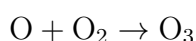


Lesson: CHEMICAL BOND

PROBLEM SHEET: QUESTIONS

1. (◆◆◆) Let us consider that the only valence electron of atom A can be described approximately using the eigenfunctions of the particle in a one-dimensional box of length L and one spin function and the electrons forming the bond in the A_2 using a box of double length. Calculate using this model the change in energy when the A_2 molecule is formed from two A atoms.
2. (◆◆◆) Let us consider that the electrons of the oxygen atom and those of the oxygen and ozone molecules can be described using the model of particles on spheres of radii R , $2R$ y $3R$ respectively. Knowing that the following reaction



gives off 107.2 kJ/mol, calculate the corresponding value of R .

3. (◆◆◆) From the values of experimental dissociation energies and internuclear equilibrium distances of different homonuclear diatomic included in the table

Molécula	D_e (eV)	r_e (Å)
H_2^+	2.79	1.06
H_2	4.75	0.741
He_2^+	2.5	1.08
He_2	0.0009	3.0
N_2^+	8.85	1.12
N_2	9.91	1.10
O_2^+	6.78	1.12
O_2	5.21	1.21

discuss following the Molecular Orbitals Theory the differences found for the neutral (A_2) and the corresponding molecular ion (A_2^+).

- ▷ 4. (◆◆◆) Experimental evidences prove that the geometry of the ozone molecule (O_3) corresponds to one central atom bonded with the two other oxygen atoms which no bond between them. The molecular angle is 116.8° and the bond distances are identical (1.272 Å). Using the Valence Bond Theory
 - a) Justify why the cyclic structure is not stable.
 - b) Justify why the two bond distances are identical.

c) Justify the value of the molecular angle.

Difficulty level: (◆◆◆) Easy, (◆◆◆) Normal, (◆◆◆) To think a bit.

PROBLEM SHEET: SOLUTIONS

Question 1 $\Rightarrow \Delta E = -\frac{3}{16} \frac{n^2 h^2}{mL^2}$

Question 2 $\Rightarrow 6.1\text{\AA}$
