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Dissociation Energy of the Ground Electronic State of MgO

M. M. Chaudhari
Dept. of Physics,
Maharashtra Mahavidyalaya,
Nilanga, Dist. Latur

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ABSTRACT

Dissociation Energy (D_e) of the ground electronic state of MgO is estimated from H-H, Materra and Extended Rydberg function. D_o values obtained from H-H and Materra functions are 3.76 eV and 3.48 eV respectively. They are in best agreement with experimental D_o value of 3.76 eV. Curve obtained from Extended Rydberg function fits best to RKRV curve as compared to other functions.

Introduction:

The potential energy measured from the minimum of the potential energy curve to the asymptotic part running parallel to the inter-nuclear distance is the dissociation energy De of the diatomic molecule.

$$D_e = D_o + G(o) \qquad \text{----------(1)}$$

Where D_o = Zero point energy of the electronic state.

$$G(o) = (\omega_e/2) - (\omega_e x_e/4) + (\omega_e y_e/8) - \ldots\ldots \qquad \text{----------(2)}$$

Dissociation energy of the diatomic molecule can be estimated by various ways. Mass spectrometric studies, pre-dissociation methods, flame photometric studies are some of the laboratory methods to determine D_e. The most commonly used method to determine D_e is the method of curve fitting. In this method RKRV curve of an electronic state of a diatomic molecule is determined. Potential energy curve determined from an

empirical function is allowed to fit to RKRV curve for a particular value of D_e. The potential function which matches the best to RKRV curve gives the estimate of D_e of a diatomic molecule under study.

D_e of MgO molecule is still uncertain. Experimental value of D_o reported [1-2] is 3.71 eV. Various workers [3-9] reported D_o values ranging from 2.80 eV to 4.34 eV. Looking at the variation in the value of D_o reported by different workers, it was thought to apply new potential function to the ground electronic state of MgO such as H-H [10-11], Materra [12] and Extended Rydberg [13] to estimate D_o of MgO.

Theory:

RKRV Method

This method is developed by Rydberg [14-15] and Klein [16]. It is further modified by Rees [17] and Vanderslice [18]. This method is based upon phase integrals and WKB [19-21] approximations, where the use of molecular constants determined from experimental data are made to construct potential energy curve. This is an established method of representing true potential energy curve of an electronic state of a diatomic molecule. According to this method the turning points are given by

$$r \pm = [(f/g) + f^2]^{1/2} \pm f \qquad \text{----------(3)}$$

where $r^+ = r_{max}$ and $r_- = r_{min}$

$$G(v) = \omega_e (v+½) - \omega_e x_e (v+½)^2 \qquad \text{----------(4)}$$

$$B(v) = B_e - \alpha (v+½) \qquad \text{----------(5)}$$

Hulbert Hirschfelder (H-H) function

This function is the modification of Morse function and is of the form [10-11]

$$U_{H\text{-}H}(r) = D_e [(1-e^{-x})^2 + Cx^3 e^{-2x} (1+bx)] \qquad \text{----------(6)}$$

Materra function

This method is based on series expansion and is given by [22]

$$V(x) = d_0 F^2(x) [1 + d_1 F(x) + d_2 F^2(x) + ...] \qquad \text{----------(7)}$$

The coefficients di are determined in terms of Dunham coefficients ai by equating the derivatives at x = 0 for V(x).

Extended Rydberg function

Huxley and Murrel [13] suggested a 3 parameter function based on the use of

Where a_1, a_2, a_3 are the constants obtained from harmonic ,cubic and quartic force constants. $\beta = r\text{-}r_e$ and D_e = dissociation energy.

Estimation of D_e of MgO

D_e of MgO is estimated using H-H, Materra and Extended Rydberg function. Details of the equations used in this paper can be obtained from the respective reference. Molecular constants are taken from Huber [23]. Constants derived to solve the above functions are presented in table 1. Corrected value of ?e [24] of MgO = 785.1 is used. RKRV turning points are determined using equation 3. A computer program is developed to plot the RKRV curve. 15 vibrational levels are used. The turning points and G(v) values are shown in table 2. RKRV curve is plotted in figure 1. Substituting these G(v) values and the corresponding r values in equation 6 of H-H function, D_e of H-H is determined. Similar method is used to compute D_e of Mattera function from equation 7.

RKRV turning points are used to calculate the G(v) values from extended Rydberg function. Experimental De = 3.76 eV is used. G(v) determined from H-H, Materra and Extended Rydberg function are presented in table 2. D_e values obtained from H-H and Materra functions are 3.76 eV and 3.48 eV respectively. They are in best agreement with experimental D_e value of 3.76 eV. RKRV curve along with H-H, Materra and Extended Rydberg are shown in figure 1. All these curves fit to RKRV curve to a good extent. Curve obtained from Extended Rydberg function fits best to RKRV curve as compared to other functions.

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Table 1 : Constants of H-H, Materra and Extended Rydberg function

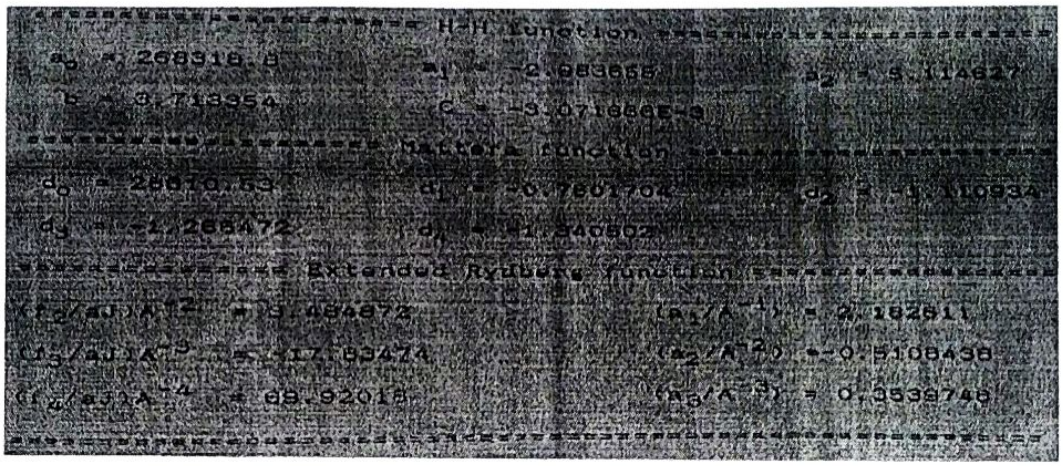


Table 2 : RKR turning points and G(v) values determined using H-H, Materra andExtended Rydberg function for ground state of MgO.

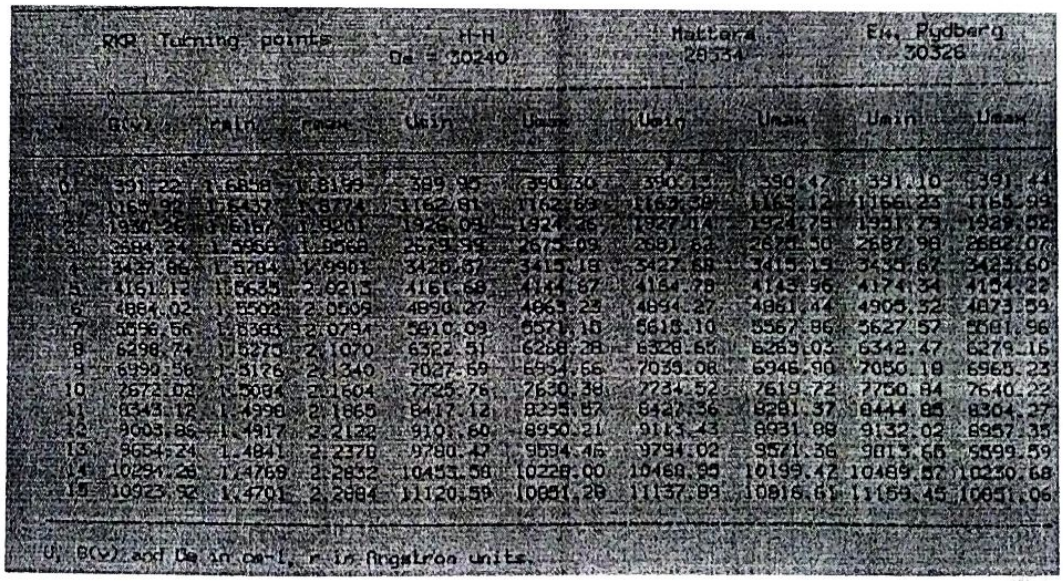
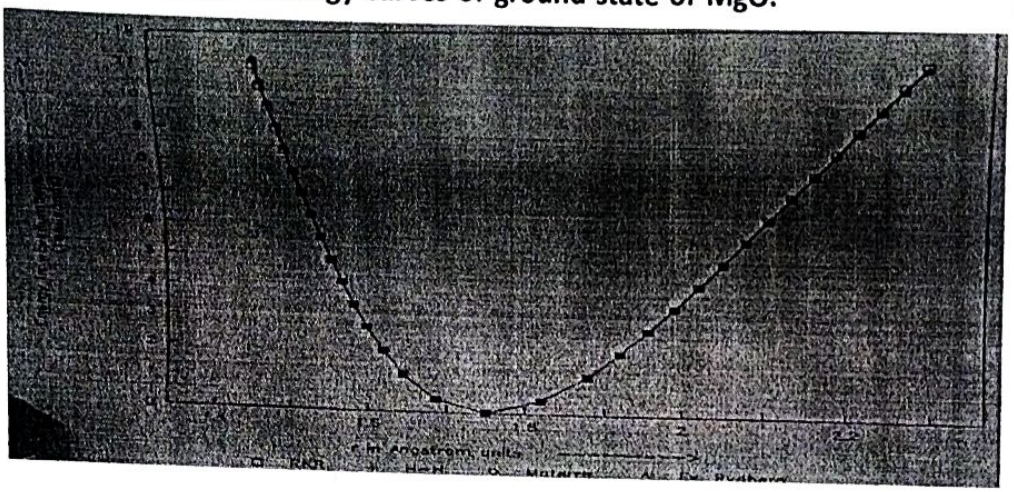


Figure 1 : Potential energy curves of ground state of MgO.



References :-

[1] Srivastava R D, High temp Sc., 8, 255,1976
[2] Farber M, Srivastava R D, High temp Sc., 8, 195, 1976
[3] Drowart J, Exsteen G, Varhagen G, Trans Far Soc, 60, 1920, 1964
[4] Veits I V, Guvrich L V, Z Phys Chem, 31, 2306, 1957
[5] Witko M, Bonacie-Koutecky, Intl J Qtm Chem, 29, 1535, 1986
[6] Thummel H, Klotz R, Peyerimhoff S D, Chem Phys, 129, 417, 1989
[7] Langhoff S R, Bauschlicher Jr, Partridge, J Chem Phys, 84, 4470, 1986
[8] Murthy N S, Bagare S P, J Phys B: Atom Mole Phys, 114, 623, 1978
[9] Badri Rai, Rai S N, Ind J Pure App Phys, 10, 401, 1972
[10] Hulbert H M, Hirschfelder J O, J Chem Phys, 9, 61, 1941
[11] Hulbert H M, Hirschfelder J O, J Chem Phys, 35, 1901, 1961
[12] Mattera L, Salvo C, Terreni S, Tommasini F, J Chem Phys, 72, 2, 1980
[13] Huxley P, Murrel, J Chem Soc Fara II, 79, 223, 1983
[14] Rydberg R, Z Phys, 73, 376, 1931
[15] Rydberg R, Z Phys, 80, 514, 1933
[16] Klein O, Z Phys, 76, 226, 1932

[17] Rees A L G, Proc Phys Soc,59, 998, 1947

[18] Vanderslice J T, Meson E A Maisch W G, Lippincott E R, J Chem Phys, 33, 614, 1960; J Mole Spectros, 3, 17, 1959 and 5, 83, 1960

[19] Wentzel G, Z Physik, 38, 518, 1926

[20] Kramers H A, Z Physik, 39, 828, 1926

[21] Brillouin L, Z Physik, 7, 353, 1926

[22] Mattera L, Salvo C, Terreni S, Tommasini F, J Chem Phys, 72, 12, 6815, 1980

[23] Huber K P, Herzberg G, Constants of diatomic molecules, IV ed., 1979

[24] Ikeda J, Wong N B, Harris D O, Field R W, J Mole Spectros, 68,452, 1977