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.

Nishio Hirai.

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,

\[ \mu_{AB} = \pm 2r_{AB}, \quad \frac{I^2}{I^2} = 1 + \frac{(E_A^0 - E_B^0)}{E'} \]  \hspace{1cm} (1)

where we will make clear the relation between \( \mu \) and the difference in electronegativity of two atoms. When the bond is completely homopolar, its energy and Hamiltonian are

\[ E_{AB}^0 = \frac{1}{2} (E_{AA} + E_{BB}), \quad H_{AB}^0 = \frac{1}{2} (H_{AA} + H_{BB}) \]  \hspace{1cm} (2)

The difference in the effective nuclear charges is \( \triangle Z \) and its effect can be considered as a perturbation to the complete homopolar bond, then

\[ H_{AB} = H_{AB}^0 + H', \quad H' = \triangle Z e^2 \left( \frac{1}{r_{AB}^2} - \frac{1}{r_{AB}^2} \right) \]  \hspace{1cm} (3)

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

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

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

\[ E' = \int \frac{e^2}{r_{AB}^2} \left( E_{AB}^0 - E_i \right)^2 \approx \triangle Z e^4 J^2 / 2 = 23 (x_A - x_B)^2 \]  \hspace{1cm} (5)

As for the amount of ionic character

\[ \left( \frac{I^2}{I^2} \right) (E_{AB}^0 - E_i)^2 = \triangle Z e^4 J^2 / 2 = \frac{1}{4} (x_A - x_B)^2 \]  \hspace{1cm} (6)

If we put \( J = \left| A(1) B(1) \right| r_{AB} \) where we assume \( L \) is 0.65, the value of hydrogen-like wave function 1S and 2S at about \( r_{AB} \approx 2A \), and \( E_{AB}^0 - E_i \approx 90 \) Kcal/mol (7) when \( \triangle Z \) 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).