# Ammonium nitrate explosions: answers

***Education in Chemistry***November 2020
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The decomposition of ammonium nitrate at temperatures above 260oC 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.

Covalentbonding within NH3 molecule
Coordinate bond between N and H+ ion
Ionic bonding between NH4+andNO3- in the lattice

1. Using the VSEPR theory and the diagrams above, state and explain the geometries of the NH4+ and NO3- ions shown.

NH4+ has four bond pairs which repel equally to give a tetrahedral geometry and a bond angle of 109.5°.
NO3- has three double bond pairs which repel equally to give a trigonal planar geometry and a bond angle of 120°.

## Task 2 – Decomposition or explosion?

Pure ammonium nitrate does not explode easily and can be handled safely. It decomposes at 230oC producing nitrous oxide gas (N2O) and water vapour.

1. Give a balanced equation for the decomposition reaction.

NH4NO3 (s)→ N2O(g) + 2H2O(g)

Above 260oC, if confined and when contaminated, ammonium nitrate will explode forming toxic gases such as NO2, responsible for the ‘orange brown fireball’ described in the article.

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

4NH4NO3(s)→ 3N2(g) + 2NO2(g) + 8H2O(g)

1. Given that the molar gas volume is 24.5 dm3 at 298K and 1atm calculate the total volume of gas produced from 80 kg of NH4NO3(s) under these conditions.

4 moles NH4NO3(s)→ 13 moles of gas
1 mole NH4NO3(s)→ 13/4 moles of gas
80kg NH4NO3(s) = 1000 moles NH4NO3(s) → 3250 moles of gas
Volume of gas = 3250 x 24.5 dm3 = 79,625 dm3

1. Use your value to calculate the total volume of gas at the same pressure and 300oC.
Scale this up to calculate the vast volume of gas produced from 2750 tonnes of NH4NO3(s) in the Beirut explosion.

80kg NH4NO3(s)→ 79,625 dm3 of gas at 298 K

V1/T1 = V2/T2; 300oC = 573 K

79,625/298 = V2/573; V2 = 153,104.4 dm3

2750 tonnes → 153,104.4/80 x 2750 x 1000 dm3 of gas = 5,262,965.3x103 dm3 of gas

## Task 3 – Calculating the enthalpy of reaction, ΔHR, and using kinetic theory to explain why this is a ‘runaway’ reaction

The data below will be used in Tasks 3 - 5

|  |  |  |
| --- | --- | --- |
| **Compound** | **ΔH0f / KJmol-1** | **S0/JK-1mol-1** |
| NH4NO3 (s) | -365.6 | +15.1 |
| N2(g)  | 0 | +153.3 |
| NO2(g)  | +33.2 | +240.1 |
| H2O(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.

1. Use the standard enthalpies of formation, ΔH0f**,** given in KJmol-1 to calculate the enthalpy change for the reaction and confirm that it is exothermic

 4NH4NO3(s)→ 3N2(g) + 2NO2(g) + 8H2O(g)

*ΔHR = sum of (ΔH0f products****) -*** *sum of (ΔH0f reactants)
ΔHR  = -1934.4 + 66.4. + 1462.4 = - 405.6KJmol-1*

1. 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, ΔHR and Eact.

Energy profile diagram B, showing reactant, NH4NO3 ,on LHS and products3N2(g),2NO2(g) and 8H2O(g) on RHS. Eact shown as the difference in energy between reactants and peak of profile.



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

For a successful collision molecules need E > or = Eact. As temperature increases kinetic energy of molecules increases and more molecules have E > or = Eact resulting in more successful collisions per unit time.

## 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.

1. Use the standard entropies, S**0,** g**i**ven in JK-1mol-1 to confirm this is the case.

4NH4NO3(s)→ 3N2(g) + 2NO2(g) + 8H2O(g)

ΔS = sum of (S0 of products) - sum of (S0 of reactants) = 459.9 + 1510.4 + 480.2 - 60.4 = +2390.1JK-1mol-1

## 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:

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

SinceΔH = -ve and ΔS = +ve, both the terms ΔH and TΔS will be -ve at all temperatures above 0K; therefore ΔG = -ve indicating a spontaneous reaction.

1. Using temperatures of 300**0**C and 5000C in amodel calculation comment on whether the decomposition is likely to become more favourable as the temperature increases.

At 300K: ΔG = -405.6 - 573 x (2390.1/1000) = -1775.1KJmol-1

At 500K: ΔG = -405.6 - 773 x (2390.1/1000) = -2253.1KJmol-1

ΔG becomes more -ve as T increases; therefore decomposition reaction becomes more favourable.

### Reminders about Gibbs equation:

**Δ**G = **Δ**H -T**Δ**S

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