

20×13×22 cm. We are now working further in construction of a more compact and lightweight high voltage supply which will be operated by small dry battery.

4. Quantum Mechanical Calculation on the Bond Moment.

Pauling's Formula about Electronegativity.

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The bond moments of diatomic (F. T. Wall: J. A. C. S. **61**, 1051 (1939)) and polyatomic (T. Ri and N. Muroyama: Proc. Imp. Acad., **20**, 93 (1944); Rev. Phys. Chem. Japan, **18**, 24 (1944)) molecules were calculated by the resonance theory and given as follow,

$$\mu_{AB} = i^2 e r_{AB}, \quad 1/i^2 = 1 + (E_{AB}^0 - E_i)/E' \quad (1)$$

Here we will make clear the relation between μ and the difference in electronegativity of two atoms. When the bond is completely homopolar, its energy and Hamiltonian are

$$E_{AB}^0 = \frac{1}{2} (E_{AA} + E_{BB}), \quad H_{AB}^0 = \frac{1}{2} (H_{AA} + H_{BB}) \quad (2)$$

The difference in the effective nuclear charges is ΔZ and its effect can be considered as a perturbation to the complete homopolar bond, then

$$H_{AB} = H_{AB}^0 + H', \quad H' = \frac{\Delta Z^2 e^2}{2r_{AB}} - \frac{\Delta Z e^2}{2r_{AB}} \left(\frac{1}{r_{A2}} - \frac{1}{r_{B1}} \right) \quad (3)$$

can be derived from (2), and corresponding to this perturbation

$$\psi_{AB} = \psi_{AB}^0 + \psi', \quad E_{AB} = E_{AB}^0 + E', \quad \psi' = iA(1)A(2) \quad (4)$$

If we put $W_A = Z_A e^2 / 2r_A \sim 110x_A$ for the atoms $r_{AB} \cong r_A + r_B = 2A$, the additional ionic resonance energy

$$E' = \iint \psi_{AB}^0 H' \psi_{AB}^0 d\tau_1 d\tau_2 \cong \frac{\Delta Z^2 e^2}{r_{AB}} = 23 (x_A - x_B)^2 \quad (5)$$

As for the amount of ionic character

$$i^2 = H_{0i}^2 / (E_{AB}^0 - E_i)^2 = \Delta Z^2 e^4 J^2 / 2(E_{AB}^0 - E_i)^2 = \frac{1}{4} (x_A - x_B)^2 \quad (6)$$

If we put $J = \int A(1)B(1) \frac{1}{r_{A1}} d\tau_1 = L/r_{AB}$ where we assume L is 0.65, the value of hydrogen-like wave function 1S and 2S at about $r_{AB} \cong 2A$, and $E_{AB}^0 - E_i \cong 90$ Kcal/mol (7) when ΔZ is small.

We can get (6) as the first term of Taylor expansion of (1) in $x_A - x_B$ from (5) and (7).

Equation (5) and (6) are the empirical formulas which are given by L. Pauling in "The Nature of the Chemical Bond." 60, 69 (1940).