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## Dissociation Energy of the Ground Electronic State of MgO

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Research Paper - Physics

### ABSTRACT

Dissociation Energy ( $D_e$ ) of the ground electronic state of MgO is estimated from H-H, Materra and Extended Rydberg function.  $D_0$  values obtained from H-H and Materra functions are 3.76 eV and 3.48 eV respectively. They are in best agreement with experimental  $D_0$  value of 3.76 eV. Curve obtained from Extended Rydberg function fits best to RKR 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  $D_e$  of the diatomic molecule.

$$D_e = D_0 + G(0) \quad \text{-----(1)}$$

Where  $D_0$  = Zero point energy of the electronic state.

$$G(0) = (\omega_e/2) - (\omega_e x_e/4) + (\omega_e y_e/8) - \dots \quad \text{-----(2)}$$

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  $D_0$ . The most commonly used method to determine  $D_e$  is the method of curve fitting. In this method RKR curve of an electronic state of a diatomic molecule is determined. Potential energy curve determined from an



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

$D_e$  of MgO molecule is still uncertain. Experimental value of  $D_0$  reported [1-2] is 3.71 eV. Various workers [3-9] reported  $D_0$  values ranging from 2.80 eV to 4.34 eV. Looking at the variation in the value of  $D_0$  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  $D_0$  of MgO.

**Theory:**

**RKR 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

$$r_{\pm} = \left[ \left( \frac{f}{g} \right) + f^2 \right]^{1/2} \pm f \quad \text{-----(3)}$$

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

$$G(v) = \omega_e (v + \frac{1}{2}) - \omega_e x_e (v + \frac{1}{2})^2 \quad \text{-----(4)}$$

$$B(v) = B_e - \alpha (v + \frac{1}{2}) \quad \text{-----(5)}$$

**Hulbert Hirschfelder (H-H) function**

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

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

**Materra function**

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

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



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

### Extended Rydberg function

Huxley and Murrell [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.  $\beta = r - r_e$  and  $D_e =$  dissociation energy.

### Estimation of $D_0$ of MgO

$D_0$  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  $\rho_e$  [24] of MgO = 785.1 is used. RKR turning points are determined using equation 3. A computer program is developed to plot the RKR curve. 15 vibrational levels are used. The turning points and  $G(v)$  values are shown in table 2. RKR curve is plotted in figure 1. Substituting these  $G(v)$  values and the corresponding  $r$  values in equation 6 of H-H function,  $D_0$  of H-H is determined. Similar method is used to compute  $D_0$  of Materra function from equation 7.

RKR turning points are used to calculate the  $G(v)$  values from extended Rydberg function. Experimental  $D_e = 3.76$  eV is used.  $G(v)$  determined from H-H, Materra and Extended Rydberg function are presented in table 2.  $D_0$  values obtained from H-H and Materra functions are 3.76 eV and 3.48 eV respectively. They are in best agreement with experimental  $D_0$  value of 3.76 eV. RKR curve along with H-H, Materra and Extended Rydberg are shown in figure 1. All these curves fit to RKR curve to a good extent. Curve obtained from Extended Rydberg function fits best to RKR curve as compared to other functions.

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

```

===== H-H function =====
a0 = 268318.8          a1 = -2.083858          a2 = 5.114627
b = 0.718954          c = -3.071866E-9
===== Materra function =====
d0 = 28070.63        d1 = -0.7601704        d2 = -1.110934
d3 = -2.285472        d4 = 41.840502
===== Extended Rydberg function =====
(r2/a0)A-2 = 13.484872          (a1/A-1) = 2.182811
(r3/a1)A-3 = -17.93474          (a2/A-2) = -0.5108438
(r4/a2)A-4 = 69.92018          (a3/A-3) = 0.3538748
  
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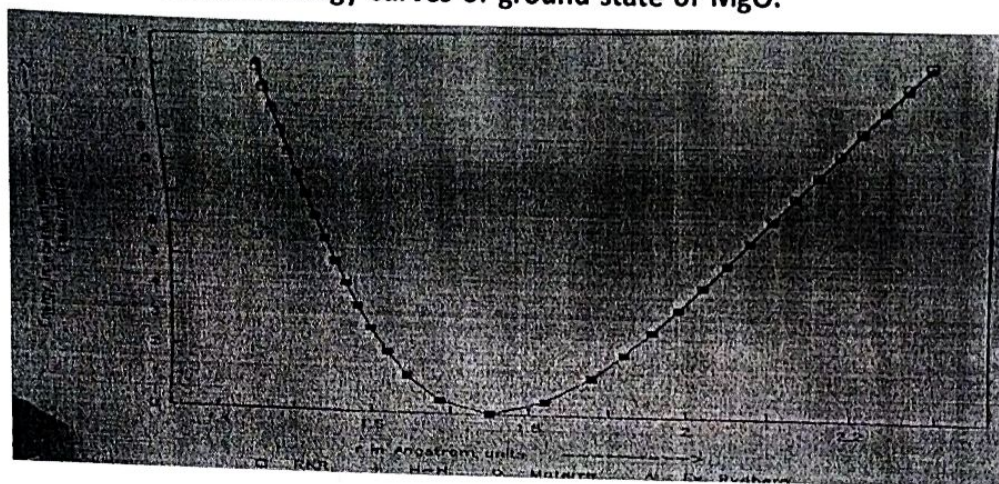
Table 2 : RKR turning points and G(v) values determined using H-H, Materra and Extended Rydberg function for ground state of MgO.

| v  | RKR turning points    |        | H-H<br>D <sub>e</sub> = 30240 |                  | Materra<br>28554 |                  | Ext. Rydberg<br>30328 |                  |          |
|----|-----------------------|--------|-------------------------------|------------------|------------------|------------------|-----------------------|------------------|----------|
|    | B(v)/cm <sup>-1</sup> | r(v)/Å | U <sub>min</sub>              | U <sub>max</sub> | U <sub>min</sub> | U <sub>max</sub> | U <sub>min</sub>      | U <sub>max</sub> |          |
| 0  | 5911.22               | 1.6858 | 1.8189                        | 399.90           | 390.30           | 390.73           | 390.47                | 391.10           | 391.44   |
| 1  | 1150.99               | 1.7537 | 1.8774                        | 1162.91          | 1162.89          | 1169.59          | 1163.12               | 1166.23          | 1165.99  |
| 2  | 1930.26               | 1.8157 | 1.9201                        | 1726.03          | 1924.76          | 1927.14          | 1924.79               | 1931.73          | 1929.02  |
| 3  | 2584.24               | 1.8666 | 1.9568                        | 2373.93          | 2575.03          | 2591.62          | 2582.30               | 2587.98          | 2582.07  |
| 4  | 3427.66               | 1.9204 | 1.9901                        | 3126.57          | 3415.18          | 3427.68          | 3415.13               | 3430.67          | 3423.60  |
| 5  | 4161.12               | 1.9683 | 2.0213                        | 4161.69          | 4144.67          | 4144.78          | 4143.96               | 4174.34          | 4154.22  |
| 6  | 4884.02               | 1.9902 | 2.0509                        | 4990.27          | 4863.23          | 4894.27          | 4861.44               | 4905.52          | 4873.59  |
| 7  | 5596.56               | 1.9993 | 2.0794                        | 5910.09          | 5571.10          | 5618.10          | 5567.86               | 5627.57          | 5581.96  |
| 8  | 6298.74               | 1.9979 | 2.1070                        | 6322.51          | 6266.28          | 6328.66          | 6263.05               | 6342.47          | 6279.16  |
| 9  | 6999.56               | 1.9916 | 2.1340                        | 7027.69          | 6954.66          | 7039.08          | 6948.90               | 7050.19          | 6963.23  |
| 10 | 7672.03               | 1.9694 | 2.1604                        | 7725.76          | 7630.38          | 7734.52          | 7619.72               | 7750.84          | 7640.22  |
| 11 | 8343.12               | 1.9398 | 2.1866                        | 8417.12          | 8293.67          | 8427.56          | 8281.37               | 8444.88          | 8304.27  |
| 12 | 9003.86               | 1.8917 | 2.2122                        | 9101.60          | 8950.21          | 9113.43          | 8931.88               | 9132.02          | 8967.35  |
| 13 | 9654.24               | 1.8441 | 2.2378                        | 9780.47          | 9594.46          | 9794.02          | 9571.36               | 9813.66          | 9599.59  |
| 14 | 10294.26              | 1.7469 | 2.2632                        | 10453.58         | 10228.00         | 10468.95         | 10199.47              | 10489.67         | 10230.68 |
| 15 | 10923.32              | 1.4701 | 2.2884                        | 11120.59         | 10851.26         | 11137.89         | 10816.61              | 11159.45         | 10851.06 |

U<sub>i</sub>, B(v)<sub>i</sub> and D<sub>e</sub> in cm<sup>-1</sup>, r in Angstrom units



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



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