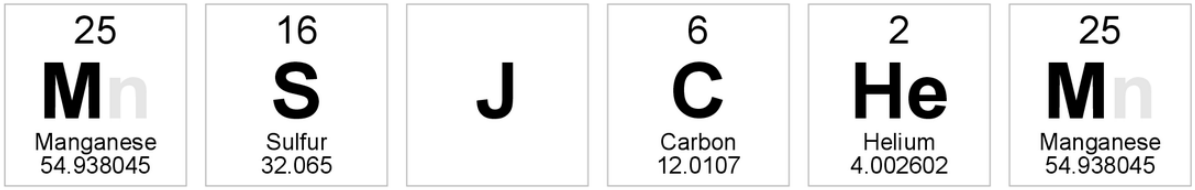
Reactivity 1.2 HL

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 ΔH_f data or ΔH_c data (1.2.4).
- $\Delta H^\ominus = \sum \Delta H_c^\ominus$ reactants $- \sum \Delta H_c^\ominus$ products
- $\Delta H^\ominus = \sum \Delta H_f^\ominus$ products $- \sum \Delta H_f^\ominus$ 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 ($\Delta H_f^\ominus$)

- The standard enthalpy change of formation ($\Delta H_f^\ominus$) 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:

$C(s) + 2H_2(g) \rightarrow CH_4(g)$ $\Delta H_f^\ominus = -74.0$ kJ mol^{-1}

$2C(s) + 3H_2(g) + ½O_2(g) \rightarrow C_2H_5OH(l)$ $\Delta H_f^\ominus = -278$ kJ mol^{-1}

$Na(s) + ½Cl_2(g) \rightarrow NaCl(s)$ $\Delta H_f^\ominus = -411$ 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. $C_3H_8(g)$
2. $CH_3OH(l)$
3. $MgCl_2(s)$

Calculating ΔH for a reaction using $\Delta H_f^\ominus$ values

$$\Delta H^\ominus = \sum \Delta H_f^\ominus \text{ products} - \sum \Delta H_f^\ominus \text{ reactants}$$

- $\Delta H_f^\ominus$ 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.

	$\Delta H_f^\ominus$ (kJ mol^{-1})
$CO_{2(g)}$	-394
$CH_{4(g)}$	-74.9
$H_2O_{(g)}$	-241.8
$H_2O_{(l)}$	-285.8
$HCl_{(g)}$	-92.3
$C_5H_{12\ (l)}$	-173
$CCl_{4(l)}$	-95.7
$NH_{3(g)}$	-45.9
$NO_{(g)}$	+90.3

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

2. $CH_4(g) + 4Cl_2(g) \rightarrow CCl_4(l) + 4HCl(g)$

3. $4NH_3(g) + 5O_2(g) \rightarrow 4NO(g) + 6H_2O(g)$

Standard enthalpy change of combustion ($\Delta H_c^\ominus$)

- The standard enthalpy change of combustion ($\Delta H_c^\ominus$) is the enthalpy change when one mole of a substance is burned completely in oxygen under standard conditions.

Example:

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

- 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, C_4H_{10}.

$$C_4H_{10}(g) + \_\_\_\ O_2(g) \rightarrow \_\_\_\ CO_2(g) + \_\_\_H_2O(l)$$

Calculating ΔH using $\Delta H_c^\ominus$ values

- The equation used to calculate the ΔH of a reaction using $\Delta H^\ominus_c$ values is given below.

$$\Delta H^\ominus = \sum \Delta H_c^\ominus \text{ reactants} - \sum \Delta H_c^\ominus \text{ products}$$

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

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

	$\Delta H_c^\ominus$
C_2H_4	-1411
H_2	-286
C_2H_6	-1561

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 ($\Delta H^{\ominus}_{lat}$)

- Lattice enthalpy ($\Delta H^{\ominus}_{lat}$) is the enthalpy change when one mole of solid ionic compound is separated into its gaseous ions under standard conditions.

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

- Note that $\Delta H^{\ominus}_{lat}$ 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 ($\Delta H^{\ominus}_{atom}$) –** the enthalpy change when one mole of gaseous atoms is formed from an element in its standard state (endothermic).

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

- **First ionisation energy ($\Delta H_i^{\ominus}$) –** the minimum energy required to remove one mole of electrons from one mole of gaseous atoms (endothermic)

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

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

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

- **First electron affinity ($\Delta H_e^{\ominus}$) –** the enthalpy change when one mole of electrons are added to one mole of gaseous atoms (exothermic).

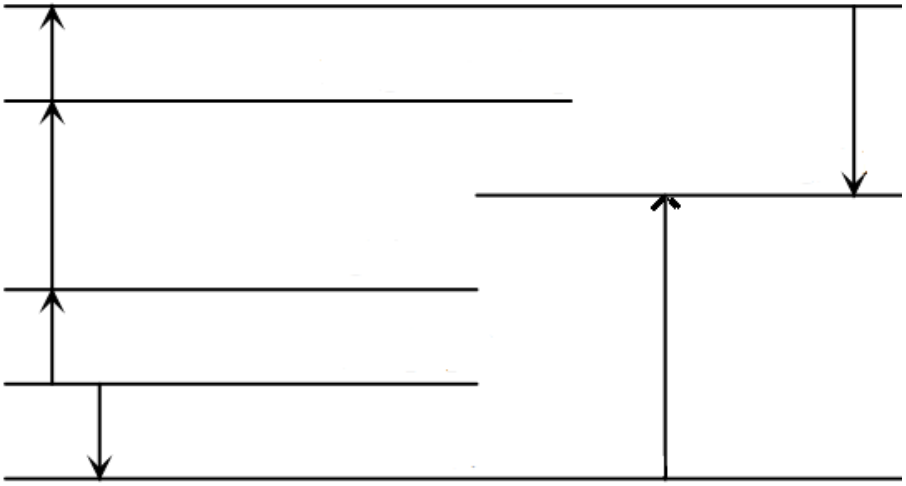
$$Cl_{(g)} + e^{-} \rightarrow Cl^{-}_{(g)} \quad (\Delta H = -349 \text{ kJ mol}^{-1})$$

- **Standard enthalpy change of formation ($\Delta H_f^{\ominus}$) –** the enthalpy change when one mole of a compound is formed from it elements in their standard states under standard conditions.

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

Exercises:

1. Using the values given above, construct a Born-Haber cycle using the template below and calculate the $\Delta H^{\ominus}_{lat}$ for NaCl.



2. Using the values given in the table below, construct a Born-Haber cycle and calculate the $\Delta H_f^{\ominus}$ for CaF_2

ΔH_{atom} $Ca_{(s)}$ (enthalpy of atomization)	+179 kJ mol^{-1}
E $F_{2(g)}$ (bond dissociation enthalpy)	+158 kJ mol^{-1}
$\Delta H^{\ominus}_i$ $Ca_{(g)}$ (1^{st} ionisation energy)	+590 kJ mol^{-1}
$\Delta H^{\ominus}_i$ $Ca^{+}_{(g)}$ (2^{nd} ionisation energy)	+1150 kJ mol^{-1}
$\Delta H^{\ominus}_e$ $F_{(g)}$ (first electron affinity)	–328 kJ mol^{-1}
ΔH_{lat} $CaF_{2(s)}$ (lattice enthalpy)	+2651 kJ mol^{-1}