

**STUDY OF ELECTRON AFFINITY FROM GAUSSIAN FORM
REPUSSION TERM POTENTIAL FUNCTION FOR
POLAR DIATOMIC MOLECULES**

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Theoretical methods (Pritchard, 1953) yield very divergent values of electron affinity of elements, which are also not in good agreement with the experimental values. Present communication reports a method of calculating the electron affinity of an element in the case of polar molecules using gaussian form repulsion term potential function.

The study of potential functions (Bleick and Mayer, 1934; Kunzmuir, 1950; Rice and Klempeter, 1957; Varshni, 1957; Varshni and Shukla, 1961) reveals that gaussian form repulsion term adequately includes the polarization, Vander wall and short range repulsion effects. Such a function may be represented by

$$U = (-e^2/r) + A \exp(-br^2) \quad \dots (1)$$

where A and b are constants and other symbols have usual meaning. Applying the following condition of suitability to equation (1)

$$\left. \begin{aligned} U(0)_{r=r_e} &= -D_e \\ (dU/dr)_{r=r_e} &= 0 \\ \text{and} \quad (d^2U/dr^2)_{r=r_e} &= -k_e \end{aligned} \right\} \quad \dots (2)$$

and then using the relation equation (3) (Gaydon, 1953)

$$D_e = D_e + I - E \quad \dots (3)$$

we get the relation equation (4), connecting the electron affinity (E), dissociation energy (D_e), ionization potential (I), force constant for infinitesimal amplitude (k_e) and equilibrium internuclear distance (r_e)

$$E = D_e + I - \frac{e^2}{r_e} \left[1 - \left\{ \frac{k_e r_e^3}{e^2} + 3 \right\}^{-1} \right] \quad \dots (4)$$

To show the applicability of this relation, the electron affinity of chlorine atom in the case of NaCl molecule has been calculated. The k_e , r_e and D_e values have

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been taken from the data of Tandon and Tandon (1964). The values of ionization potential are taken from Hodgman's data (1963). The result obtained is compared with that obtained by other theoretical and experimental methods (Table I). It is of interest to note that the linear extrapolation methods yield higher values whereas the quadratic ones yield lower ones. The values obtained by equation (4) are in close agreement with the observed magnetron and electron impact methods.

This method has been applied to calculate electron affinities of twenty elements in about one hundred and fifty diatomic molecules. The results are in good agreement with experimental values (Pritchard, 1953, Page, 1965).

TABLE I

Comparison of values of electron affinity $E(e.v)$ of chlorine atom by different methods

$E(e.v)$	Method	Author
3.9183 ± 0.05	by equation (4)	Present
4.8	linear extrapolation of ionization potential	Pritchard (1953)
3.7	quadratic extrapolation of ionization potential	Glockler*
3.1	do	Bates*
3.05	do	Pritchard (1953)
3.58 ± 0.13	surface ionization measurements	Dukel'ski and Tonov
3.913	lattice energies	Pritchard (1953)
3.93 ± 0.174	magnetron	Mitchell and Mayer (1940)
3.724 ± 0.434	do	James <i>et al.</i> (1943)
3.999 ± 0.26	electron impact	Hanson*

*From Pritchard (1953)

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