ENTHALPY OF FORMATION

ENTHALPY OF FORMATION

Standard enthalpy of formation ($\Delta H_f°$): Also called the standard heat of formation of a substance

Standard heat of formation: The amount of heat absorbed or released when one mole of the substance is formed at 25°C and 100kPa (SATP) from its elements <u>in their standard states</u>

$\Delta H_f°$ units are always in kJ/mol

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Standard heat of formation: The amount of heat absorbed or released when one mole of the substance is formed at 25°C and 100kPa (SATP) from its **elements** <u>in their standard states</u>

Example: What equation represents the formation of nitric acid?

Nitric acid = $HNO_{3(l)}$

Elements: hydrogen nitrogen oxygen

What are these elements in their standard (most common) states?

$$\frac{1}{2} H_{2(g)} + \frac{1}{2} N_{2(g)} + 3/2\ O_{2(g)} \rightarrow HNO_{3(l)}$$

ENTHALPY OF FORMATION

The **$\Delta H_f°$** for elements in their standard states are zero

Table A-6

Thermodynamic Properties (at standard states)

$\Delta H_f°$ in kJ/mol $\Delta G_f°$ in kJ/mol $S°$ in J/mol·K
concentration of aqueous solutions is 1*M*

Substance	$\Delta H_f°$	$\Delta G_f°$	$S°$
Ag	0	0	42.7
AgCl	−127	−110	96.1
AgCN	−146	−164	83.7
Al	0	0	28.3
Al_2O_3	−1670	−1580	51.0
$BaCl_2$(aq)	−873	−823	121
$BaSO_4$	−1470	−1350	132
Be	0	0	9.54
Be_3N_2	−568	−512	—
Bi	0	0	56.9
$BiCl_3$	−379	−319	190
Bi_2S_3	−183	−164	146
Br_2	0	0	152
CH_4	−74.8	−50.8	186
C_2H_4	+52.3	+68.1	219
C_2H_6	−84.7	−32.9	229
C_4H_{10}	−125	−15.7	310
CO	−111	−137	198
CO_2	−393.5	−394.4	214
CS_2	+87.9	+63.6	151
Ca	0	0	41.6
$Ca(OH)_2$	−987	−897	—
Cl_2	0	0	223
$CoCO_3$	−723	−650	—
CoO	−239	−213	43.9
Cr_2O_3	−1130	−1050	81.2
CsCl(aq)	−415	−371	188
Cs_2SO_4(aq)	−1400	−1310	283
CuI	−67.8	−69.5	96.7
CuS	−53.1	−53.7	66.5
Cu_2S	−79.5	−86.2	121
$CuSO_4$	−770	−662	113
F_2	0	0	203
$FeCl_3$	−405	—	—
FeO	−267	—	—
Fe_2O_3	−822	−741	90.0
H	+218	—	115
H_2	0	0	131
HBr	−36.2	−53.2	198
HCl	−92.3	−95.3	187
HCl(aq)	−167	−131	56.5
HCN(aq)	+151	+172	94.1
HF	−269	−271	174
HI	+25.9	+1.30	206
H_2O(l)	−286	−237	70.0
H_2O(g)	−242	−229	189
H_2O_2	—	−118	110
H_3PO_2	−609	—	—
H_3PO_3	−972	—	—
H_3PO_4	−1280	−1120	110
H_2S	−20.1	−33.0	206
H_2SO_3(aq)	−614	−538	232
H_2SO_4(aq)	−908	−742	17.2
$HgCl_2$	−230	−177	—
Hg_2Cl_2	−265	−211	196
Hg_2SO_4	−742	−624	201
I_2	0	0	117
K	0	0	63.6
KBr	−392	−379	96.4
$KMnO_4$	−813	−714	172
KOH	−426	—	—
LiBr	−350	—	—
LiOH	−487	−444	50.2
Mn	0	0	32.0
$MnCl_2$(aq)	−555	−491	38.9
$Mn(NO_3)_2$(aq)	−636	−451	218
MnO_2	−521	−466	53.1
MnS	−214	—	—
N_2	0	0	192
NH_3	−46.2	−16.6	193
NH_4Br	−270	−175	113
NO	+90.4	—	211
NO_2	+33.8	+51.8	240
Na	0	0	51.0
NaBr	−360	—	—
NaCl	−411	−384	72.4
$NaNO_3$(aq)	−447	—	—
NaOH	−427	—	—
Na_2S(aq)	−437	—	—
Na_2SO_4	−1380	−1270	149
O_2	0	0	205
P_4O_6	−1640	—	—
P_4O_{10}	−2980	−2700	229
$PbBr_2$	−277	−260	162
$PbCl_2$	−359	−314	136
S	0	0	31.9
SO_2	−297	−300	249
SO_3	−438	−368	95.6
SrO	−590	−560	54.4
Ti	0	0	30.3
TiO_2	—	−853	50.2
TlI	−50.2	−83.3	236
UCl_4	−1050	−962	198
UCl_5	−1100	−993	259
Zn	0	0	41.6
$ZnCl_2$(aq)	−487	−410	3.72
$ZnSO_4$(aq)	−1063	−892	−92.0

ENTHALPY OF FORMATION

Determine the equations for the formation of:

a) $KBrO_3$

b) C_2H_5OH

c) $NaHCO_3$

Don't forget that the equation must result in the formation of **one** mole of the desired compound.

ENTHALPY OF FORMATION

Now we can assign the $\Delta H°_f$ of the product as the $\Delta H°$ of the whole reaction

$2C_{(s)} + 3H_{2(g)} + 1/2O_{2(g)} \rightarrow C_2H_5OH_{(l)}$ $\Delta H° = -235.2 kJ/mol$

This additional equation may assist solving Hess' Law questions.

ENTHALPY OF FORMATION

How are these equations and $\Delta H°_f$ values useful?

$$CaO_{(s)} + H_2O_{(l)} \rightarrow Ca(OH)_{2(s)}$$

By knowing the $\Delta H°_f$ of each of the chemicals in the above reaction, you can calculate the $\Delta H°$ of the reaction without using thermochemical equations and Hess' Law

ENTHALPY OF FORMATION

$$\Delta H^\circ_f$$

Formation reactions and their ΔH°_f values may be manipulated to determine balanced equation and the ΔH° value of chemical reactions.

$$\Delta H^\circ = \Sigma\Delta H^\circ_{f(products)} - \Sigma\Delta H^\circ_{f(reactants)}$$

Σ = "sum of"

Don't forget that the equations should be multiplied by the appropriate factor, as necessary.

ENTHALPY OF FORMATION

Using $\Delta H°_f$ values, calculate the $\Delta H°$ of combustion of one mole of ethanol to produce carbon dioxide gas and liquid water.

$$C_2H_5OH_{(l)} + 3\ O_{2(g)} \rightarrow 2\ CO_{2(g)} + 3\ H_2O_{(l)}$$

-235.2kJ/mol 0.0000kJ/mol -393.5kJ/mol -285.8kJ/mol

$$\Delta H° = \Sigma\Delta H°_{f(products)} - \Sigma\Delta H°_{f(reactants)}$$

$$= [(2\text{ mol} \times -393.5\text{kJ/mol}) + (3\text{ mol} \times -285.8\text{kJ/mol})] - [(1\text{ mol} \times -235.2\text{kJ/mol}) + (3\text{ mol} \times 0.0000\text{kJ/mol})]$$

$$= -1644.4\text{kJ} - (-235.2\text{kJ})$$

$$= -1409.2\text{kJ}$$

Since this equation already combusts 1 mole of ethanol, then the final answer is:

Therefore the heat of combustion is -1409kJ/mol of ethanol

ENTHALPY OF FORMATION

Using $\Delta H°_f$ values, calculate the $\Delta H°$ for the following reaction:

$$NaOH_{(s)} + HCl_{(g)} \rightarrow NaCl_{(s)} + H_2O_{(l)}$$

-425.6kJ/mol -92.30kJ/mol -411.2kJ/mol -285.8kJ/mol

$\Delta H° = \Sigma\Delta H°_{f(products)} - \Sigma\Delta H°_{f(reactants)}$

$= [(1 \text{ mol} \times -411.2\text{kJ/mol}) + (1 \text{ mol} \times -285.8\text{kJ/mol})] - [(1 \text{ mol} \times -425.6\text{kJ/mol}) + (1 \text{ mol} \times -92.30\text{kJ/mol})]$

$= -697.0\text{kJ} - (-517.9\text{kJ})$

$= -179.1\text{kJ}$

Therefore the heat of the reaction is -179.1kJ

ENTHALPY OF FORMATION

Enthalpy of Combustion:

What is the reaction to produce $C_6H_{12}O_6$?

$$6\ CO_2 + 6\ H_2O \rightarrow 6\ O_2 + C_6H_{12}O_6$$

Where does this naturally occur?

How do we measure it?

In plant chloroplasts; it is not easy to measure.

ENTHALPY OF FORMATION

Enthalpy of Combustion:

$$C_6H_{12}O_6 + 6\ O_2 \rightarrow 6\ CO_2 + 6\ H_2O$$

For complex organics, such as $C_6H_{12}O_6$, it is difficult to directly measure its formation. Instead, the compound is combusted and the products analyzed to determine $\Delta H°_f$ for the original compound.

ENTHALPY OF FORMATION

Enthalpy of Combustion:

$$\Delta H^\circ_c$$

standard heat of combustion - the ΔH° for the combustion of one mole of compound

Ex. $CH_3OH_{(g)} + O_{2(g)} \rightarrow CO_{2(g)} + H_2O_{(l)}$ $\Delta H^\circ_c = -727kJ$

ENTHALPY OF FORMATION

Calculate the $\Delta H°_f$ for C_2H_4.

$$C_2H_{4(g)} + 3\ O_{2(g)} \rightarrow 2\ CO_{2(g)} + 2\ H_2O_{(l)} \quad \Delta H°_c = -1386\ \text{kJ}$$

x　　0.000kJ　　-393.5kJ　　-285.8kJ

$$\Delta H° = \sum\Delta H°_{f(products)} - \sum\Delta H°_{f(reactants)}$$

$$-1386\text{kJ} = [(2\text{ mol} \times -393.5\text{kJ/mol}) + (2\text{ mol} \times -285.8\text{kJ/mol})] - [(1\text{ mol} \times x) + (3\text{ mol} \times 0.000\text{kJ/mol})]$$

$$-1386\text{kJ} = -1358.6\text{kJ} - x$$

$$x = 27.4\text{kJ}$$

Therefore the heat of formation is 27.4kJ/mol

ENTHALPY OF FORMATION

Enthalpy of Combustion:

$C_2H_{4(g)} + 3\ O_{2(g)} \rightarrow 2\ CO_{2(g)} + 2\ H_2O_{(l)} \quad \Delta H°_c = -1386\ kJ$

Calculate the $\Delta H°_f$ for C_2H_4.

$2C_{(s)} + 2H_{2(g)} \rightarrow C_2H_{4(g)} \quad \Delta H_f° = ?$

1 $2\ CO_{2(g)} + 2\ H_2O_{(l)} \rightarrow C_2H_{4(g)} + 3\ O_{2(g)} \quad \Delta H° = +1386\ kJ$

2 $C_{(s)} + O_{2(g)} \rightarrow CO_{2(g)} \quad \Delta H° = -393.5\ kJ$

3 $H_{2(g)} + 1/2O_{2(g)} \rightarrow H_2O_{(l)} \quad \Delta H° = -285.8\ kJ$

ENTHALPY OF FORMATION

Enthalpy of Combustion:

$C_2H_{4(g)} + 3\ O_{2(g)} \rightarrow 2\ CO_{2(g)} + 2\ H_2O_{(l)} \quad \Delta H°_c = -1386\ kJ$

Calculate the $\Delta H°_f$ for C_2H_4.

$2C_{(s)} + 2H_{2(g)} \rightarrow C_2H_{4(g)} \quad \Delta H_f° = ?$

1 $\cancel{2\ CO_{2(g)}} + \cancel{2\ H_2O_{(l)}} \rightarrow C_2H_{4(g)} + \cancel{3\ O_{2(g)}} \quad \Delta H° = +1386\ kJ$

2 x 2 $\quad 2C_{(s)} + \cancel{2O_{2(g)}} \rightarrow \cancel{2CO_{2(g)}} \quad \Delta H° = -787\ kJ$

3 x 2 $\quad 2H_{2(g)} + \cancel{O_{2(g)}} \rightarrow \cancel{2H_2O_{(l)}} \quad \Delta H° = -571.6\ kJ$

$2C_{(s)} + 2H_{2(g)} \rightarrow C_2H_{4(g)} \quad \Delta H_f° = 27.4kJ$

Table 6.2 • Selected Standard Molar Enthalpies of Formation at 298 K

Substance	Name	Standard Molar Enthalpy of Formation (kJ/mol)
C(graphite)	graphite	0
C(diamond)	diamond	+1.8
$CH_4(g)$	methane	−74.87
$C_2H_6(g)$	ethane	−83.85
$C_3H_8(g)$	propane	−104.7
$C_4H_{10}(g)$	butane	−127.1
$C_2H_4(g)$	ethene (ethylene)	+52.47
$CH_3OH(\ell)$	methanol	−238.4
$C_2H_5OH(\ell)$	ethanol	−277.0
$C_{12}H_{22}O_{11}(s)$	sucrose	−2,221.2
CO(g)	carbon monoxide	−110.53
$CO_2(g)$	carbon dioxide	−393.51
$CaCO_3(s)$*	calcium carbonate	−1207.6
CaO(s)	calcium oxide	−635.0
$H_2(g)$	hydrogen	0
HCl(g)	hydrogen chloride	−92.31
HCl(aq)*	hydrochloric acid (1 M)	−167.2