

Reactivity 1.2 · Energy cycles in reactions

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Reactivity 1.2, Energy cycles in reactions, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

Prerequisites: enthalpy change, exothermic and endothermic reactions, and calorimetry from Reactivity 1.1; covalent bonds from Structure 2.2; lattice enthalpy and ionization energy from Structures 2.1 and 1.3. You will use bond enthalpies and enthalpy data from the data booklet.

Bond enthalpy

■ Where does the energy of a reaction come from?

Burning one mole of methane in a gas cooker releases about 800 kJ. No atoms are created or destroyed, so the energy must come from the bonds: the bonds in the products are stronger than the bonds in the reactants. This unit shows how to calculate enthalpy changes from bond data and from **energy cycles** when they cannot be measured directly.

■ Breaking and making bonds

- Breaking a bond **needs** energy: bond breaking is **endothermic**.
- Making a bond **releases** energy: bond making is **exothermic**.

The **bond enthalpy** is the energy needed to break one mole of a covalent bond, with the substances in the **gaseous** state. It is always positive. For example, $\text{H}_2(\text{g}) \rightarrow 2\text{H}(\text{g})$, $\Delta H = +436 \text{ kJ mol}^{-1}$.

The value for a bond such as C–H differs a little from one molecule to another, so the data booklet gives an **average bond enthalpy**: the mean over many compounds.

■ Calculating ΔH from bond enthalpies

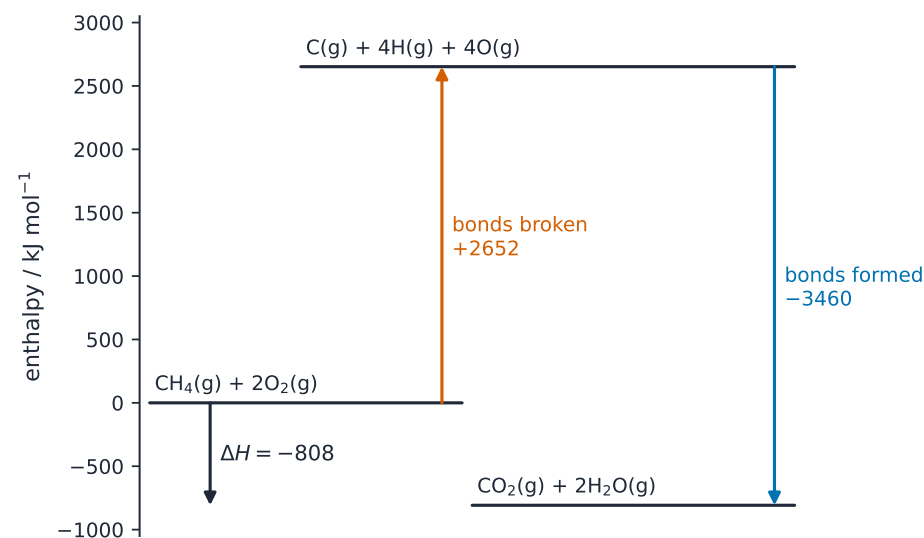
$$\Delta H = \sum(\text{bonds broken}) - \sum(\text{bonds formed})$$

Worked example: $\text{CH}_4(\text{g}) + 2\text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g}) + 2\text{H}_2\text{O}(\text{g})$.

Bonds broken	Energy / kJ	Bonds formed	Energy / kJ
4 C–H: 4×414	1656	2 C=O: 2×804	1608
2 O=O: 2×498	996	4 O–H: 4×463	1852
total	2652	total	3460

$\Delta H = 2652 - 3460 = -808 \text{ kJ mol}^{-1}$. More energy is released by forming bonds than

is needed to break them, so the reaction is exothermic.



Every bond is broken to gaseous atoms, then the new bonds form; ΔH is the difference

■ Why the answer is only approximate

The measured value for this reaction is -802 kJ mol^{-1} (with water as a gas). The bond enthalpy answer differs because:

- **average** bond enthalpies are used, not the values for these exact molecules;
- bond enthalpies apply only to **gases**. If a substance is a liquid or solid, the energy to change its state is missing. With liquid water as a product the true value is -890 kJ mol^{-1} .

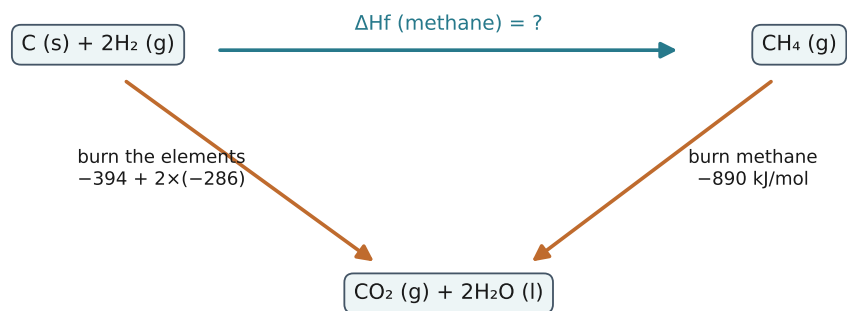
Hess's law

■ Same start, same end

Hess's law: the enthalpy change of a reaction is the same whatever route is taken, as long as the initial and final conditions are the same. Enthalpy is a **state function**: it depends only on where you start and where you finish, like the difference in height between the bottom and the top of a mountain, whichever path you climb.

This lets you calculate enthalpy changes that cannot be measured directly. Build an **energy cycle** with the target reaction on one route and reactions with known ΔH on the other.

Hess cycle: same start, same end → same total energy change



Same start, same end: $\Delta H_f = -394 + 2(-286) - (-890) = -76 \text{ kJ/mol}$

■ Working with equations

You can also combine equations directly, like algebra:

- If you **reverse** an equation, change the sign of ΔH .
- If you **multiply** an equation by a number, multiply ΔH by the same number.
- Add the equations and their ΔH values; species that appear on both sides cancel.

Worked example: find ΔH for $\text{C(s)} + \frac{1}{2}\text{O}_2(\text{g}) \rightarrow \text{CO(g)}$, which cannot be measured because some CO_2 always forms.

- (1) $\text{C(s)} + \text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g})$, $\Delta H = -394 \text{ kJ mol}^{-1}$
- (2) $\text{CO(g)} + \frac{1}{2}\text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g})$, $\Delta H = -283 \text{ kJ mol}^{-1}$

Keep (1) and reverse (2): $\text{CO}_2 \rightarrow \text{CO} + \frac{1}{2}\text{O}_2$, $\Delta H = +283$. Adding them, CO_2 cancels and $\frac{1}{2}\text{O}_2$ is left on the left:

$$\Delta H = -394 + 283 = -111 \text{ kJ mol}^{-1}$$

■ Worked example: three equations

Find ΔH for $2\text{C(s)} + \text{H}_2(\text{g}) \rightarrow \text{C}_2\text{H}_2(\text{g})$, given:

- (1) $\text{C(s)} + \text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g})$, $\Delta H = -394$
- (2) $\text{H}_2(\text{g}) + \frac{1}{2}\text{O}_2(\text{g}) \rightarrow \text{H}_2\text{O(l)}$, $\Delta H = -286$
- (3) $\text{C}_2\text{H}_2(\text{g}) + \frac{5}{2}\text{O}_2(\text{g}) \rightarrow 2\text{CO}_2(\text{g}) + \text{H}_2\text{O(l)}$, $\Delta H = -1301$

Take $2 \times (1)$ (two C on the left), $1 \times (2)$, and reverse (3) (C_2H_2 on the right):

$$\Delta H = 2(-394) + (-286) + 1301 = +227 \text{ kJ mol}^{-1}$$

Check that the oxygen, CO_2 and water cancel: $\frac{5}{2}\text{O}_2$ on each side, 2CO_2 on each side, one H_2O on each side.

AHL: Formation and combustion cycles

■ Standard enthalpy changes

Standard conditions are 100 kPa and a stated temperature, usually 298 K, written with the symbol $\ominus$.

- The **standard enthalpy change of formation**, $\Delta H_f^\ominus$, is the enthalpy change when one mole of a substance forms from its elements in their standard states. For an element in its standard state, $\Delta H_f^\ominus = 0$.
- The **standard enthalpy change of combustion**, $\Delta H_c^\ominus$, is the enthalpy change when one mole of a substance burns completely in oxygen under standard conditions.

■ Using formation data

When $\Delta H_f^\ominus$ values are known for every substance, use the products-minus-reactants rule, which comes from a cycle through the elements:

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

Worked example: the combustion of ethanol, $\text{C}_2\text{H}_5\text{OH(l)} + 3\text{O}_2(\text{g}) \rightarrow 2\text{CO}_2(\text{g}) + 3\text{H}_2\text{O(l)}$. Data: $\Delta H_f^\ominus$ ethanol -278 , CO_2 -394 , $\text{H}_2\text{O(l)}$ -286 kJ mol^{-1} ; O_2 is an element, so 0.

$$\Delta H_c^\ominus = [2(-394) + 3(-286)] - [(-278) + 0] = -1646 + 278 = -1368 \text{ kJ mol}^{-1}$$

■ Using combustion data

When combustion values are known, the arrows of the cycle point **down** to the combustion products, and the rule turns round:

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

Worked example: the formation of methane, $\text{C(s)} + 2\text{H}_2(\text{g}) \rightarrow \text{CH}_4(\text{g})$. Data: $\Delta H_c^\ominus$ carbon -394 , hydrogen -286 , methane -890 kJ mol^{-1} .

$$\Delta H_f^\ominus = [(-394) + 2(-286)] - (-890) = -966 + 890 = -76 \text{ kJ mol}^{-1}$$

This is the cycle in the Hess's law figure above.

AHL: Born–Haber cycles

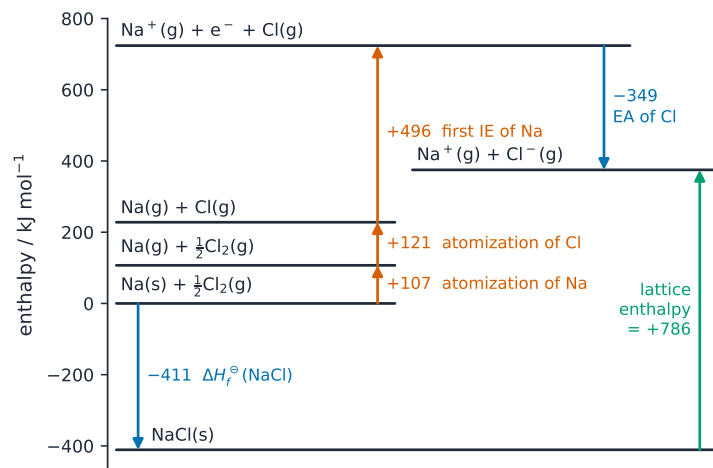
■ Lattice enthalpy from a cycle

Lattice enthalpy cannot be measured directly, because you cannot separate a crystal into gaseous ions in one step. A **Born–Haber cycle** is an energy cycle for forming an ionic compound from its elements, through gaseous atoms and gaseous ions. All the other steps can be measured, so the lattice enthalpy can be calculated.

The steps for sodium chloride:

Step	Process	$\Delta H / \text{kJ mol}^{-1}$
atomization of Na	$\text{Na(s)} \rightarrow \text{Na(g)}$	+107
atomization of Cl	$\frac{1}{2}\text{Cl}_2(\text{g}) \rightarrow \text{Cl(g)}$	+121
first ionization energy of Na	$\text{Na(g)} \rightarrow \text{Na}^+(\text{g}) + \text{e}^-$	+496
first electron affinity of Cl	$\text{Cl(g)} + \text{e}^- \rightarrow \text{Cl}^-(\text{g})$	−349
formation of NaCl	$\text{Na(s)} + \frac{1}{2}\text{Cl}_2(\text{g}) \rightarrow \text{NaCl(s)}$	−411
lattice enthalpy	$\text{NaCl(s)} \rightarrow \text{Na}^+(\text{g}) + \text{Cl}^-(\text{g})$	?

The **enthalpy of atomization** is the enthalpy change to form one mole of gaseous atoms from the element in its standard state. For chlorine it is half the Cl–Cl bond enthalpy, because one mole of Cl atoms comes from half a mole of Cl₂.



Two routes from NaCl(s) to the gaseous ions have the same total enthalpy change

■ Calculating the lattice enthalpy

Going round the cycle, the route from NaCl(s) to the gaseous ions directly must equal the route back through the elements:

$$\Delta H_{\text{latt}} = -\Delta H_f^\ominus + \Delta H_{\text{at}}(\text{Na}) + \Delta H_{\text{at}}(\text{Cl}) + \text{IE}(\text{Na}) + \text{EA}(\text{Cl})$$

$$\Delta H_{\text{latt}} = 411 + 107 + 121 + 496 - 349 = +786 \text{ kJ mol}^{-1}$$

The data booklet value, 790 kJ mol⁻¹, differs only by rounding in the data.

For a group 2 compound such as MgO, the cycle includes the first **and** second ionization energies of magnesium, and the first **and** second electron affinities of oxygen. The second electron affinity is positive: adding an electron to O⁻ means pushing it against the negative charge already there.

Practice

- Explain, in terms of bonds, why the combustion of methane is exothermic.
- Use bond enthalpies (H–H 436, Cl–Cl 242, H–Cl 431 kJ mol⁻¹) to calculate ΔH for $\text{H}_2(\text{g}) + \text{Cl}_2(\text{g}) \rightarrow 2\text{HCl}(\text{g})$.
- Use bond enthalpies (C=C 614, H–H 436, C–C 346, C–H 414 kJ mol⁻¹) to calculate ΔH for $\text{C}_2\text{H}_4(\text{g}) + \text{H}_2(\text{g}) \rightarrow \text{C}_2\text{H}_6(\text{g})$.
- Give two reasons why an enthalpy change calculated from average bond enthalpies differs from the measured value.
- State Hess's law.
- Given $\text{S(s)} + \text{O}_2(\text{g}) \rightarrow \text{SO}_2(\text{g})$, $\Delta H = -297$, and $2\text{SO}_2(\text{g}) + \text{O}_2(\text{g}) \rightarrow 2\text{SO}_3(\text{g})$, $\Delta H = -198 \text{ kJ mol}^{-1}$, calculate ΔH for $\text{S(s)} + \frac{3}{2}\text{O}_2(\text{g}) \rightarrow \text{SO}_3(\text{g})$.
- AHL.** Use $\Delta H_f^\ominus$ values (NH₃ −46, NO +90, H₂O(g) −242 kJ mol⁻¹) to calculate $\Delta H^\ominus$ for $4\text{NH}_3(\text{g}) + 5\text{O}_2(\text{g}) \rightarrow 4\text{NO}(\text{g}) + 6\text{H}_2\text{O}(\text{g})$.
- AHL.** Use $\Delta H_c^\ominus$ values (C −394, H₂ −286, C₂H₆ −1560 kJ mol⁻¹) to calculate $\Delta H_f^\ominus$ of ethane.
- AHL.** Write the equations, with state symbols, for the first electron affinity of oxygen and the lattice enthalpy of magnesium oxide.
- AHL.** Data for KCl: $\Delta H_{\text{at}}(\text{K}) +89$, $\Delta H_{\text{at}}(\text{Cl}) +121$, $\text{IE}(\text{K}) +419$, $\text{EA}(\text{Cl}) -349$, $\Delta H_f^\ominus(\text{KCl}) -437 \text{ kJ mol}^{-1}$. Calculate the lattice enthalpy of KCl.

Answers.

- Bonds broken: 4 C–H and 2 O=O need 2652 kJ. Bonds formed: 2 C=O and 4 O–H release 3460 kJ. More energy is released forming the new bonds than is needed to break the old ones.
- Broken: $436 + 242 = 678$. Formed: $2 \times 431 = 862$. $\Delta H = 678 - 862 = -184 \text{ kJ mol}^{-1}$.

3. Broken: C=C 614 and H-H 436, total 1050 (the four C-H bonds are not broken).
Formed: C-C 346 and two new C-H $2 \times 414 = 828$, total 1174. $\Delta H = 1050 - 1174 = -124 \text{ kJ mol}^{-1}$.
4. Average bond enthalpies are means over many compounds, not the values for these molecules; bond enthalpies apply to gases, so any liquid or solid needs extra energy for the change of state.
5. The enthalpy change of a reaction is independent of the route taken, provided the initial and final conditions are the same.
6. Keep the first equation and halve the second: $\Delta H = -297 + \frac{1}{2}(-198) = -297 - 99 = -396 \text{ kJ mol}^{-1}$.
7. **AHL.** $[4(+90) + 6(-242)] - [4(-46) + 0] = (360 - 1452) - (-184) = -1092 + 184 = -908 \text{ kJ mol}^{-1}$.
8. **AHL.** $2\text{C} + 3\text{H}_2 \rightarrow \text{C}_2\text{H}_6$: $\Delta H_f^\ominus = [2(-394) + 3(-286)] - (-1560) = -1646 + 1560 = -86 \text{ kJ mol}^{-1}$.
9. **AHL.** $\text{O}(\text{g}) + \text{e}^- \rightarrow \text{O}^-(\text{g})$; $\text{MgO}(\text{s}) \rightarrow \text{Mg}^{2+}(\text{g}) + \text{O}^{2-}(\text{g})$.
10. **AHL.** $\Delta H_{\text{latt}} = 437 + 89 + 121 + 419 - 349 = +717 \text{ kJ mol}^{-1}$ (data booklet 720).

Exam tips

- Bond breaking is endothermic and bond making exothermic; write “**broken minus formed**” before you substitute numbers.
- Count every bond: draw the structural formula, and leave out bonds that are not broken.
- Bond enthalpies are for **gases**; say so when you explain why a calculated value differs.
- When you reverse an equation, change the **sign**; when you multiply it, multiply ΔH .
- **AHL.** Formation data: products minus reactants. Combustion data: **reactants minus products**.
- **AHL.** Elements in their standard states have $\Delta H_f^\ominus = 0$; do not forget the coefficients.
- **AHL.** In the IB convention, lattice enthalpy is the endothermic separation of the solid into gaseous ions, so it is positive.