The *Reaction* module

Use *Reaction* to calculate the thermochemical properties of a species or a chemical reaction.

Reaction accesses only compound type databases.

Note that *Reaction* assumes all gases to be ideal and ignores expansivities and compressibilities of solids and liquids.

Table of contents

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

The *Reaction* module

Click on *Reaction* in the main *FactSage* window.

The simplest possible application of the **Reaction** module is the calculation of thermodynamic properties of a pure substance.

In order to do that the input in the Reactants window is not a balanced reaction but a single line with one substance name.

The properties of this substance are calculated as a function of temperature depending upon the choice of the phase state given in the Reactants window. If a particular phase state is chosen, the properties of this phase are calculated, if the option most stable is used, the phase state that corresponds to the temperature that is used in the calculation is chosen.

A graph is given which shows the Gibbs energy minimum principle in order to determine the most stable state.

Reactants window **-** entry of a species

Add a Product

Add a Reactant

Open

New Reaction

Reaction has two windows – **Reactants** and **Table**

Entry of reactant species

Compound databases available

Go to the Table window

Table window – calculating thermodynamic properties of a species

Open

Save

New Reaction

Stop Calculation

F Table Reaction

File Units Output Figure Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

Summary of the **Reactants** window entry

Cu
(T)

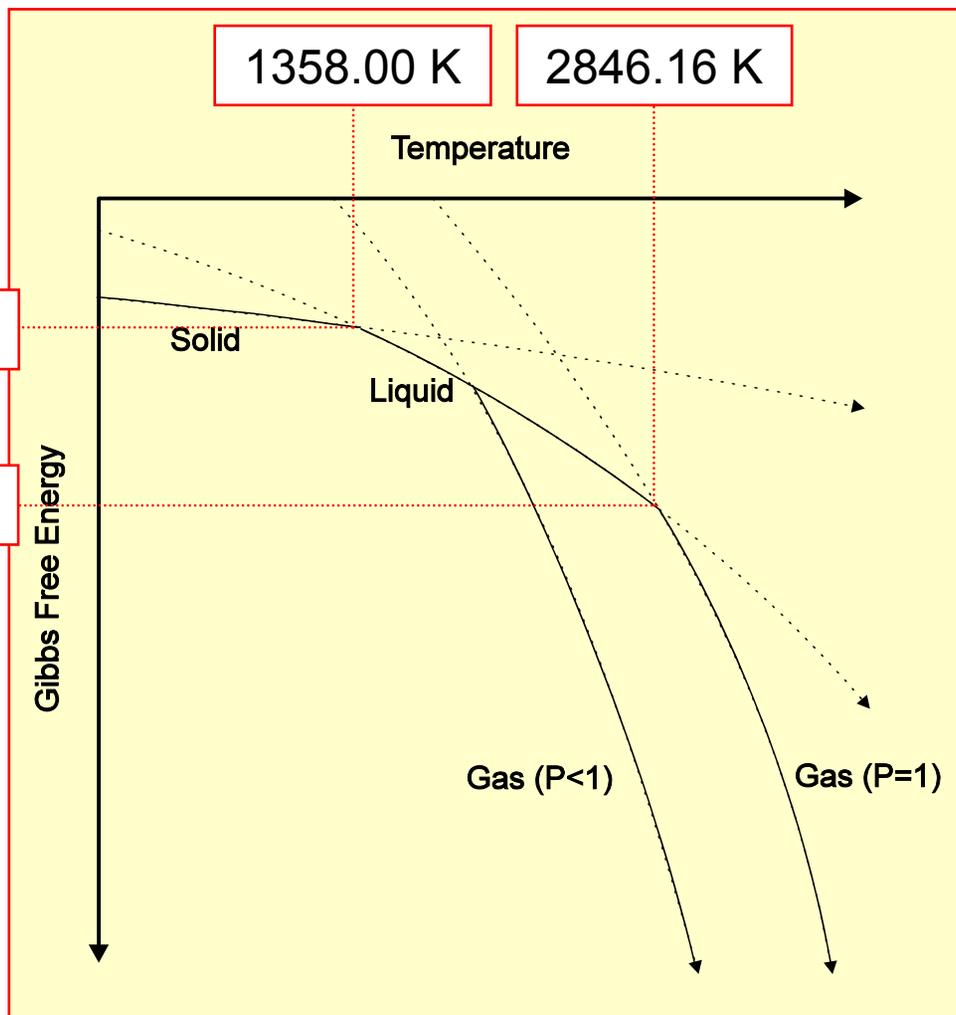| T(K)	H(J)	G(J)	Vol(l)	S(J/K)	Cp(J/K)	A (J)	T
------	Cu(s)	------					
300.00	45.3	-9949.3	7.1240E-03	33.315	24.468	-9950.1	
800.00	13120.4	-33868.0	7.1240E-03	58.736	27.481	-33868.8	
1300.00	27758.9	-66968.6	7.1240E-03	72.867	32.201	-66969.4	
1358.00	29659.9	-71236.5	7.1240E-03	74.298	33.362	-71237.2	
------	Cu(l)	------					
Cu(1 mol):	DH = 13138.0	DG = 0	------	DS = 9.674			
1358.00	42797.9	-71236.5	7.1240E-03	83.972	32.844	-71237.2	
1800.00	57314.9	-110493.4	7.1240E-03	93.227	32.844	-110494.1	
2300.00	73736.9	-159201.7	7.1240E-03	101.278	32.844	-159202.4	
2800.00	90158.9	-211508.6	7.1240E-03	107.738	32.844	-211509.4	
2846.16	91675.0	-216494.2	7.1240E-03	108.275	32.844	-216494.9	
------	Cu(g)	------					
Cu(1 mol):	DH = 300653.1	DG = 0	------	DS = 105.635			
2846.16	392328.1	-216494.2	2.3355E+02	213.910	24.400	-240158.6	
3300.00	403914.1	-314439.8	2.7079E+02	217.683	26.675	-341877.7	

`300 3300 500`

Calculate

<< Back

Clear

A multiple entry for **T**: **min**, **max** and **step**. This results in the computation of the **transition temperatures**.

Return to the **Reactants** window

Determination of most stable phase by **Gibbs energy minimization**

Phase with **lowest** Gibbs energy is the **most** stable.

1358.00 K   2846.16 K

Temperature

-71236.5 J

Solid

Liquid

-216494.2 J

Gibbs Free Energy

Gas (P<1)   Gas (P=1)

Points on the solid lines for **P = 1 atm** are given in column «**T**» and «**G**» of the previous figure for copper.

fact*Sage*™

Isothermal standard state reactions (oxidation of copper)

The classical use of the *Reaction* module is the determination of the isothermal reaction properties of a stoichiometric reaction.

From the names of the reactants and products as well as their respective stoichiometric coefficients it is possible to calculate from the data stored in a *Compound* type database the values for ΔH, ΔS, ΔG, ΔV, ΔA and K (the equilibrium constant) as functions of temperature.

The results are shown in a table (but can also be plotted using the *Figure* module, see Figure Help, section 8).

As an example the reaction $4\ Cu + O_2 = 2\ Cu_2O$ is used.

Simple isothermal standard state reaction: **oxidation of copper**

> Entry of an isothermal standard state reaction: **4 Cu + O$_2$ = 2 Cu$_2$O**

An alternative way to enter this data is from the **Slide Show Examples Directory**. Go to the **menu bar** and click on: **File** > **Directories…** > **Slide Show Examples** and **double-click** on a file.

Isothermal means same "**T**" throughout

Non-standard states checkbox is **not** selected

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Oxidation of copper at **various temperatures**

Entry: T_{min}=**300K**, T_{max}=**2000K** and **step=300K.** Note the **transition temperatures**.

F Table Reaction   _ ☐ ✕

File   Units   Output   Figure   Help

☐ 🖿 🖫   ⊗   T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

```
4 Cu  +  O2  =   2 Cu2O
 (T)         (T)          (T)
```

T(K)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Keq	T
------	Cu(s)	O2(g)	Cu2O(s)	------			
300.00	-341417.7	-295521.9	-2.4598E+01	-152.986	-1.922	2.8421E+51	
600.00	-339925.3	-249958.6	-4.9215E+01	-149.945	8.923	5.7581E+21	
900.00	-336636.3	-205643.5	-7.3833E+01	-145.548	12.414	8.6087E+11	
1200.00	-332624.3	-162561.9	-9.8450E+01	-141.719	14.604	1.1911E+07	
1358.00	-330450.9	-140311.2	-1.1142E+02	-140.015	12.551	2.4937E+05	
------	Cu(l)	O2(g)	Cu2O(s)	------			
Cu(1 mol):	DH = 13138.0	DG = 0	------	DS = 9.675			
1358.00	-383002.9	-140311.2	-1.1142E+02	-178.713	14.623	2.4937E+05	
1500.00	-380261.0	-115060.9	-1.2307E+02	-176.800	24.076	1.0155E+04	
1516.70	-379849.5	-112110.6	-1.2444E+02	-176.527	25.211	7.2603E+03	
------	Cu(l)	O2(g)	Cu2O(l)	------			
Cu2O(1 mol):	DH = 64768.0	DG = 0	------	DS = 42.703			
1516.70	-250313.5	-112110.6	-1.2444E+02	-91.121	31.880	7.2603E+03	
1800.00	-241381.7	-87085.7	-1.4768E+02	-85.720	31.181	3.3659E+02	
2000.00	-235193.2	-70274.4	-1.6410E+02	-82.459	30.706	6.8444E+01	

300 2000 300

[Calculate]   [<< Back]   [Clear]

The equilibrium constant column appears for an **isothermal** standard state reaction.
Note: $\Delta G^o = -RT \ln K$. (For the values of the gas constant R, click on the **Units** menu)

Using non-standard states in equilibrium reaction

A more advanced application of the ***Reaction*** module is the use of non-standard states for the reactants and/or products of a reaction.

This option permits to fix certain activities or partial pressures of the species and to resolve the equation $\Delta G° = -RT \ln K_{eq}$ for a suitable variable.

It is for example possible to fix all activites/partial pressures of the reactants and products and thus fix K, set the equilibrium condition $\Delta G=0$ and then resolve for the temperature that fits the fixed value of K.

Simple chemical equilibrium: **non standard state** oxidation of copper

Reaction   5.1

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Specifying an extensive property change to deal with chemical equilibrium

For simple chemical equilibrium: $\Delta G = \Delta G^0 + RT \ln\left(\dfrac{a_{Cu_2O}^2}{a_{Cu}^4 \cdot P_{O_2}}\right)$ and $\Delta G^0 = -RT \ln K_{eq}$

Table provides ΔG using: $\Delta G = \Delta G^0 + RT \ln\left(\dfrac{1}{X^4 \cdot P}\right)$ and $K_{eq} = \dfrac{1}{X^4 \cdot P}$ when $\Delta G = 0$.

Table Reaction

File Units Output Figure Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

4 Cu	+	O2	=	2 Cu2O
(T,s,X)		(T,P,g)		(T,s)

T(K)	P(atm)	Activity X	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	T
1000.00	1.0000E+00	1.0000E+00	-335381.1	-191155.7	-8.2039E+01	-144.225	
1000.00	1.0359E-10	1.0000E+00	-335381.1	0.0	-7.9216E+11	-335.381	
1000.00	1.0000E+00	3.1903E-03	-335381.1	0.0	-8.2039E+01	-335.381	
897.01	1.0000E-12	1.0000E+00	-336673.3	0.0	-7.3607E+13	-375.327	T

1e-12   1   0

Calculate   << Back   Clear

Specify 3 variables.

For the last entry:
- $P_{O_{2}(g)} = 10^{-12}$
- $a_{Cu(s)} = 1$
- $\Delta G = 0$, equilibrium

A further use of the *Reaction* module lies in the calculation of non-isothermal non-equilibrium balances of the extensive property changes ΔH, ΔS, ΔG, ΔV, ΔF for a given reaction.

It is assumed that this reaction does not represent an equilibrium but a complete transition from the reactants to the products. Under this condition it is possible to attribute the reactants one temperature and the products another.

Thus the above mentioned extensive property changes from one state (reactants at reactant temperature) to the other (products at product temperature) can be calculated using data from a *Compound* type database.

As an example the heating of Al is demonstrated by use of the reaction Al(300K) = Al(T).

Heating **Al** from **300 K** to the temperature **T**

phase transition, $Al_{(s)} \rightarrow Al_{(l)}$
(i.e. *fusion*) at 933.45 K

$$\Delta H°_{fusion} = T_{fusion} \cdot \Delta S°_{fusion}$$
$$= 28649.1J - 17938.1J$$
$$= 10711.0 \ J$$

Reactants - Reaction

File Edit Units Data Search Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
1	Al	most stable	300	1.0	1.0	
= 1	Al	most stable	T	1.0	1.0	

☐ non standard states

Next >>

FactSage 5.1   Compound: FACT   ELEM   SGPS   SGSL

Table Reaction

File Units Output Figure Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

Al   = Al
(300K)   (T)

T(K)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Delta A (J)	T
------	Al(s)	Al(s)	------			
300.00	0.0	0.0	0.0000E+00	0.000	0.000	0.0
400.00	2508.7	-3216.4	0.0000E+00	7.207	1.533	-3216.4
500.00	5141.0	-7082.0	0.0000E+00	13.076	2.594	-7082.0
600.00	7876.6	-11487.3	0.0000E+00	18.061	3.644	-11487.3
700.00	10724.5	-16359.3	0.0000E+00	22.448	4.858	-16359.3
800.00	13705.6	-21648.4	0.0000E+00	26.427	6.317	-21648.4
900.00	16846.7	-27320.4	0.0000E+00	30.125	8.061	-27320.4
933.45	17938.1	-29298.8	0.0000E+00	31.315	8.711	-29298.8
------	Al(s)	Al(l)	------			
Al(1 mol):	DH = 10711.0	DG = 0	------	DS = 11.475		
933.45	28649.1	-29298.8	0.0000E+00	42.790	7.505	-29298.8
1000.00	30762.2	-34111.8	0.0000E+00	44.977	7.505	-34111.8
1100.00	33937.3	-41605.6	0.0000E+00	48.003	7.505	-41605.6
1200.00	37112.4	-49388.5	0.0000E+00	50.765	7.505	-49388.5
1300.00	40287.5	-57436.3	0.0000E+00	53.307	7.505	-57436.3

300 1300 100

Calculate   << Back   Clear

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Heating **Al**: setting the graphical display with *Figure*

Heating **Al**: a few thermodynamic considerations

$$\Delta H_T = \int_{300}^{933} C_p(solid)\, dT + \Delta H_{fusion}^0 + \int_{933}^{T} C_p(liquid)\, dT$$

liquid

$$\Delta H_{fusion}^o = 10711.0 \text{ J}$$

17.9 kJ

Point the mouse to read the coordinates of the melting point.

solid

$$\Delta H_T = \int_{300}^{T} C_p(solid)\, dT$$

933 K
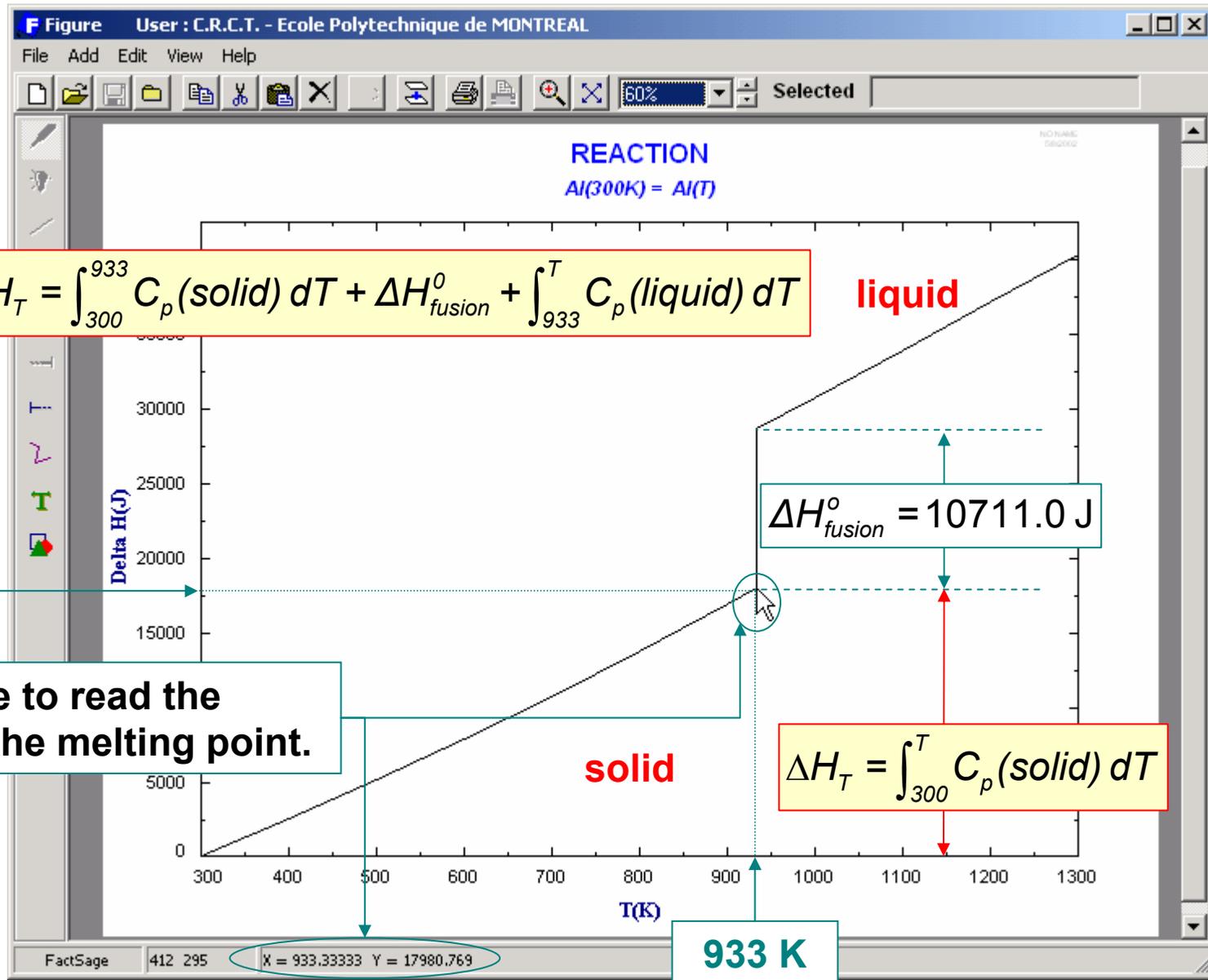
An thermodynamically more advanced application of the ***Reaction*** module is its use in the calculation of the equilibrium of pure solid with its liquid under the assumption that this liquid is dissolved in a solvent (some other liquid which is not explicitely given) under the condition of ideal mixing.

This situation is reflected in an equilibrium of the type:

Me(pure solid,T) = Me (liquid,a(Me) = x(Me),T)

In the example Cu is used. A graph for the phase boundary of the ideal liquid in equilibrium with the pure solid is given.

Computation of Cu **liquidus** in an ideal binary system: **data entry**

Cu(solid) **= Cu**(liquid)

$a_{Cu(solid)}$ **= 1**, pure solid copper

$a_{Cu(liquid)}$ **= X**

Your choice of phases:
- **liquid** phase from the *FACT* database;
- **2 compound databases** are included in your data search.

Computation of Cu **liquidus** in an ideal binary system: **database entry**

2. Follow the instructions if you want to **include** or **exclude** a **database** in the **data search**.

1. To connect databases, click on the **Data Search** menu, select **Databases…** to open the Databases dialog box.

3. Follow the instructions if you want to **add** or **remove** (and this does not delete) a **database** from your **list**.

Reaction   **7.2**

Computation of Cu **liquidus** in an **ideal binary system**: tabular and graphical output

Calculated activity of **Cu**(liquid) in **equilibrium (△G=0)** with pure **Cu**(solid) at **various temperatures T**.

Table Reaction

File Units Output Figure Help

T(K) P(atm)

Reactants

Cu =
(T,s-FACT)   (T

T(K)	Activity X	Delta H(J)	Delta G(J)
300.00	2.3836E-02	11856.1	0.0
375.00	6.1674E-02	11857.4	0.0
450.00	1.1625E-01	11857.4	0.0
525.00	1.8280E-01	11855.7	0.0
600.00	2.5669E-01	11854.3	0.0
675.00	3.3426E-01	11854.5	0.0
750.00	4.1288E-01	11856.1	0.0
825.00	4.9078E-01	11858.2	0.0
900.00	5.6684E-01	11858.8	0.0
975.00	6.4144E-01	12200.3	0.0
1050.00	7.1519E-01	12503.8	0.0
1125.00	7.8763E-01	12766.1	0.0
1200.00	8.5840E-01	12979.5	0.0
1275.00	9.2706E-01	13112.0	0.0
1350.00	9.9313E-01	13141.5	0.0

300 1350 75   0

Calculate   Specify 2 variables.   < Back
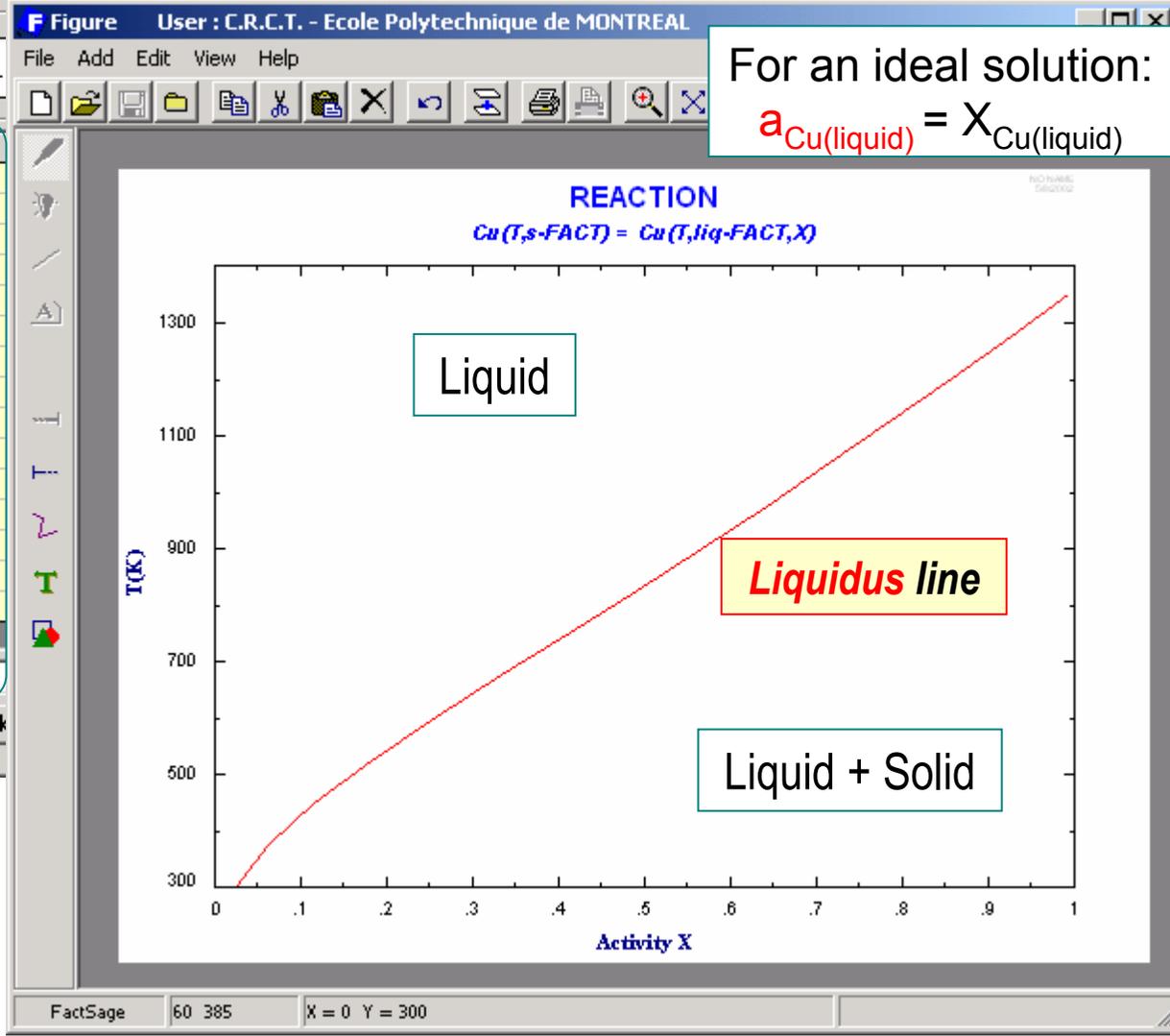
The 2 specified variables, **T** and **△G**, are highlighted.

Note: When **△G = 0**, the reaction must be isothermal.

Figure   User : C.R.C.T. - Ecole Polytechnique de MONTREAL

File Add Edit View Help

For an ideal solution:
$$a_{Cu(liquid)} = X_{Cu(liquid)}$$

REACTION
Cu (T,s-FACT) = Cu (T,liq-FACT,X)

Liquid

Liquidus line

Liquid + Solid

T(K) vs Activity X graph

FactSage   60 385   X = 0 Y = 300

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The following example shows how a variable amount for a reactant can be used to simulate an excess of this substance, i.e. its appearance both among the reactants and the products.

As an example the combustion reaction

$$CH_4 + (2 + \textbf{\textit{excess}}) \, O_2 = CO_2 + 2 \, H_2O + (\textbf{\textit{excess}}) \, O_2$$

is used. The **A**lpha variable is introduced to handle the **excess** amount.

In the example is also shown how the **autobalance feature** can be used to generate stoichiometric coefficient that satisfy the mass-balances automatically.

Combustion of methane in excess **<Alpha>** O_2 – data entry

The **reactants** are at **298 K** but the **products** are at an unspecified **T**.

Variable quantity
<Alpha>

The **phase** of each species is specified.

The reaction is **non-isothermal** (except when T = 298 K). Hence:
- K_{eq} will not appear as a column in the **Table** window.
- Setting Δ**G = 0** is meaningless (except when product T = 298 K).

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Combustion of methane in excess **<Alpha>** O_2 – **adiabatic** reactions

Stoichiometric reaction (A = 2):
$CH_4 + 2 O_2 = CO_2 + 2 H_2O$

Reaction with *excess* O_2 (A > 2):
$CH_4 + (2 + excess) O_2 = CO_2 + 2 H_2O + (excess) O_2$

Exothermic reaction

F Table Reaction

File Units Output Figure Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

$$CH4 + \langle A \rangle \; O2 = CO2 + 2\,H2O + \langle A-2 \rangle \; O2$$
(298K,g)　　(298K,g)　　(T,g)　　(T,g)　　(T,g)

<A>	T(K)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	T
2.0000	298.00	-802318.5	-800835.2	0.0000E+00	-4.978	9.923	
8.0000	298.00	-802318.5	-800835.2	0.0000E+00	-4.978	9.923	
2.0000	2000.00	-565283.1	-2064845.8	4.1899E+02	242.441	68.308	
8.0000	2000.00	-210211.4	-4566836.7	1.2570E+03	624.126	118.504	
8.0000	2530.20	0.0	-5891566.4	1.6485E+03	717.294	132.503	T
8.1553	2500.00	0.0	-5900779.7	1.6543E+03	723.662	133.274	
10.0000	2196.28	0.0	-5991619.2	1.7135E+03	795.161	141.768	T

Adiabatic reaction: $\Delta H = 0$

Product flame temperature

As **<A>** increases, the flame temperature decreases.
Energy is required to heat the ***excess*** O_2.

| 10 | | 0 | | | | | |

Calculate　　　　<< Back　　　　Clear

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Heating the products of the methane combustion. *Reaction* «auto-balance» feature

Step wise **heat balance** in treating methane combustion

Table Reaction

File   Units   Output   Figure   Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

CH4   +   <A> O2   =   CO2   +   2 H2O   +   <A-2> O2
(298K,g)   (298K,g)   (T,g)   (T,g)   (T,g)

<A>	T(K)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	T
2.0000	298.00	-802318.5	-800835.2	0.0000E+00	-4.978	9.923	
8.0000	298.00	-802318.5	-800835.2	0.0000E+00	-4.978	9.923	
2.0000	2000.00	-565283.1	-2064845.8	4.1899E+02	242.441	68.308	
8.0000	2000.00	-210211.4	-4566836.7	1.2570E+03	624.126	118.504	
8.0000	2530.20						
8.1553	2500.00						
10.0000	2196.28						

Different thermodynamic paths, **same** variation of **extensive** properties (here Δ**H**).

2000 K

Overall Process ΔH = - 210211.4 J

Warming Products ΔH = + 592107.1 J

298 K

Isothermal Reaction
Heat ΔH = **- 802318.5 J**
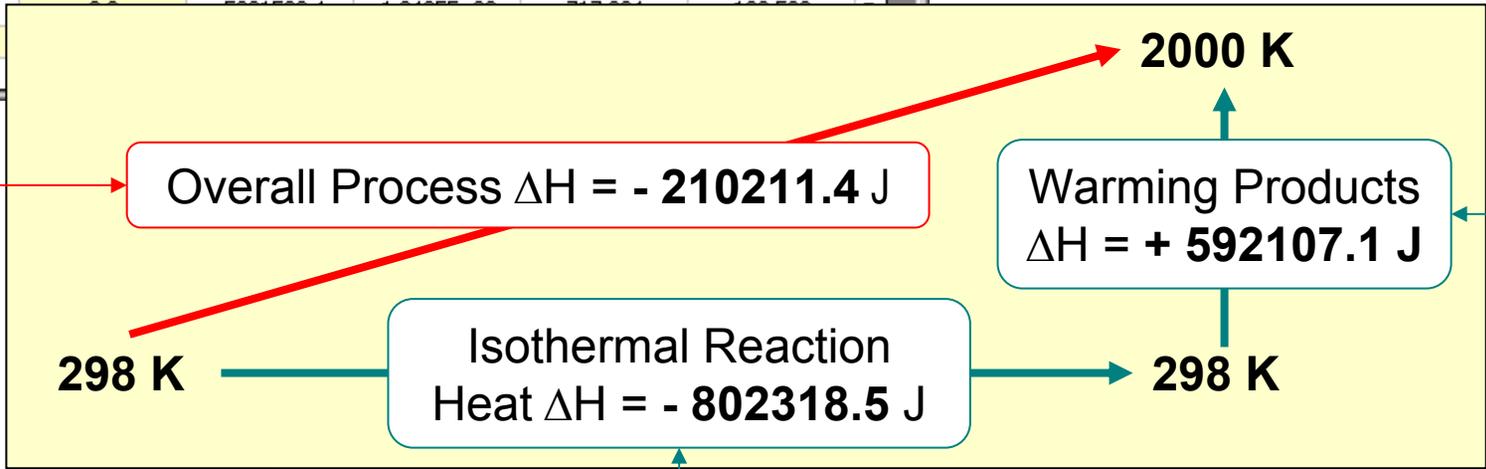
298 K

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

CO2   +   2 H2O   +   6 O2   =   CO2   +   2 H2O   +   6 O2
(298K,g)   (298K,g)   (298K,g)   (T,g)   (T,g)   (T,g)

T(K)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Delta A (J)	T
2000.00	592107.1	-3766001.5	1.2570E+03	629.104	108.581	-3893363.2	
2530.20	802320.1	-5090741.2	1.6485E+03	722.272	122.580	-5257778.0	

The following five slides show how various aspects of the Pidgeon process (production of Mg vapor from MgO in a redox reaction with Si) can be treated using reaction thermochemistry.

Pidgeon Process for the Production of Magnesium

Apparatus Schema:

Equilibrium **Mg partial pressure** developed at the hot end of the retort

Radiation Baffles

Ni-Cr Alloy Retort

Mg (Ca) O + Fe - Si

heated to **1423 K** for Mg reduction

Water-cooled vacuum connection also condenses alkalis

Mg condensed on removable sleeve
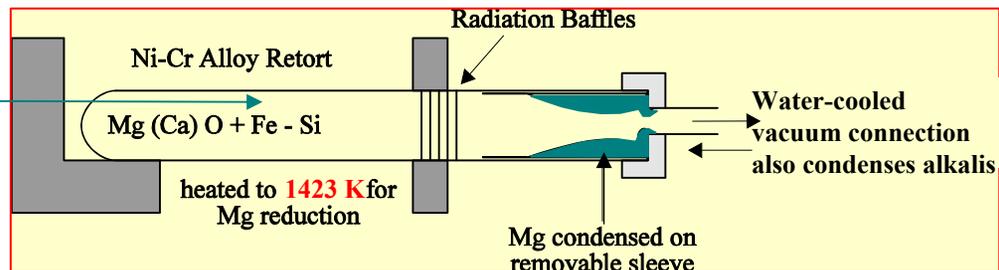
MgO-SiO$_2$ phase diagram:

Note: MgO(s) and SiO$_2$(s) can **not** coexist.

MgO-SiO$_2$

Periclase & Liquid   1850°

Liquid

Two Liquids   1695°

Periclase & Fosterite

Liquid

Cristobalite & Liquid

Cristobalite & Liquid

Liquid & Fosterite

Clinoenstatite & Liquid

1557°

1543°

Fosterite & Clinoenstatite

Clinoenstatite & Cristobalite

Temperature (°C)

0   20   40   60   80   100
MgO   (MgO)$_2$•SiO$_2$ SiO$_2$

Weight Percentage

Pidgeon Process for the Production of Magnesium: **Data Entry**

In the reaction, the hydrostatic pressure above the condensed phases: MgO(s), Si(s) and SiO$_2$(s2) is 1 atm – i.e. has no effect.

The reaction is **isothermal** (same "*T*" throughout), hence $\Delta G = 0$ gives equilibrium.

F Reactants - Reaction

File   Edit   Units   Data Search   Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

	Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
	2	MgO	solid periclase	T	1.0	1.0	
+	1	Si	solid	T	1.0	1.0	
=	2	Mg	gas	T	P	1.0	
+	1	SiO2	solid-2 quartz(h)	T	1.0	X	

The activity of SiO$_2$ is: $a_{SiO_2} = X$.

** For a gas species, P(atm/bar/psi) is its ideal partial pressure.
For a liquid or solid, P is the hydrostatic pressure above the phase
- molar volume (but not compressibility) data are employed in the 'VdP' term

☑ non standard states

The partial pressure of Mg$_{(g)}$ is: $P_{Mg_{(g)}} = P$ atm.

Next >>

FactSage 5.1   Compound: FACT   ELEM   SGPS   SGSL

Allotrope s2(solid-2) has been selected for **SiO$_2$** in order to fully specify the phase – **if the phase is not completely specified, equilibrium calculations ($\Delta G = 0$) can not be performed**.

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Note: There are an infinite number of values of ($P_{Mg(g)}$, $a_{SiO_2(s2)}$) which satisfy K_{eq} . Here we select 3 special cases.

Standard state reaction at **1423 K**: $P_{Mg\ eq}$ = **1 atm** and $a_{SiO_2(s2)}$ = **1**
$\Delta G° $ = 221.39 kJ = $-RT \ln K_{eq}$, hence K_{eq} = 7.4723 × 10^{-9} $\Delta G°$ > 0 but Mg can be produced by reducing $P_{Mg(g)}$ and/or a_{SiO_2}.

F Table Reaction

File   Units   Output   Figure   Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

2 MgO	+	Si	=	2 Mg	+	SiO2
(T,s)		(T,s)		(T,P,g)		(T,s2X)

T(K)	P(atm)	Activity X	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	T
1423.00	1.0000E+00	1.0000E+00	570269.4	221392.6	2.3352E+02	245.170	
1423.00	1.0000E+00	7.4723E-09	570269.4	0.0	2.3352E+02	400.751	
1423.00	8.6443E-05	1.0000E+00	570269.4	0.0	2.7016E+06	400.751	
1423.00	1.0876E-03	6.3170E-03	570269.4	0.0	2.1472E+05	400.751	

At equilibrium(ΔG=0), when $a_{SiO_2(s2)}$=**1.0** and T=**1423 K**, $P_{Mg\ eq}$=**8.6443 × 10^{-5}** atm

At equilibrium(ΔG=0), when $P_{Mg\ eq}$=**1atm** and T=**1423 K**, $a_{SiO_2(s2)\ eq}$=**7.4723 × 10^{-9}**

When ΔG=0, T=**1423 K** and $a_{SiO_2(s2)}$=**0.006317** then $P_{Mg(g)\ eq}$=**1.0876 × 10^{-3} atm**. This value of $a_{SiO_2(s2)}$ is taken from the next page calculation.

Computation of SiO₂ activity when MgO coexists with (MgO)₂•SiO₂

Pure MgO

Pure (MgO)₂•SiO₂

SiO₂(s2) at activity **X**

MgO-SiO₂

Gives the equilibrium value of the **activity of SiO₂(s2)** at 1423 K: **a_SiO₂(s2)=0.006317**

Isothermal…

…and at equilibrium

Alternative way to calculate equilibrium **Mg partial pressure**

Remember, $\Delta G = 0$ (equilibrium) calculations are only meaningful for **isothermal** reactions (**«T»** throughout).

Reactants – Reaction

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T(K) P(atm) Energy

Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
4	MgO	solid periclase	T	1	1.0	
+ 1	Si	solid	T	1	1.0	
= 2	Mg	gas	T	P	1.0	
+ 1	Mg2SiO4	solid-1 forsterite	T	1	1.0	

** For a gas species, P(atm/ba
For a liquid or solid, P is the hydr
- molar volume (but not compressibilit

☑ non standard states

Table Reaction

File Units Output Figure Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

$$4\ MgO\ +\ Si\ =\ 2\ Mg\ +\ Mg2SiO4$$
$$(T,s)\quad (T,s)\quad (T,P,g)\quad (T,s1)$$

T(K)	P(atm)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	T
1423.00	1.0876E-03	506709.7	0.0	2.1472E+05	356.086	-12.832	

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FactSage 5.1   Compound: FACT   ELEM   SGPS   SGSL

Magnesium production is enhanced by:
- reducing the total pressure (**<0.0010876 atm**);
- reducing a_{SiO_2} – this is done automatically due to $(MgO)_2 SiO_2$ formation, but the addition of say CaO (slag formation) reduces a_{SiO_2} further.

Aqueous applications

In the following two slides examples are given for the use of the **Reaction** module in aqueous thermochemistry.

It should be noted however, that ideal behaviour of the aqueous species is assumed since **Reaction** accesses **Compound** type databases. If a system requires non-ideal behaviour of the aqueous phase the **Equilib** module must be used.

Hydrogen reduction of aqueous copper ion - **Reactants** and **Table** windows

Reactants - Reaction

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	Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
	1	Cu^{++}	aqueous	T	1.0	X	
+	1	H2	gas	T	P		1.0
=	1	Cu	solid	T	1.0	1.0	
+	2	H^{+}	aqueous	T	1.0	1.0	

The standard Gibbs energy change underlined yields standard reduction potential of Cu^{2+} when divided by -2 Faradays. (Remember: $\Delta G° = -nFE°$, where **F** (= 96485 C/mol) is the Faraday constant)

The molality of Cu^{2+} is given by "**X**".

$H_2(g)$ pressure is "**P**" atm.

Standard state reaction at **298.15 K**

** For a gas species, P(atm/bar/psi) is its ideal partial pressure.
For a liquid or solid, P is the hydrostatic pressure above the phase
- molar volume (but not compressibility) data are employed in the 'VdP' te

☑ non standard states

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FactSage 5.1   Compound: FACT   ELEM   SGPS   SGSL

Table Reaction

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T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

Cu^{++}	+	H2	=	Cu	+	2 H^{+}
(T,aq1 X)		(T,P,g)		(T,s)		(T,aq)

T(K)	P(atm)	Activity X	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	T
298.15	1.0000E+00	1.0000E+00	-64852.0	-65499.8	-2.4458E+01	2.173	
308.15	1.0000E+00	1.0000E+00	-65088.5	-65517.5	-2.5279E+01	1.392	
318.15	1.0000E+00	1.0000E+00	-65301.1	-65528.0	-2.6100E+01	0.713	
328.15	1.0000E+00	1.0000E+00	-65491.3	-65532.1	-2.6920E+01	0.124	
338.15	1.0000E+00	1.0000E+00	-65660.1	-65530.7	-2.7741E+01	-0.383	
348.15	1.0000E+00	1.0000E+00	-65808.6	-65524.7	-2.8561E+01	-0.816	
358.15	1.0000E+00	1.0000E+00	-65937.8	-65514.6	-2.9382E+01	-1.182	
368.15	1.0000E+00	1.0000E+00	-66048.4	-65501.2	-3.0202E+01	-1.486	
370.00	1.0000E+00	1.0000E+00	-66066.9	-65498.4	-3.0354E+01	-1.536	
315.00	1.0000E+00	1.3633E-11	-65236.6	0.0	-2.5841E+01	-207.100	
315.00	2.0000E+00	6.8163E-12	-65236.6	0.0	-1.2917E+01	-207.100	
315.00	3.0000E+00	4.5442E-12	-65236.6	0.0	-8.6089E+00	-207.100	
315.00	4.0000E+00	3.4081E-12	-65236.6	0.0	-6.4549E+00	-207.100	
315.00	5.0000E+00	2.7265E-12	-65236.6	0.0	-5.1625E+00	-207.100	
315.00	6.0000E+00	2.2721E-12	-65236.6	0.0	-4.3009E+00	-207.100	
315.00	7.0000E+00	1.9475E-12	-65236.6	0.0	-3.6855E+00	-207.100	

| 315 | 1 7 1 | | | 0 | | |

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Standard state reaction at various temperatures

Equilibrium molality at various P_{H_2}

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Reaction   10.1

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Thermal balance for leaching of zinc oxide

The reaction is exothermic: **ΔH < 0**.

This entry calculates the product temperature for an adiabatic reaction: **ΔH = 0**.

The following two slides show how ***Reaction*** is used on a system with polymer formation in the gas phase (Na(l) ↔ Na$_1$ + Na$_2$) and on a pure substance system that is submitted to very high pressure (C).

Computation of **Na** and **Na$_2$ partial pressure** in equilibrium with **liquid Na**

Both reactions are **isothermal**, hence **ΔG=0** gives **equilibrium**.

Reactants – Reaction

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Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
1	Na	liquid	T	1.0	1.0	
= 1	Na	gas	T	P		

$Na_{(l)} \rightarrow \textbf{Na}_{(g)}$ (monomer)

1. Calculate **T** when **P$_{Na}$ = 1 atm**

- molar volume (but not compressibility) data are employed in the 'VdP' term.

☑ non standard states

2. Calculate **P$_{Na}$** when **T = 1158 K**

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Reactants – Reaction

Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
2	Na	liquid	T	1.0	1.0	
= 1	Na2	gas	T	P		

$2\,Na_{(l)} \rightarrow \textbf{Na}_{2(g)}$ (dimer)

** For a gas species, P(atm/bar/psi) is its ideal partial pressure.
For a liquid or solid, P is the hydrostatic pressure above the phase
- molar volume (but not compressibility) data are employed in the 'VdP' term.

☑ non standard states

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FactSage 5.1   Compound: FACT   ELEM   SGPS   SGSL

Table Reaction

File Units Output Figure Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

Na   =   Na
(T,liq)   (T,P,g)

T(K)	P(atm)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	T
1171.80	1.0000E+00	97012.3	0.0	9.6132E+01	82.789	-8.871	T
1158.00	8.8805E-01	97134.3	0.0	1.0698E+02	83.881	-8.802	

3. Calculate **P$_{Na_2}$** when **T=1158 K**

Table Reaction

File Units Output

Reactants

2 Na   =   Na2
(T,liq)   (T,P,g)

T(K)	P(atm)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	T
1158.00	1.1067E-01	119358.8	0.0	8.5854E+02	103.073	-20.353	

Na also forms a gaseous dimer **Na$_2$(g)**. The proportion of **Na$_2$/Na** near the boiling point (**1171.8 K**) of **Na** is: **0.111/0.888** at **1158 K**; and the total vapor pressure over **Na(l)** would be: **P$_{Na}$** + **P$_{Na_2}$** (**0.888 + 0.111 ≅ 1**).

Effect of **high pressure** on the **graphite** to **diamond** transition

Where available, **density** (i.e. molar volume) data for solids and liquids are employed in *REACTION* (the "**VdP**" term) although their effect only becomes significant at high pressures. (However, unlike *EQUILIB*, compressibility and expansivity data are **NOT** employed.)

Reactants - Reaction

File Edit Units Data Search Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

1 - 2

Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
1	C	solid-1 graphite	T	P	1.0	
= 1	C	solid-2 diamond	T	P	1.0	

** For a gas species, P(atm/bar/psi) is its ideal partial pressure.
For a liquid or solid, P is the hydrostatic pressure above the phase
- molar volume (but not compressibility) data are employed in the 'VdP' term.

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FactSage 5.1   Compound: FACT ELEM SGPS SGSL

Here, carbon **density** data are employed to calculate the high pressure required to convert *graphite* to diamond at **1000 K**.

At **1000 K** and **30597 atm**, **graphite** and **diamond** are at equilibrium **(∆G=0)**

Table Reaction

File Units Output Figure Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

$$C = C$$
$$(T,P,s1) \quad (T,P,s2)$$

T(K)	P(atm)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	T
1000.00	1.0000E+04	-574.7	3926.0	-1.8812E-03	-4.501	-0.581	
1000.00	2.0000E+04	-2480.8	2019.9	-1.8812E-03	-4.501	-0.581	
1000.00	3.0000E+04	-4386.9	113.8	-1.8812E-03	-4.501	-0.581	
1000.00	4.0000E+04	-6293.0	-1792.3	-1.8812E-03	-4.501	-0.581	
1000.00	5.0000E+04	-8199.0	-3698.4	-1.8812E-03	-4.501	-0.581	
1000.00	3.0597E+04	-4500.7	0.0	-1.8812E-03	-4.501	-0.581	

The volume of diamond is smaller than graphite. Hence, at high pressures, the "**VdP**" term creates a **favorable negative contribution to the enthalpy change** associated with the **graphite → diamond** transition.

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Reaction   **11.2**

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