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PRESENTATION ON

OXYGEN BALANCE AND ITS IMPORTANCE

CUFS 2416 EXPLOSIVE AND POST BLAST INVESTIGATION

B.SC. FORENSIC SCIENCE (SEM 6)
SCHOOL OF FORENSIC SCIENCES
BHUBANESHWAR CAMPUS

CONTENT

- OXYGEN BALANCE
- IMPORTANCE OF OXYGEN BALANCE
- CALCULATION OF OXYGEN BALANCE

OXYGEN BALANCE-

- Oxygen balance is an expression that is used to indicate the degree to which an explosive can be oxidised.
- It is usually expressed as a percentage of the molar mass of the explosive.
- It is also the mass of oxygen either in excess or in deficit of that required for complete oxidation of C and H.

IMPORTANT OF OXYGEN BALANCE-

- The chemical structure of the explosive material and the types of bond present have a greater influence on its properties.
- Helps to determine if an explosive molecule contains enough oxygen to fully oxidize the other atoms in the explosive.
- The oxygen balance is very important when we are creating a mixtures of explosives.
- E.g-Amatol, it is the mixtures of ammonium nitrate and TNT.

Types of Oxygen Balance

- Zero oxygen balance: The explosive molecule contains just enough oxygen to form carbon dioxide from carbon, water from hydrogen molecules, all of its sulfur dioxide from sulfur, and all metal oxides from metals with no excess.
- A molecule is said to have a positive oxygen balance if it contains more oxygen than is needed and a negative oxygen balance if it contains less oxygen than is needed.

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- Negative oxygen balance
e.g. trinitrotoluene (TNT) requires extra oxygen for complete formation of all the CO_2 and H_2O
Thus, despite being an high explosive, TNT is only efficient in the presence of an external oxidant, which may be air or another compound that provides a positive oxygen balance.
 - Zero oxygen balance
example: Performic acid has all the oxygen it needs for complete combustion, and hence only requires energy to detonate making it a much more dangerous compound per se than TNT.
 - Positive oxygen balance means that the compound liberates oxygen surplus to its own needs
Example the decomposition of ammonium nitrate provides one atom of oxygen per molecule. Any compound with a positive oxygen balance makes a good oxidizer and is highly incompatible with combustible chemicals.

Oxygen balance Values of selected compounds

Element or Compound	Oxygen balance (%)
Carbon	-266.7
Sulfur	-100
Aluminum powder	-89
Trinitrotoluene	-74
Nitroglycerine	+3.5
Ammonium nitrate	+20
Ammonium perchlorate	+27
Potassium chlorate	+26
Sodium chlorate	+45
Sodium nitrate	+37
Tetranitromethane	+57
Lithium perchlorate	+45

CALCULATION OF OXYGEN BALANCE

- 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

$C_a H_b N_c O_d$ is $16d - 16(2a + b/2)$ all divided by $12a + b + 14c + 16d$ multiplied by 100%.

Quantification of oxygen balance

- A quantification of oxygen balance allows for the determination of approximate ratio of reagents to optimize combustion/explosion. In this regard *oxygen balance* is defined as the number of moles of oxygen (excess or deficient) for 100 g of a compound of a known molecular weight (M_w), (1.8.9) where x = number of atoms of carbon, y = number of atoms of hydrogen, z = number of atoms of oxygen, and m = number of atoms of metal oxide produced.

$$OB\% = -1600 / M_w * (2x + y / 2 + m - z)$$

- In the case of TNT, the $M_w = 227.1$ g/ mol, the number of carbon atoms (x) = 7, the number of hydrogen atoms (y) = 5, the number of oxygen atoms (z) = 6, and the number of atoms of metal oxide produced (m) = 0. Therefore:
- $OB\% = -1600 / 227.1 * (14 + 2.5 + 0 - 6) = -74\%$

THANK YOU.

