Reactivity 1.2 HL Answers

IB CHEMISTRY HL













Reactivity 1.2.3 and 1.2.4

Understandings:

- Standard enthalpy changes of combustion, ΔH_c , and enthalpy of formation, ΔH_f , data are used in thermodynamic calculations (1.2.3).
- An application of Hess's law uses enthalpy of formation data or enthalpy of combustion data to calculate the enthalpy change (1.2.4).

Learning outcomes:

- Deduce equations and solutions to problems involving these terms (1.2.3).
- Calculate enthalpy changes of a reaction using $\Delta H_{\rm f}$ data or $\Delta H_{\rm c}$ data (1.2.4).
- $\Delta H^{\Theta} = \sum \Delta H_{c}^{\Theta}$ reactants $-\sum \Delta H_{c}^{\Theta}$ products
- $\Delta H^{\Theta} = \sum \Delta H^{\Theta}$ products $-\sum \Delta H^{\Theta}$ reactants

Additional notes:

- Enthalpy of combustion and formation data are given in the data booklet.
- The above equations are given in the data booklet.

Linking questions:

• Structure 2.2 Would you expect allotropes of an element, such as diamond and graphite, to have different ΔH values?

Standard enthalpy change of formation (ΔH_{f}°)

- The standard enthalpy change of formation (ΔH_f^e) is the enthalpy change when one mole of a substance is formed from its elements in their standard states under standard conditions.
- Standard state is the normal, most pure stable state of a substance measured at a pressure of 100 kPa.

Examples:

C(s) + 2H₂(g) → CH₄(g) 2C(s) + 3H₂(g) + $\frac{1}{2}O_2(g) \rightarrow C_2H_5OH(I)$ ΔH_f^Θ = -278 kJ mol⁻¹ Na(s) + $\frac{1}{2}Cl_2(g) \rightarrow NaCl(s)$ ΔH_f^Θ = -411 kJ mol⁻¹

• Note that fractional coefficients are used because the equation is written for the formation of one mole of product.

Exercise: Write equations for the formation of one mole of the following compounds.

- **1.** $C_3H_8(g)$ **3C**(graphite) + $4H_2(g) \rightarrow C_3H_8(g)$
- 2. CH₃OH(I) C_(graphite) + 2H₂(g) + $\frac{1}{2}O_2(g) \rightarrow CH_3OH(I)$
- **3.** MgCl₂(s) Mg(s) + Cl₂(g) \rightarrow MgCl₂(s)

Calculating ΔH for a reaction using ΔH_{f}^{e} values

 $\Delta H^{e} = \sum \Delta H^{e}_{f^{e} \text{ products}} - \sum \Delta H^{e}_{f^{e} \text{ reactants}}$

- $\Delta H_{\rm f}^{\rm o}$ values can be found in table 12 of the data booklet.
- Elements have a standard enthalpy change of formation of zero.

Exercise: Calculate the enthalpy change for each of the reactions below, given the data in the table.

	Δ <i>H</i> f ^e (kJ mol⁻¹)	
CO _{2(g)}	-394	
CH _{4(g)}	-74.9	
$H_2O(g)$	-241.8	
H ₂ O _(I)	-285.8	
HCI _(g)	-92.3	
C5H12 (I)	-173	
CCI _{4(I)}	-95.7	
NH _{3(g)}	-45.9	
NO _(g)	+90.3	

1. $C_5H_{12}(I) + 8O_2(g) \rightarrow 5CO_2(g) + 6H_2O(I)$

 $\Delta H = [(5 \times -394) + (6 \times -286)] - (-173) = -3513 \text{ kJ mol}^{-1}$

2. CH₄(g) + 4Cl₂(g) → CCl₄(l) + 4HCl(g) $\Delta H = [(4 \times -92.3) + (-95.7)] - [(-74.9)] = -390 \text{ kJ mol}^{-1}$

3. $4NH_3(g) + 5O_2(g) \rightarrow 4NO(g) + 6H_2O(g)$ $\Delta H = [(6 \times -241.8) + (4 \times + 90.3)] - [(4 \times -45.9)] = -906 \text{ kJ mol}^{-1}$

Standard enthalpy change of combustion (ΔH_c^{o})

 The standard enthalpy change of combustion (ΔH_c^e) is the enthalpy change when one mole of a substance is burned completely in oxygen under standard conditions.

Example:

 $C_2H_5OH(I) + 3O_2(g) \rightarrow 2CO_2(g) + 3H_2O(I) \qquad \Delta H_c{}^{\rm e} = -1367 \ kJ \ mol^{-1}$

- Note that the equation is balanced for one mole of reactant and the oxygen is assumed to be the excess reactant.
- Write an equation for the complete combustion of one mole of butane, C₄H₁₀.

$$C_4H_{10}(g) + \frac{61}{2}O_2(g) \rightarrow 4CO_2(g) + \frac{5}{2}H_2O(I)$$

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Calculating ΔH using ΔH_c^{e} values

• The equation used to calculate the ΔH of a reaction using $\Delta H^{e_{c}}$ values is given below.

 $\Delta H^{e} = \sum \Delta H_{c}^{e} \text{ reactants} - \sum \Delta H_{c}^{e} \text{ products}$

Example: Determine the ΔH of the following reaction using the values given in the table.

 $C_2H_4(g) + H_2(g) \rightarrow C_2H_6(g)$

	ΔH _c e
C ₂ H ₄	-1411
H ₂	-286
C_2H_6	-1561

 $\Delta H^{\rm e} = (-1411 + -286) - (-1561)$ $\Delta H^{\rm e} = -136 \text{ kJ mol}^{-1}$

Reactivity 1.2.5

Understandings:

• A Born–Haber cycle is an application of Hess's law, used to show energy changes in the formation of an ionic compound.

Learning outcomes:

• Interpret and determine values from a Born–Haber cycle for compounds composed of univalent and divalent ions.

Additional notes:

- The cycle includes: ionization energies, enthalpy of atomization (using sublimation and/or bond enthalpies), electron affinities, lattice enthalpy, enthalpy of formation.
- The construction of a complete Born–Haber cycle will not be assessed.

Linking questions:

• Structure 2.1 What are the factors that influence the strength of lattice enthalpy in an ionic compound?

Lattice enthalpy (ΔH^{o}_{lat})

• Lattice enthalpy (ΔH^{e}_{lat}) is the enthalpy change when one mole of solid ionic compound is separated into its gaseous ions under standard conditions.

 $NaCl_{(s)} \rightarrow Na^{+}_{(g)} + Cl^{-}_{(g)} \Delta H^{e}_{lat} = +790 \text{ kJ mol}^{-1}$

- Note that ΔH^{e}_{lat} is endothermic and has a positive ΔH .
- A Born-Haber cycle is an enthalpy cycle that can be used to calculate the lattice enthalpy or enthalpy of formation of an ionic compound.
- Enthalpy of atomisation (ΔH^o_{atom}) the enthalpy change when one mole of gaseous atoms is formed from an element in its standard state (endothermic).

 $Na_{(s)} \rightarrow Na_{(g)}$ ($\Delta H = +107 \text{ kJ mol}^{-1}$)

 First ionisation energy (ΔHi^e) – the minimum energy required to remove one mole of electrons from one mole of gaseous atoms (endothermic)

 $Na_{(g)} \rightarrow Na^{+}_{(g)} + e^{-} (\Delta H = +496 \text{ kJ mol}^{-1})$

• Bond dissociation enthalpy (E) – the enthalpy change when one mole of bonds is broken in the gaseous state (endothermic).

 $Cl_{2(g)} \rightarrow 2Cl_{(g)}$ ($\Delta H = +242 \text{ kJ mol}^{-1}$)

 First electron affinity (ΔHe^o) – the enthalpy change when one mole of electrons are added to one mole of gaseous atoms (exothermic).

 $CI_{(g)} + e^{-} \rightarrow CI^{-}_{(g)}$ ($\Delta H = -349 \text{ kJ mol}^{-1}$)

• Standard enthalpy change of formation (ΔH_{f}^{e}) – the enthalpy change when one mole of a compound is formed from it elements in their standard states under standard conditions.

$$Na_{(s)} + \frac{1}{2}Cl_{2(g)} \rightarrow NaCl_{(s)}$$
 ($\Delta H = -411 \text{ kJ mol}^{-1}$)

Exercises:

1. Using the values given above, construct a Born-Haber cycle using the template below and calculate the ΔH^{e}_{lat} for NaCl.



$$\begin{split} \Delta H^{\Theta}_{lat} &= \Delta H^{\Theta}_{atom} \, \text{Na}_{(s)} + \Delta H^{\Theta}_{i} \, \text{Na}_{(g)} + \frac{1}{2} \, E \, \text{Cl}_{2(g)} + \Delta H^{\Theta}_{e} \, \text{Cl}_{(g)} - \Delta H^{\Theta}_{f} \, \text{NaCl} \\ \Delta H^{\Theta}_{lat} &= (+107) + (+496) + (+121) + (-349) - (-411) \\ \Delta H^{\Theta}_{lat} &= +786 \text{ kJ mol}^{-1} \end{split}$$

2. Using the values given in the table below, construct a Born-Haber cycle and calculate the ΔH_{l}^{e} for CaF₂

$\Delta H_{\text{atom}} \operatorname{Ca}_{(s)}$ (enthalpy of atomization)	+179 kJ mol ⁻¹
$E F_{2(g)}$ (bond dissociation enthalpy)	+158 kJ mol ⁻¹
$\Delta H^{\Theta_i} \operatorname{Ca}_{(g)} (1^{st} \text{ ionisation energy})$	+590 kJ mol⁻¹
$\Delta H^{\Theta_i} \operatorname{Ca}^{+}_{(g)}$ (2 nd ionisation energy)	+1150 kJ mol ^{−1}
$\Delta H^{\Theta}_{e} F_{(g)}$ (first electron affinity)	–328 kJ mol ^{–1}
$\Delta H_{lat} \operatorname{CaF}_{2(s)}$ (lattice enthalpy)	+2651 kJ mol ⁻¹



$$\begin{split} \Delta H^{\Theta}{}_{f} &= \Delta H^{\Theta}{}_{atom} \operatorname{Ca}_{(s)} + \Delta H^{\Theta}{}_{i} \operatorname{Ca}_{(g)} + \Delta H^{\Theta}{}_{i} \operatorname{Ca}^{+}{}_{(g)} + E \operatorname{F}_{2(g)} + 2(\Delta H^{\Theta}{}_{e} \operatorname{F}_{(g)}) - \Delta H^{\Theta}{}_{lat} \operatorname{Ca}{}_{F_{2(s)}} \\ \Delta H^{\Theta}{}_{f} &= (+179) + (+590) + (+1150) + (+158) + 2(-328) - (+2651) \\ \Delta H^{\Theta}{}_{f} &= -1230 \text{ kJ mol}{}^{-1} \end{split}$$