Writing 'explosive' equations (question 3, 2011 paper)
Video transcript

This question is all about explosives and how explosives work.

The question starts with an introduction into explosives and shows us the skeletal formulae of two common explosives, TNT and RDX. It states that some high explosives have a general formula of $C_aH_bN_cO_d$. The oxidiser (the oxygen atoms) and the fuel (the carbon and hydrogen atoms) are all present in the same molecule. The nitrogen atoms are present so that there is the highly exothermic production of hot nitrogen gas.

Part a

Part (a) of the question asks you to find an expression for d in terms of a, b and c that must be satisfied for an explosive of general formula $C_aH_bN_cO_d$ to decompose to form CO_2, H_2O and N_2 only. To answer this question, we can begin by writing out a simple equation to represent the reaction taking place. The key information is that the oxidiser and the fuel are all present in the same molecule and hence the only reactant is the explosive itself. The products are CO_2, H_2O and N_2. If we now balance the equation, we must produce a molecules of CO_2, $b/2$ molecules of H_2O (as each water molecule has two hydrogen atoms) and $c/2$ molecules of N_2. Now balancing the oxygen atoms, we have d atoms of oxygen on the left and $2a + b/2$ atoms of oxygen on the right. Thus for an explosive of general formula $C_aH_bN_cO_d$ to decompose to form CO_2, H_2O and N_2 only, $d = 2a + b/2$.

Part b

The question now moves on to explain the meaning of the *oxygen balance* of an explosive and how it can be calculated. The *oxygen balance* of an explosive is the mass of oxygen either in excess or in deficit of that required for the complete oxidation of the carbon and hydrogen atoms present in the explosive, ie how much oxygen is present in the molecule compared to the amount needed for the complete combustion of all the fuel in the molecule. It is expressed as a percentage of the molar mass of the explosive.

Part (b) asks you to write a general expression for the *oxygen balance* of $C_aH_bN_cO_d$. Remembering that the mass of a substance in grams is equal to the number of moles of that substance multiplied by its molar mass in g per mole, then the mass of oxygen present in the molecule $C_aH_bN_cO_d$ is equal to the number of moles of oxygen present, d, multiplied by the molar mass of oxygen which is 16 g per mole. This is the mass of oxygen present. The mass of oxygen required for the complete combustion of the explosive is effectively the mass of oxygen on the right hand side of the equation we wrote in part (a), since these are the products if complete combustion occurred. Thus the mass of oxygen required for the complete combustion of the fuel is the number of moles of oxygen produced = $2a + b/2$ multiplied by the molar mass of oxygen, ie 16 g per mole. The difference between these two values is therefore $16d – 16(2a + b/2)$.

The question tells us that the oxygen balance is expressed as a percentage of the molar mass of the explosive. Again using the equation mass = moles times molar mass, the molar mass of the explosive can be calculated as $12a + b + 14c + 16d$. Therefore the oxygen balance of $C_aH_bN_cO_d$ is $16d – 16(2a + b/2)$ all divided by $12a + b + 14c + 16d$ multiplied by 100%.

Part c

In part (c) of the question, you are asked to calculate the oxygen balance for RDX, whose structure is given at the start of the question. This can be calculated using the answer to part (b). In order to use this equation it is necessary to determine the molecular formula of RDX from its skeletal formula. If you have not come across skeletal formulae in your studies, at each junction between the bonds and at the end of each bond it is assumed that there is a carbon atom. In addition, the hydrogen atoms are not drawn in. It is therefore important that when determining a molecular formula from a skeletal formula that you add in the correct number of hydrogen atoms such that each atom has the correct number of bonds, ie each carbon atom must have four bonds.

It is best to draw out the structural formula of the molecule and then count up the number of carbon, hydrogen, nitrogen and oxygen atoms. If we do this, we determine that the molecular formula for RDX is $C_3H_6N_6O_6$ and hence for substitution into our equation for oxygen balance, $a = 3$, $b = 6$, $c = 6$, $d = 6$.

To complete the question, it is now simply a matter of substituting each of these values into the equation. Thus, the oxygen balance of RDX is -21.6%.

Part d

The final part of the question describes what happens if an explosive does not contain enough oxygen. If this is the case, there is incomplete oxidation of C and/or H. For nitrated aromatic compounds the products are determined by a following a set of rules.

Part (d) of the question asks us to apply these rules to determine the products from the explosion of TNT and hence write an equation for its explosion. Once again, our first step is to determine the molecular formula of TNT from its skeletal formula. Drawing out the structural formula of TNT we can see that it contains 7 carbon atoms, 5 hydrogen atoms, 3 nitrogen atoms and 6 oxygen atoms and hence has a molecular formula of $C_7H_5N_3O_6$. Before proceeding we can check that it does not contain sufficient oxygen for complete combustion by looking back at our answer to part (a). Here we determined that for complete combustion, the number of atoms of oxygen in the explosive must be equal to the two times the number of atoms of carbon plus half the number of atoms of hydrogen. In this case by doing a quick sum we can see that the oxygen content is insufficient and so incomplete combustion will occur. As TNT is a nitrated aromatic compound we can follow the rules to determine the products from its explosion.

Let's follow each of the bullet points in turn. The first bullet point tells us that the carbon atoms react with the available oxygen to form CO. Thus, the 7 carbon atoms in TNT react with the six available oxygen atoms to form 6 molecules of CO and a single C atom. Following the second bullet point, the 3 nitrogen atoms combine to form 1½ molecules of N_2. Looking now at the third and fourth bullet points, one third of the 6 molecules of CO formed (ie 2) are converted into C and CO_2. In addition, one sixth of the 6 molecules of CO formed (ie 1) react with 2 atoms of hydrogen in TNT to form C and H_2O. Thus we can write the equation as $C_7H_5N_3O_6$ forms 3CO + C + 1½ N_2, + C + CO_2, + C + H_2O. However finally we must balance the hydrogen atoms to form H_2 gas. If we do this we determine the final equation for the explosion of TNT as:

$$C_7H_5N_3O_6 \rightarrow 3CO + 3C + 1\tfrac{1}{2}\,N_2 + CO_2 + H_2O + 1\tfrac{1}{2}\,H_2$$

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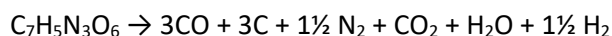
Part e

The last part of the question, part (e), asks us to calculate the mass of TNT that will explode to produce 1.0 dm^3 of gas at room temperature and pressure. In order to do this, we need to use the equation for the explosion of TNT produced in part (d). At room temperature and pressure, of the products from the explosion, carbon monoxide, nitrogen, carbon dioxide and hydrogen will all be gases. Thus one mole of TNT explodes to produce seven moles of gas.

To use this fact, we now need to find out the number of moles in 1.0 dm^3 of gas at RTP. If we know that the molar volume of any gas at RTP is 24 dm^3, then we can calculate that the number of moles in 1.0 dm^3 of gas is 1 dm^3 ÷ 24 dm^3 mol^{-1} = 0.0417 mol. Since one mole of TNT produces 7 moles of gas, then the number of moles of TNT which must have exploded to produce 0.0417 moles of gas is equal to 0.0417 moles divided by 7 = 5.95×10^{-3} moles of TNT.

The question however asks us to calculate the mass of TNT that will explode to produce this volume of gas. The molar mass of TNT can be calculated to be 227.14 g mol^{-1}. Therefore, using the equation, mass = moles × molar mass, we can calculate the mass of 5.95×10^{-3} moles of TNT as 1.35 g. As we have only been given the accuracy of the volume of gas to 2 significant figures, our final answer should only be given to the same degree of accuracy. Therefore, the mass of TNT that will explode to produce 1.0 dm^3 of gas at room temperature and pressure is 1.4 g.