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ROLE OF MNDO APPROXIMATION METHOD IN MOLECULAR PROPERTIES & STRUCTURAL CHEMICAL ASPECTS

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ABSTRACT

As the quantum mechanics developed and advanced, the scientists working in this field tried to explain the various aspects of electronic structure of chemical species. The invention of computer and their application to quantum chemistry gave a strong base for thorough study. Starting from hydrogen atom they are now capable to get more detailed discussion of the actual calculation of orbital for many electron systems. The LCAD approximation from Hartee (Hartee & D. R. Proc, 1978) – Fock orbitals (Fock, V:Z – Physik, 1930) to Rootham equation (C.C.J. Rootham, 1951) served as theoretical basis for approximate molecular orbital theories which are by nature semi – empirical. In semi – empirical methods the molecular properties are not only derived for the principles of quantum mechanics but are also use to interprete and correlate the theoretical data with the experimental data.

KEYWORDS: LCAD, MNDO

Various approximation theories were given from time to time to explain various structural aspects which are commonly known as CNDO (Pople et. al., 1965) (Complete neglect of differential overlap) CNDO/1, CNDO/2 (Pople and Segal, 1966), INDO (Intermediate Neglect of differential overlap), MINDO (Bingham et. al., 1975). But the chemist interested in this field were still in search of an approximation method which would give an accurate reliable and involving less computational time for the quantitative treatment of molecular properties. The advancement & further development of this method are commonly known as A.M.-I (Austin Model-I) P.M.-3 (Parametric method number -3) are also use recently.

METHODOLOGY

M.J.S. Dewar and his co-workers positioned a milestone in this field by developing MNDO (Dewar and Thiel, 1977) (Modified Neglect of diatomic overlapping) approximate method. This involve the use of atomic parameters instead of pair parameters which were used in previous approximation method. The data and statistics by using MNDO approximation for heat of formation, molecular geometries, Ionization – Potential, dipole-moment and charge distribution were quite close to experimental observation. The data obtained from MNDO method about eigen-values, Atomic Orbital Electron Population, bond-length, bond–angle twist-angle, dihedral-angle, inter atomic distance and other various thermodynamic and structural properties were very accurate when compared to experimental values. It contributed upto a large extent in study of reaction mechanism and verification of other synthetic aspects. Although MNDO approximately method is not accurate in all cases but this method dominated over previous approximation methods.

For getting the softness values of in ion or atom Klopman equation (Klopman, 1968) is to be solved. The Klopman equation is given below:-

Klopmann Equation

$$Em^{\neq} = IP_m - a^2(I P_m - E_{Am}) - Xr (C_r^m)^2 \text{----------} (1\text{-}1/\epsilon) [q_r + 2 b^2 Xr(C_r^m)^2]$$

Rr

$$En^{\neq} = IP_n - b2 (IP_n\text{-}E_{An}) - Xs(C_s^n)^2 \text{----------} (1 - 1/\epsilon) [q_s +2b^2 xs(C_s^n)^2]$$

Rs

Where $Em^{\neq}$ = softness of Lewis base.

$En^{\neq}$ = Softness of Metal ion. (Lewis acid)

IP = Ionization potential of atom.

E_A = Electron affinity of atom.

e = Dielectric constant of the medium in which reaction is carried.

R & q = Radius and charge of atom s & r.

C = electron density

$X = q-(q^{-1}) K$ and $K = 0.75$

a & b = Variational parameter defined as $a^2+b^2 = 1$

RESULTS AND DISCUSSION

For the solution of Klopman equation of neutral molecule we invariably used to obtain the values of Ionization potential (I.P.), electron affinity (E_A) charge (q) on the atom and electron density (C).

The above values were available for single atom or ions but for bigger molecule these values were not available. Singh et. al., 1992 developed method for

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evaluation of Ionization potential (I.P.), electron affinity (E_A) charge (q) on the atom and electron density (C) for simple molecules but these values only approximate. The MNDO (Modified Neglect of Diatomic Overlap) approximation method calculation developed by Dewar M.J.S. have made it possible to obtained Ionization potential (I.P.), electron affinity (E_A) charge (q) and electron density (C) of any atom in a molecule containing 70 or 80 atoms. With the help of MNDO approximation method calculation we have been able to evaluate softness parameters at any site in a molecule.

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