Ammonium nitrate explosions

Education in Chemistry
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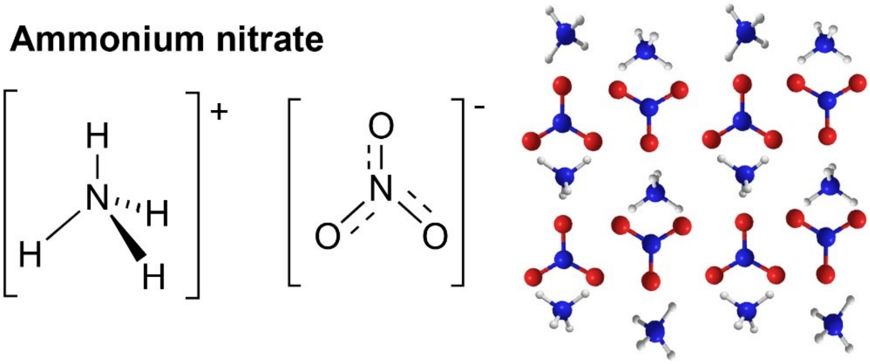
The decomposition of ammonium nitrate at temperatures above 260°C leads to a 'runaway' explosive reaction. Many aspects of this 'runaway' reaction can be explained by concepts such as enthalpy change and by taking a closer look at the structure and bonding of ammonium nitrate.

Task 1 – Structure and bonding in ammonium nitrate

The structure and geometry of ammonium nitrate are shown in the diagrams below.



1. Ammonium nitrate is composed of two polyatomic ions – identify the different type(s) of bonding within its structure.

2. Using the VSEPR theory and the diagrams above, state and explain the geometries of the NH_4^+ and NO_3^- ions shown.

Task 2 – Decomposition or explosion?

Pure ammonium nitrate does not explode easily and can be handled safely. It decomposes at 230°C producing nitrous oxide gas (N_2O) and water vapour.

3. Give a balanced equation for the decomposition reaction.

Above 260°C, if confined and when contaminated, ammonium nitrate will explode forming toxic gases such as NO_2, responsible for the 'orange brown fireball' described in the article.

The following equation represents one of the reactions contributing to the explosion:

$$4NH_4NO_3(s) \rightarrow 3N_2(g) + 2NO_2(g) + 8H_2O(g)$$

4. Given that the molar gas volume is 24.5 dm^3 at 298K and 1atm calculate the total volume of gas produced from 80 kg of $NH_4NO_3(s)$ under these conditions.

5. Use your value to calculate the total volume of gas at the same pressure and 300°C.
   Scale this up to calculate the vast volume of gas produced from 2750 tonnes of $NH_4NO_3(s)$ in the Beirut explosion.

Task 3 – Calculating the enthalpy of reaction, ΔH_R, and using kinetic theory to explain why this is a 'runaway' reaction

The data below will be used in Tasks 3 - 5

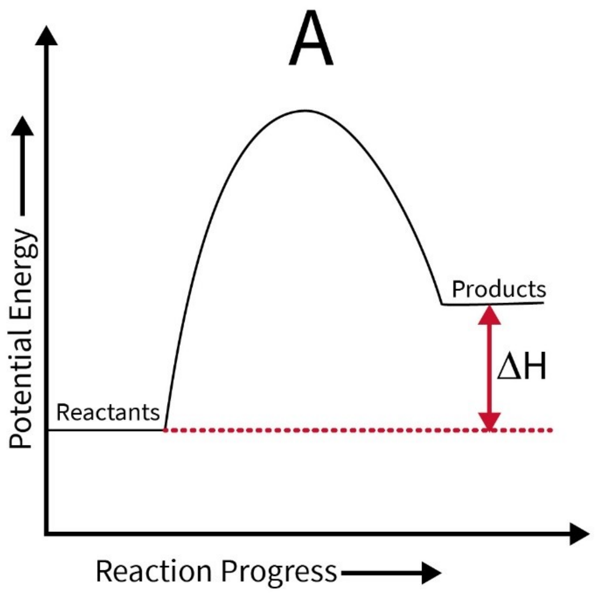
Compound	ΔH^0f / $KJmol^{-1}$	$S^0/JK^{-1}mol^{-1}$
NH_4NO_3 (s)	-365.6	+15.1
N_2(g)	0	+153.3
NO_2(g)	+33.2	+240.1
H_2O(g)	-241.8	+188.8

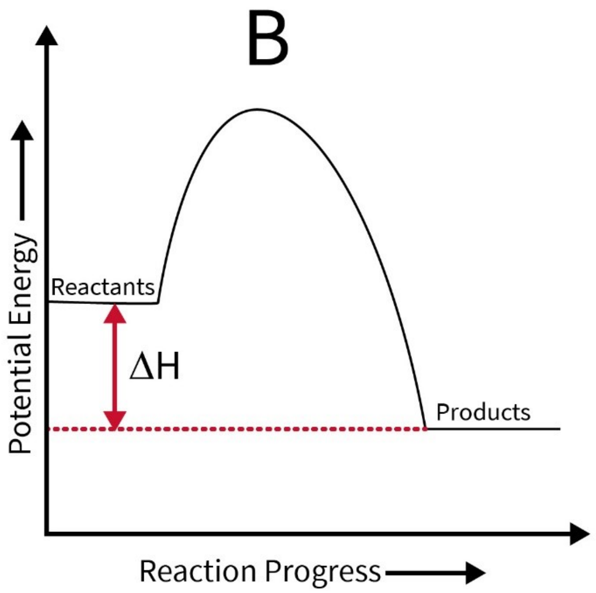
Once decomposition begins a 'runaway' reaction occurs. In a runaway reaction an exothermic reaction goes out of control. The heat evolved raises the temperature of the reacting mixture leading to an increase in reaction rate, which causes a further increase in temperature and a further increase in reaction rate until an explosion occurs.

6. Use the standard enthalpies of formation, ΔH^0f, given in $KJmol^{-1}$ to calculate the enthalpy change for the reaction and confirm that it is exothermic

$$4NH_4NO_3(s) \rightarrow 3N_2(g) + 2NO_2(g) + 8H_2O(g)$$

7. Select which of the energy profile templates below (A or B) correctly represents the enthalpy change you have calculated and label it showing reactants, products, ΔH_R and E_{act}.





8. Use kinetic theory to explain why an increase in temperature causes an increase in reaction rate.

Task 4 – Calculating the entropy change, ΔS, for the reaction

The changes in state during the decomposition reaction below suggest there will be a significant increase in the disorder, entropy, for the reaction – ie ΔS will be highly positive.

9. Use the standard entropies, S^0, given in $JK^{-1}mol^{-1}$ to confirm this is the case.

$$4NH_4NO_3(s) \rightarrow 3N_2(g) + 2NO_2(g) + 8H_2O(g)$$

Task 5 – Assessing the spontaneity of the reaction

To assess the spontaneity of a reaction both enthalpy and entropy changes need to be considered together in Gibb's Equation.

Using your enthalpy and entropy changes from Tasks 3 and 4 and Gibbs equation below:

10. Comment on whether the decomposition reaction is likely to be spontaneous at all temperatures.

11. Using temperatures of 300^0C and 500^0C in a model calculation comment on whether the decomposition is likely to become more favourable as the temperature increases.

Reminders about Gibbs equation:

$$\Delta G = \Delta H - T\Delta S$$

For a reaction to be spontaneous ΔG must be negative.
Take care with units!
ΔG and ΔH in $KJmol^{-1}$, ΔS in $JK^{-1}mol^{-1}$ and T is in K.