	G
CuO2 [2-]	FACT	Aq	
Cu2O	FACT	S	L

Help is provided through a slide show presentation

Help

Slide Shows...

FACT-Demo slide show ...

Regular 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**.

3 Phases

Name: Copper
Formula Weight: 63.546

Phase	Cp Range, K	Density, g/ml	Ref.
S	298.15 - 1100.00	8.92	128
	1100.00 - 2000.00		
	2000.00 - 2001.00		
L	298.15 - 900.00	ideal	
	900.00 - 4000.00		
G	298.15 - 1800.00		
	1800.00 - 4100.00		
	4100.00 - 6000.00		

FactSage 5.0 C:\FactWin\FACTDATA\FACTBASE.CDB

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

References

F Cu Units: P(bar) Energy(J)

File Edit Units Summary Databases Table Graph Help

3 Phases FACT - Main FACT pure substances database

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

Name: Copper

References

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

FactSage 5.0 C:\FactWin\FACTDATA\FACTBASE.CDB

Bibliographic data

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

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:

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

F Cu Units: P(bar) Energy(J)

File Edit Units Summary Databases Table Graph Help

3 Phases FACT - Main FACT pure substances database

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

Name: Copper

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

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]	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	298 - 1100
			212626.807	-2	6.86736674E-06	2	
			-2799.24538	-1			
S	-139473.47	-326.232701	-1111.31788	0	9.34944879E-02	1	1100 - 2000
			3.60627463E+08	-2	-1909966.88	-1	
			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	298 - 1800
			111381.781	-2	8.03042639E-07	2	
			-837.115980	-1			
G	621512.53	858.835719	658.909214	0	-2.20262268E-02	1	1800 - 4100
			-4.41758515E+08	-2	1658224.92	-1	
			-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 ΔH_{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**, $G(T)$.

$$H(T) = \Delta H_{298} + \int_{298}^T C_p(T) dT$$

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

Combined in the Gibbs-Helmholtz equation:

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

Enthalpy expressions – H(T)

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

F Cu Units: P(bar) Energy(J)

File Edit Units Summary Databases Table Graph Help

3 Phases FACT - Main FACT pure substances database

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

Name: Copper

H(T) /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	
L	+ 259407.3009 T ⁻¹	+ 1197.884960 ln(T)		298 - 900
L	- 1804.281775	+ 32.84400000 T		
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
FactS	- 148798.7903 ln(T)	+ 7687.867779 T ^{0.5}		

Entropy expressions – S(T)

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

FactSage Software Interface: Cu Units: P(bar) Energy(J)

File Edit Units Summary Databases Table Graph Help

3 Phases FACT - Main FACT pure substances database

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

Name: Copper

S(T) J/mol-K - 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	
L	-152.9567158	+ 32.84400000 ln(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	
G	-55690.89057 T ⁻²	+ 4.015213196E-07 T ²	+ 837.1159795 T ⁻¹	298 - 1800
	- 6608.530023	+ 658.9092143 ln(T)	- 2.202622682E-02 T	
G	+ 220879257.5 T ⁻²	- 1658224.917 T ⁻¹	+ 117358.4583 T ^{-0.5}	1800 - 4100
	210.0730345	+ 11.45164074 ln(T)	+ 40677945.71 T ⁻²	
G	+ 148798.7903 T ⁻¹	- 7687.867779 T ^{-0.5}		4100 - 6000

Gibbs Energy expressions – G(T)

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

FactSage software interface showing Gibbs energy data for Copper. The window title is "F Cu Units: P(bar) Energy(J)". The "G(T)" tab is selected. The name is "Copper". The units are "G(T) J/mol - 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)			
FactS 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 that 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

View Data

Enter a list of e-l-e-m-e-n-t-s or a compound or 'ALL'

Examples:
 Al-S-O - compounds of Al, S and/or O
 SiO2 - compound
 Fe2(SO4)3 - compound
 Cu[++] - cation
 OH[-] - anion
 ALL - all compounds

Pressure: atm bar
 Energy: J cal
 Data Type: Compound Solution

Compound Databases (1)
 Add... Remove FACT
 C:\FactWin\FACTDATA\FACTBASE.CDB
 Main FACT pure substances database

e-l-e-m-e-n-t-s or compound or 'ALL': **Fe**

Exit OK

F Fe Units: P(bar) Energy(J)

File Edit Units Summary Databases Table Graph Help

4 Phases FACT - Main FACT pure substances database

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

Name: Iron

Magnetic Properties

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

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

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

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

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

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

F Fe Units: P(bar) Energy(J)

File Edit Units Summary Databases Table Graph Help

4 Phases FACT - Main FACT pure substances database

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

Name: Iron
 Formula Weight: 55.847

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

F Fe Units: P(bar) Energy(J)

File Edit Units Summary Databases Table Graph Help

4 Phases FACT - Main FACT pure substances database

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

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) (J)	S(298.15) (J/K)	C(i)	P(i)	C(i)	P(i)	Cp (K)
S1	9149.45	36.863493	23.5143000	0	8.79504000E-03	1	298 - 1811
			-154717.000	-2	3.53561400E-07	2	
S1	+ H(magnetic) + S(magnetic) + Cp(magnetic)						1811 - 1812
S2	7973.03	35.902097	24.6643000	0	7.51504000E-03	1	298 - 1811
			-154717.000	-2	3.53561400E-07	2	
S2	+ H(magnetic) + S(magnetic) + Cp(magnetic)						1811 - 1812
L	21189.62	43.421941	23.5143000	0	8.79504000E-03	1	298 - 1811
			-154717.000	-2	3.53561400E-07	2	
L	+ H(magnetic) + S(magnetic) + Cp(magnetic)						1811 - 1812
L	2876.06	16.787452	46.0000000	0			1811 - 6000
G	406173.01	172.960265	27.0621120	0			298 - 6000

Real gas coefficients for carbon dioxide CO₂

View Data

Enter a list of e-l-e-m-e-n-t-s or a compound or 'ALL'

Examples:
Al-S-O - compounds of Al, S and/or O
SiO2 - compound
Fe2(SO4)3 - compound
Cu[++] - cation
OH[-] - anion
ALL - all compounds

Pressure: atm bar
Energy: J cal
Data Type: Compound Solution

Compound Databases (1):
Add ... Remove FACT
C:\FactWin\FACTDATA\FACTBASE.CDB
Main FACT pure substances database

e-l-e-m-e-n-t-s or compound or 'ALL': CO2

Exit OK

For example, CO₂

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 ω (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.

F CO2 Units: P[bar] Energy[J]

File Edit Units Summary Databases Table Graph Help

2 Phases FACT - Main FACT pure substances database

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

Name: Carbon Dioxide
Volume data

Non-ideal gas properties

	Tc (K)	Pc (bar)	Vc (cc/mol)	Omega	Dipole Moment (Debyes)
G	304.100	73.800	93.900	0.239	0.000

Expansivities / Compressibilities / Derivative of Bulk Modulus
(-none-)

FactSage 5.0 C:\FactWin\FACTDATA\FACTBASE.CDB

Data for SiO_2

View Data

Enter a list of e-l-e-m-e-n-t-s or a compound or 'ALL'

Examples:
 Al-S-O - compounds of Al, S and/or O
 SiO2 - compound
 Fe2(SO4)3 - compound
 Cu(++) - cation
 OH(-) - anion
 ALL - all compounds

Pressure
 atm
 bar

Energy
 J
 cal

Data Type
 Compound
 Solution

Compound Databases (1)
 FACT
 C:\FactWin\FACTDATA\FACTBASE.CDB
 Main FACT pure substances database

e-l-e-m-e-n-t-s or compound or 'ALL':

F SiO2 Units: P(bar) Energy(J)

File Edit Units Summary Databases Table Graph Help

9 Phases FACT - Main FACT pure substances database

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

Name: silicon dioxide
 Formula Weight: 60.0843

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

For example, SiO_2

Volume data - expansivities, compressibilities and derivative of bulk modulus

FactSage 5.0 Units: P[bar] Energy[J]

File Edit Units Summary Databases Table Graph Help

9 Phases [FACT - Main FACT pure substances database]

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

Name: silicon dioxide
Volume data

Non-ideal gas properties
(-none-)

Expansivities / Compressibilities / Derivative of Bulk Modulus

	Expansivity [1/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

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)

Compressibility expression (compressibilities):

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

	Compressibility [1/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):

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

	Expansivity [1/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:

Table

- 300 - 2000 K (all phases) ...
- Temperature limits, TK; min, max, step ...
- Phases
 - ✓ all phases
 - gas
 - liquid
 - solid
 - aqueous
 - most stable

Selection of the temperature range and step.

Selection of the phase(s).

Graph Menu:

Graph

- 300 - 2000 K (all phases) ... *
- Temperature limits, TK; min, max, step ...
- Phases
 - ✓ all phases
 - gas
 - liquid
 - solid
 - aqueous

* Selection of thermodynamic data:
 C_p , H, G or S ... vs T

Graph

- 300 - 2000 K (all phases) ...
- Temperature limits, TK; min, max, step ...
- Phases
 - Cp vs T ...
 - H vs T ...
 - G vs T ...
 - S vs T ...

F Cu Units: P(bar) Energy(J)

File Edit Units Summary **Databases** Table Graph Help

FACT - Main FACT pure substances database

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

Name: Copper
Formula Weight: 63.546

Databases Menu: Databases
✓ FACT

	Phase	Cp Range, K	Density, g/ml	Ref.
S	solid-1	298.15 - 1100.00	8.92	128
		1100.00 - 2000.00		
		2000.00 - 2001.00		
L	liquid-1	298.15 - 900.00	ideal	
		900.00 - 4000.00		
G	gas-1	298.15 - 1800.00	ideal	
		1800.00 - 4100.00		
		4100.00 - 6000.00		

FactSage 5.0 C:\FactWin\FACTDATA\FACTBASE.CDB

Thermodynamic Data for Cu: Tabular Output

Table

500 - 2500 K (all phases) ...

Temperature limits, TK; min, max, step ...

Phases

Close

Save

Table

500 - 2500 K (liquid) ...

Temperature limits, TK; min, max, step ...

Phases

- all phases
- gas
- ✓ liquid
- solid
- aqueous
- most stable

all phases (S, L, G)

T(K):

Enter temperature limits, K (range 100 to 20000): 'min max step'

Click on 'Cancel' for the default values 300 2000 100

500 2500 500

**From 500 K to 2500 K
in steps of 500 K**

Output Menu:

- Output
- Save Output ...
- Print
- Printer Font ...
- Printer Setup ...

F Cu

Output

Print

Cu - Copper

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 -

standard state

S

T (K)	Cp (J/K)	H (J)	G (J)	S (J/K)
298.15	24.449	0.0	-9887.8	33.164
500.00	25.961	5104.1	-17997.9	46.204
1000.00	28.707	18733.8	-46259.7	64.994
1500.00	36.401	34611.1	-82033.3	77.763
2000.00	32.844	55533.0	-123918.8	89.726
2500.00	32.844	71955.0	-170682.1	97.055

L

T (K)	Cp (J/K)	H (J)	G (J)	S (J/K)
298.15	24.441	11856.1	-551.9	41.617
500.00	25.936	16960.4	-10368.7	54.658
1000.00	32.844	31039.7	-42881.9	73.922
1500.00	32.844	47461.7	-83396.3	87.239
2000.00	32.844	63883.7	-129490.9	96.687
2500.00	32.844	80305.7	-179734.9	104.016

G

T (K)	Cp (J/K)	H (J)	G (J)	S (J/K)
298.15	20.791	337600.0	287988.7	166.397
500.00	20.793	341794.7	253224.3	177.141
1000.00	20.774	352189.4	160637.4	191.552
1500.00	20.871	362590.4	62612.5	199.985
2000.00	21.422	373127.8	-38961.1	206.044
2500.00	22.868	384156.1	-143244.6	210.960

+ thermodynamic data at T = 298.15 K

Tabular output for Fe

Table
Temperature limits, TK; min, max, step ...
Phases

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
 $S1 \rightarrow S2$
 (alpha \rightarrow gamma)
 at **1184.81 K**

The allotropic transition reverses at
1667.47 K
 where $S2 \rightarrow S1$
 (gamma \rightarrow delta).

Phase transitions
 $S1 \rightarrow S2 \rightarrow S1 \rightarrow L \rightarrow G$
 as **T** increases.

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

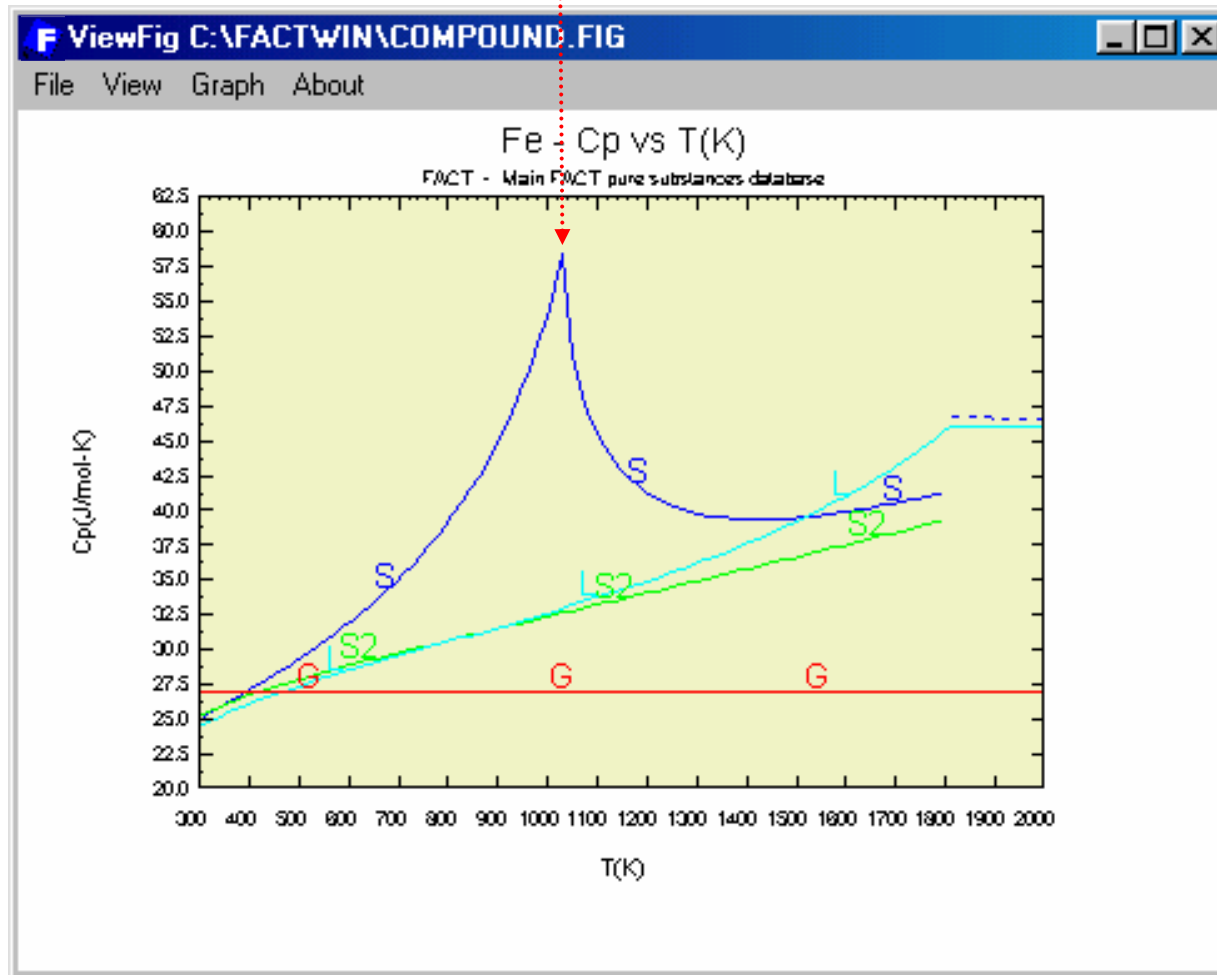
At this temperature $G(S1) = G(S2)$ (two phases in equilibrium).

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

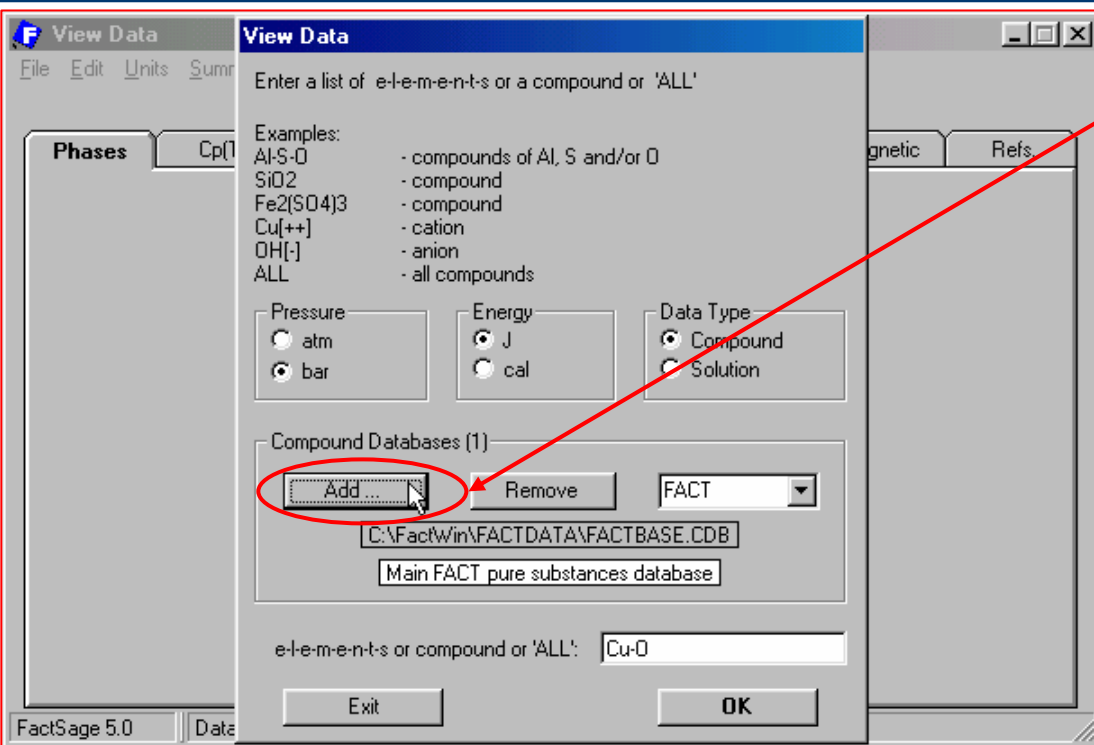


The following slides show how the View Data module is used in order to **link additional Compound databases** with the **FactSage** program.

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.

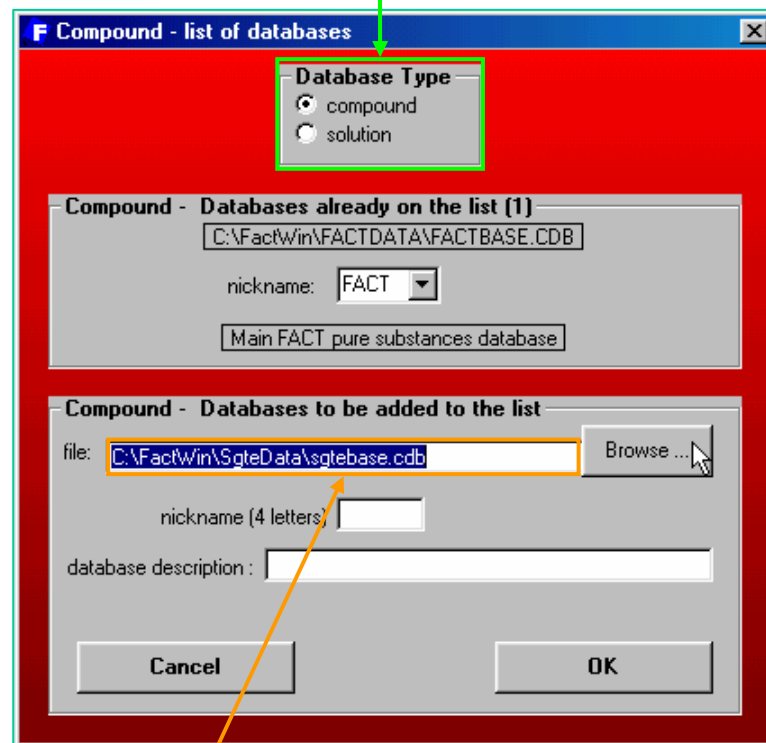
NOTE: The additionally linked databases are also available for use in other modules. Thus View Data can be considered a general entry point for databases.

Adding a compound database to the list

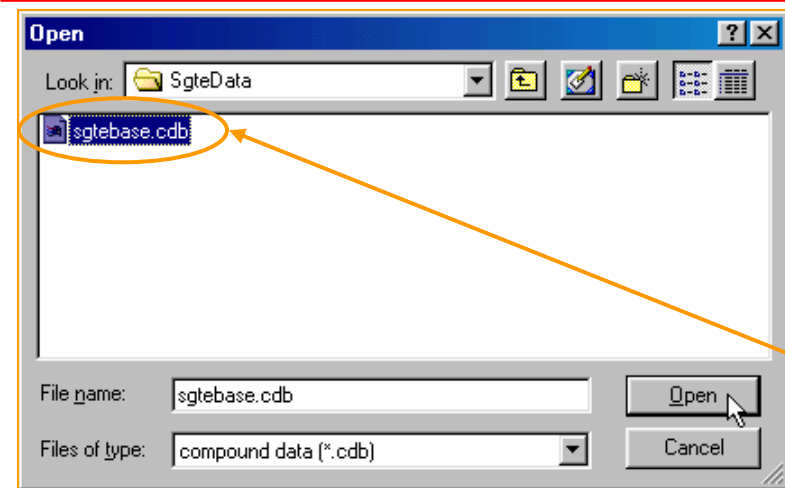


1. Press the « Add... » button in the Compound Databases (1) frame.

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)

Compound - list of databases

Database Type

- compound
- solution

Compound - Databases already on the list (1)

file: C:\FactWin\FACTDATA\FACTBASE.CDB

nickname: FACT

Main FACT pure substances database

Compound - Databases to be added to the list

file: C:\FactWin\SgteData\sgtebase.cdb

nickname (4 letters) SGTE

database description: SGTE compound database.

Cancel OK

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

View Data

Enter a list of e-l-e-m-e-n-t-s

Examples:
Ca-Al-O-S - solutions with Ca, Al, O and/or S
H-O-Fe-S - solutions (including aqueous) of H, O, Fe and/or S

Pressure
 atm
 bar

Energy
 J
 cal

Data Type
 Compound
 Solution

Solution Databases (2)

Add ... Remove

SGTE
FACT
SGTE
All Databases

C:\FactWin\SgteData\sgtesol

SGTE solution database

e-l-e-m-e-n-t-s: Cu-O

Exit OK

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

Data in 2 or more compound databases

View Data

Enter a list of e-l-e-m-e-n-t-s or a compound or 'ALL'

Examples:

- Al-S-O - compounds of Al, S and/or O
- SiO2 - compound
- Fe2(SO4)3 - compound
- Cu[++] - cation
- OH[-] - anion
- ALL - all compounds

Pressure: atm bar

Energy: J cal

Data Type: Compound Solution

Compound Databases (2):

Add ... Remove **All Databases**

All Databases

- 2 Compound Databases

e-l-e-m-e-n-t-s or compound or 'ALL': Cu-O

Exit OK

« All Databases »

F Cu-O Units: P(bar) Energy(J)

File Edit Units Summary Databases Table Graph Help

17 Compounds All Databases

Cu	FACT	S	L	G
Cu	SGTE	S	L	
Cu2	FACT	G		
Cu2O	FACT	S	L	
CuO	FACT	S	G	
CuO2 [2-]	FACT	Aq		
Cu[+]	FACT	G	Aq	
Cu[-]	FACT	G		
Cu[2+]	FACT	Aq		
O	FACT	G		
O	SGTE	L		
O2	FACT	G	Aq	
O2[+]	FACT	G		
O2[-]	FACT	G		
O3	FACT	G		
O[+]	FACT	G		
O[-]	FACT	G		

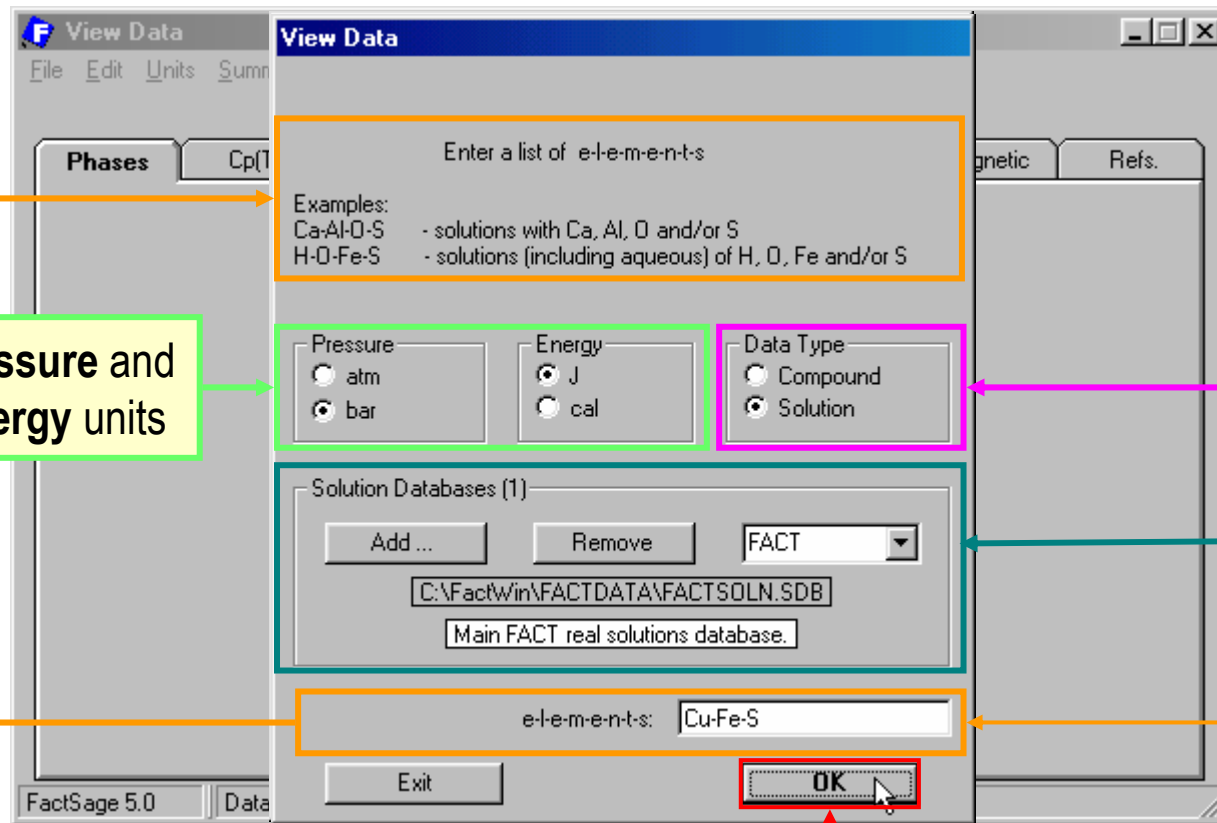
FactSage 5.8 All compound databases

15 compounds from the **FACTBASE** database and **2** from the **SGTEBASE** database for a total of **17** compounds.

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.

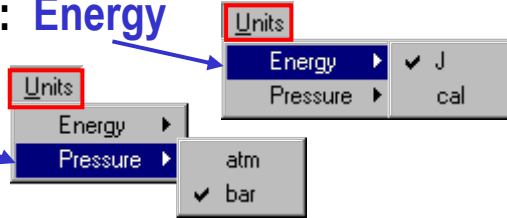
For example, the elements **Cu**, **Fe** and **S**

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

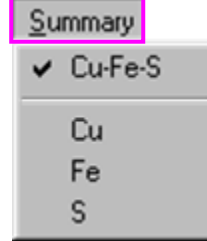
The solution datasets window

Units Menu: Energy

Pressure

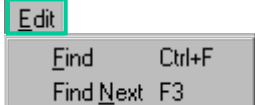


Summary Menu:

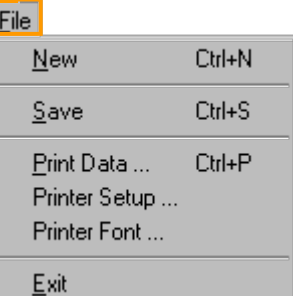


- All solutions containing **Cu**, **Fe** or **O**
- All solutions containing **Cu**
- All solutions containing **Fe**
- All solutions containing **O**

Edit Menu:



File Menu:



F Cu-Fe-S - solution datasets

File Edit **Units** Summary Databases Table Graph Help

4 Solutions [FACT - Main FACT real solutions database.]

Solution	Data	Information
FACT-FES	FACT	FeS-liq (solvent) with Fe, FeO, MgS, MnS, TiS & Na2S Valid only for FeS - rich compositions.
	Fe	
	FeS	0.30 > X > 1.0
FACT-FELQ	FACT	Fe-liq steel with solutes Ag, Al, B, C, Ca, Ce, Co, Cr, Cu, H, La, Mn, Mo, N, Nb, Ni, O, P, Pb, Pd, S, Si, Sn, Ta, Ti, U, V, W and Zr
	Fe	
	Cu	0.0 < X < 0.10
FACT-CULQ	FACT	Cu-liq or speiss (presence of Cu not essential.) <50 mol% As, <15 mol% S (300-1300 C). <10 mol% O in Cu-Pb (good around
	Cu	
	Fe	0.0 < X < 0.50
FACT-MATT	FACT	Matte S-Cu-Fe-Ni-Co-Pb-Zn-As; < 10 mol% As, 30 - 60 mol% S. Do not use for calculation of equilibria with solid sulphide phases.
	S	0.20 > X > 1.0
	Fe	
	Cu	

FactSage 5.0 C:\FactWin\FACTDATA\FACTSOLN.SDB

Help is provided through a slide show presentation



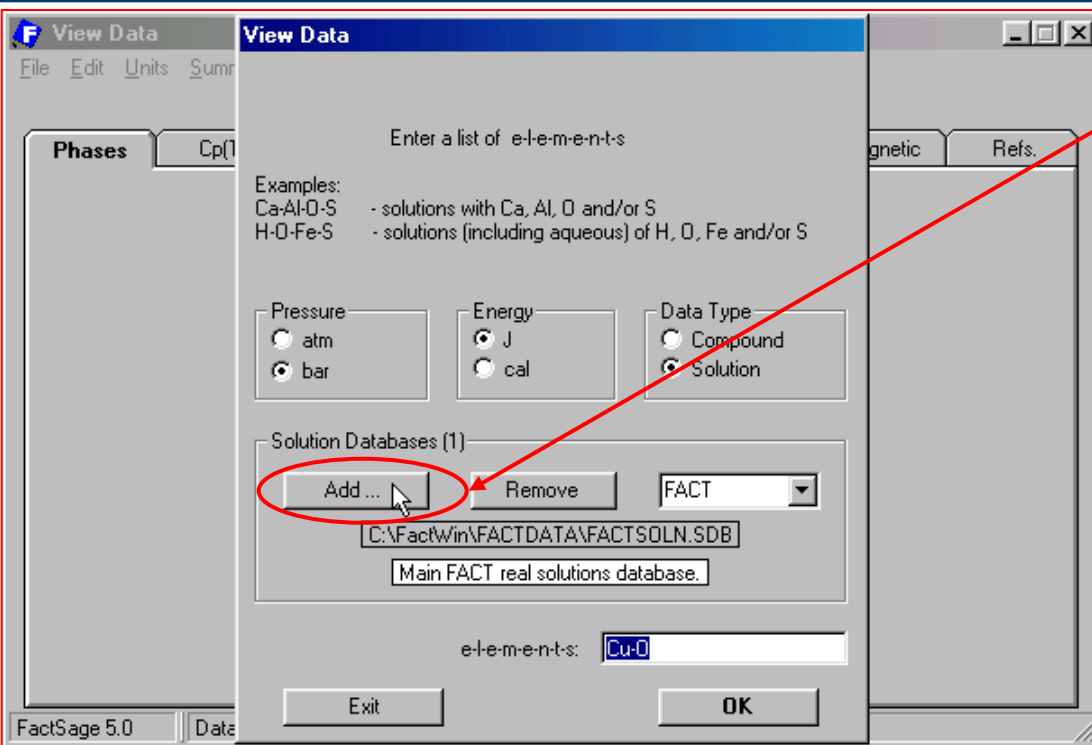
The full name of the Main **FACT** real solutions database appears in the Status Bar:
[C:\FactWin\FACTDATA\FACTSOLN.SDB].

The 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.

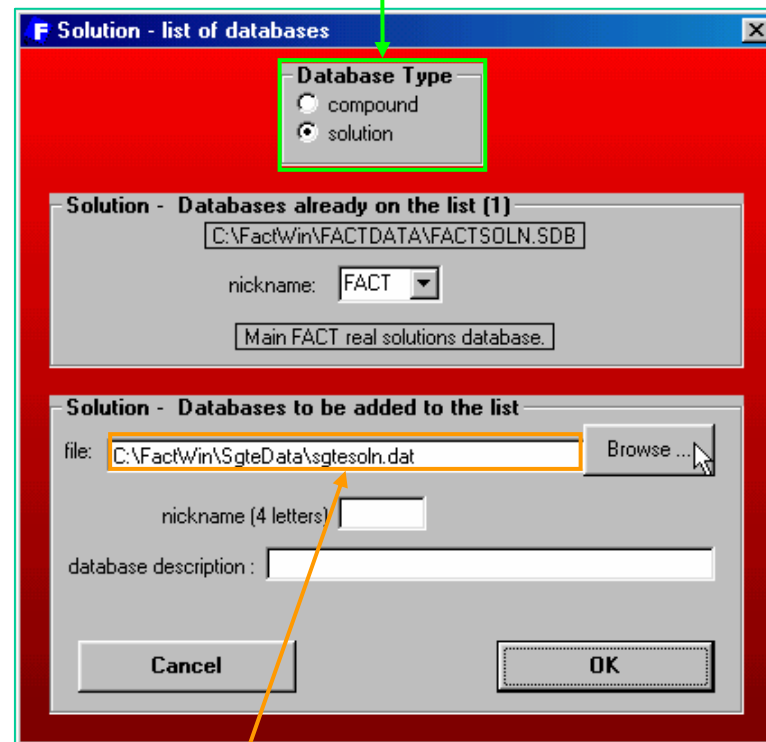
NOTE: The additionally linked databases are also available for use in other modules. Thus View Data can be considered a general entry point for databases.

Adding a solution database to the list

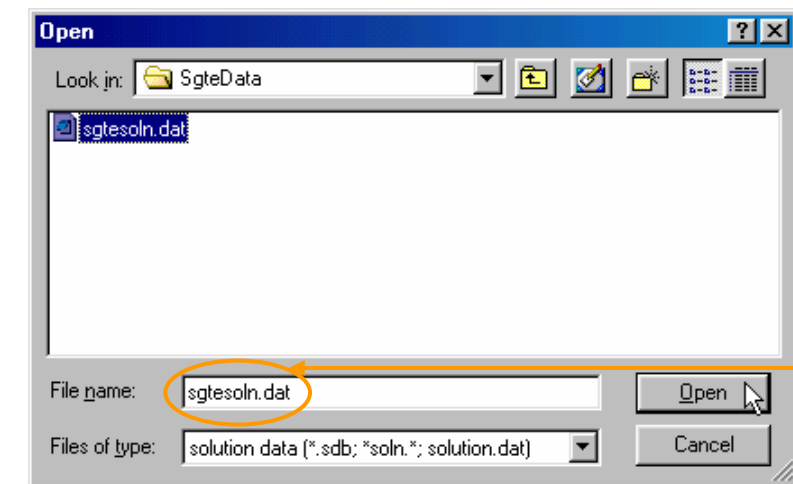


1. Press « Add... » button in the Solution Databases (1) frame.

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)

Solution - list of databases

Database Type
 compound
 solution

Solution - Databases already on the list (1)
C:\FactWin\FACTDATA\FACTSOLN.SDB
nickname: FACT
Main FACT real solutions database.

Solution - Databases to be added to the list
file: C:\FactWin\SgteData\sgtesoln.dat
nickname (4 letters) SGTE
database description: SGTE solution database.

Cancel OK

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

View Data

Enter a list of e-l-e-m-e-n-t-s

Examples:
Ca-Al-O-S - solutions with Ca, Al, O and/or S
H-O-Fe-S - solutions (including aqueous) of H, O, Fe and/or S

Pressure
 atm
 bar

Energy
 J
 cal

Data Type
 Compound
 Solution

Solution Databases (2)
Add ... Remove SGTE
C:\FactWin\SgteData\sgtesoln.dat
FACT
SGTE
All databases
SGTE solution database.

e-l-e-m-e-n-t-s: Cu-Fe-S

Exit OK

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

Data in 2 or more solution databases

« All Databases »

View Data

Enter a list of e-l-e-m-e-n-t-s

Examples:
 Ca-Al-O-S - solutions with Ca, Al, O and/or S
 H-O-Fe-S - solutions (including aqueous) of H, O, Fe and/or S

Pressure: atm bar
 Energy: J cal
 Data Type: Compound Solution

Solution Databases (2):
 Add ... Remove **All Databases** (dropdown)
 All Databases
 - 2 Solution Databases

e-l-e-m-e-n-t-s: Cu-Fe-S

Exit OK

F Cu-Fe-S - solution datasets

File Edit Units Summary Databases Table Graph Help

10 Solutions (highlighted)

Solution	Data	Information
FACT-FES	FACT	FeS-liq (solvent) with Fe, FeO, MgS, MnS, TiS & Na2S Valid only for FeS - rich compositions.
	Fe	
	FeS	0.30 > X > 1.0
FACT-FELQ	FACT	Fe-liq steel with solutes Ag, Al, B, C, Ca, Ce, Co, Cr, Cu, H, La, Mn, Mo, N, Nb, Ni, O, P, Pb, Pd, S, Si, Sn, Ta, Ti, U, V, W and Zr
	Fe	
	Cu	0.0 < X < 0.10
	S	0.0 < X < 0.10
FACT-CULQ	FACT	Cu-liq or speiss (presence of Cu not essential.) <50 mol% As, <15 mol% S (300-1300 C). <10 mol% O in Cu-Pb (good around
	Cu	
	Fe	0.0 < X < 0.50
	S	0.0 < X < 0.18
FACT-MATT	FACT	Matte S-Cu-Fe-Ni-Co-Pb-Zn-As; < 10 mol% As, 30 - 60 mol% S. Do not use for calculation of equilibria with solid sulphide phases.
	S	0.20 > X > 1.0
	Fe	
	Cu	
SGTE-1	SGTE	FCC_A1 This is also the MC(1-x) carbide or nitride!
	Cu1Va1	
	Fe1Va1	
	S1Va1	
SGTE-2	SGTE	BCC_A2
	Cu1Va3	
	Fe1Va3	
	S1Va3	
SGTE-3	SGTE	HCP_A3 This is also the M2C carbide and M2N nitride!
	Cu	
	Fe	
SGTE-13	SGTE	LIQUID
	Cu1Va1	
	Fe1Va1	
	S1Va1	
SGTE-62	SGTE	B2_BCC This is B2 ordered BCC!
	Cu1Cu1Va6	
	Cu1Fe1Va6	
	Fe1Cu1Va6	
	Fe1Fe1Va6	
SGTE-101	SGTE	B2_BCC BCC_A2 This is B2 ordered BCC!
	Cu1Cu1Va6	
	Cu1Fe1Va6	
	Fe1Cu1Va6	
	Fe1Fe1Va6	

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