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

$$\mathrm{O} + \mathrm{O_2} \rightarrow \mathrm{O_3}$$

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 whith 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.

Dificulty level: (♦♢♢) Easy, (♦♦♢) Normal, (♦♦♦) To think a bit.

PROBLEM SHEET: SOLUTIONS

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

Question 2 $\Rightarrow$ 6.1Å