

# Potential energy curves and dissociation energies for some diatomic molecules by using two different functions

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## Abstract:

This study has been carried out of calculating potential energy curves (Deng-Fan potential and Morse potential) of ground state and dissociation energies of diatomic molecule (AlBr, AlI). Potential energy curves and dissociation energies depended on spectroscopic Parameters ( $\omega_e$ ,  $\omega_e x_e$ ,  $r_e$ ,  $\alpha$ ,  $\mu$ ,  $\beta$ ).

**Keywords:** diatomic molecule, Potential energy function

## Introduction:

A potential energy curve is a graphical representation of the change in potential energy of the molecule as a function of the distortion of the bond of the molecule from its equilibrium distance. The knowledge of potential energy curves is of prime importance in the study of diatomic molecular spectra [1]. In the calculations of Franck Condon factor, dissociation energy and thermodynamic quantities etc, the studies of potential energy curves are necessary. The empirical potential energy functions like Morse [2] and Deng-Fan potential [3] are usually applied and the potential energy curves are drawn. Naturally to compute the turning points of various vibrational levels the accurate spectroscopic constants are required. The empirical potential energy functions also require these molecular constants.

## Theory:

### Potential energy functions and Dissociation energy:

The height of an asymptote of a potential energy curve, above the lowest vibrational level, is equal to the work that must be done in order to dissociate that molecule, and is known as the heat of dissociation or dissociation energy  $D_0$ . Another constant  $D_e$  is also the dissociation energy but it is taken as a height of an asymptote from x-axis or measured from minima of the potential energy curve. The relation between  $D_0$  and  $D_e$  is here [4]

$$D_e = D_0 + G(0) \dots\dots\dots (1)$$

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

$$D_e = \Delta G_{\max}(v) \dots\dots\dots (3)$$

The relation in defining the dissociation energy  $D_e$  in terms of molecular constants is

$$D_e = \omega_e^2 / 4\omega_e x_e \dots\dots\dots (4)$$

One of functions of potential is Morse function which had written as [5]:

$$U(x) = D_e (1 - e^{-\beta x})^2 \dots\dots\dots (5)$$

$$x = r - r_e$$

$$\beta = \left[ \frac{8\pi^2 \mu (\omega_e \chi_e) c}{h} \right]^{1/2} \dots\dots\dots(6)$$

where  $\beta$ ,  $r_e$ ,  $\omega_e \chi_e$  spectroscopic constants,  $\mu$  : reduced mass,  $c$ : speed of light and  $h$  :plank constant.

On the other hand, another function of potential called Deng-Fan potential function has the form[3]:

$$U_{Deng-Fan}(r) = P_1 + \frac{P_2}{e^{\alpha r} - 1} + \frac{P_3}{(e^{\alpha r} - 1)^2} \dots\dots\dots(7)$$

$P_1=D_e$  ;  $P_2=-2D_e (e^{\alpha r_e} - 1)$  ;  $P_3=D_e (e^{\alpha r_e} - 1)^2$  ;  $\alpha$ : spectroscopic parameter

**Results and discussion:**

In the present work, the spectroscopic parameters for diatomic molecule (AlBr and AlI) are summarized in table1 [1,6,7], dissociation energy is obtained using (eq.4) compared with another energy. and potential energy curves for two functions began with Morse potential function for ground state (eq. 13) and other function "Deng- Fan potential function " for ground state (eq. 14).

Table 1. Spectroscopic parameters of ground state of AlBr and AlI molecules measured in (cm<sup>-1</sup>) and  $r_e$  in (Å°) [1,6]

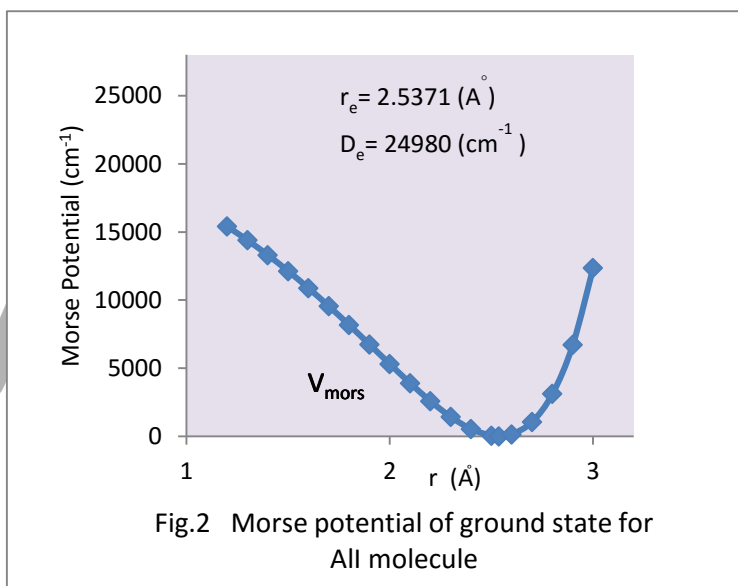
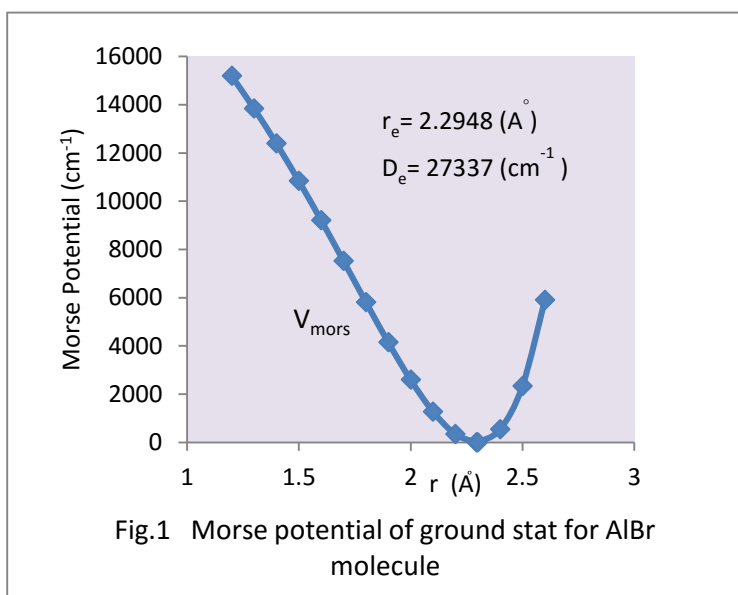
parameter	AlBr	AlI
$\omega_e$	378.1	316.1
$\omega_e \chi_e$	1.307	1
$r_e$	2.2948	2.5371
$B_e$	0.1591	0.1176
$\alpha$	0.0008	0.0005
$\mu$ a.m.u	20.107	22.25

The  $D_e$  value of these molecule is found to be (27343 cm<sup>-1</sup>) for ground state of AlBr molecule, and (24979 cm<sup>-1</sup>) for ground state of AlI molecule that dissociation due to approaching the bond length ( $r$ ) from infinity values, where this is one of three conditions of potential curve. These results are in good agreement with the experimental values[1] as in table below.

Table 2. Dissociation energy of ground state of AlBr and AlI molecules measured in (cm<sup>-1</sup>)

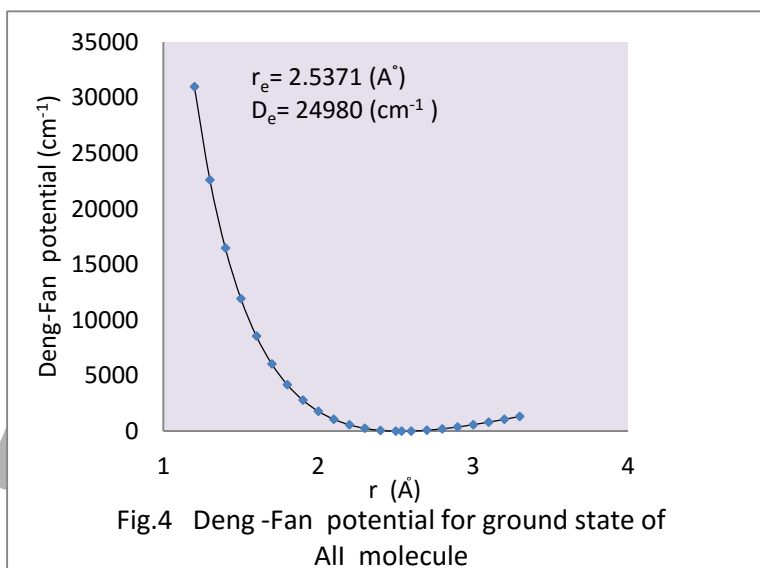
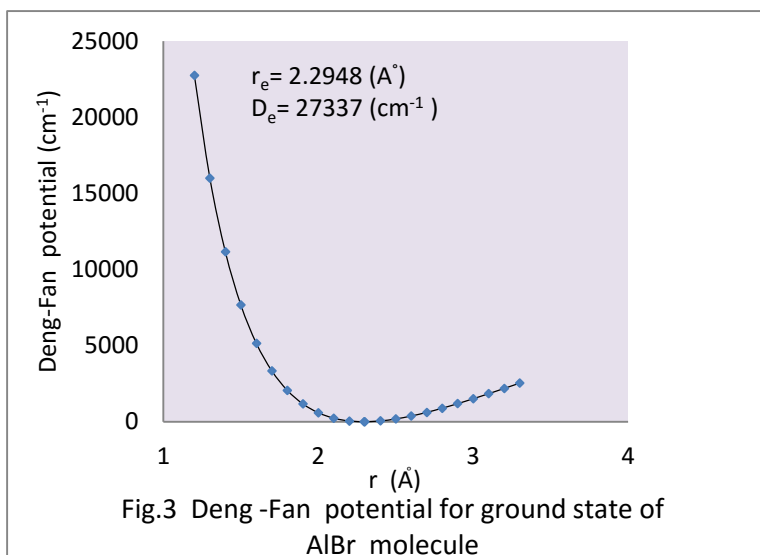
Result	AlBr	AlI
Calc.	27343	24979
Expt. [1]	27227	23889

This theoretical values are agreement with experimental results. In calculating Morse potential for these molecules (eq. 5) is used for the ground state, and here are the results as figures (1,2).



The calculations of two molecules appeared the maximum value of Morse potential is at ( $r = 1.2 \text{\AA}$ ) that mean the minimum value of bond length give us maximum potential in ground state of these molecules. At bond length ( $r = 2.2984 \text{\AA}$  and  $2.5371 \text{\AA}$ ), the potential equal (zero), then the potential increase by increasing bond length until reach at the point which happen in it the dissociation because that the diatomic molecules dissociate when the value of ( $r$ ) increase to determinate limit.

To calculate Deng-Fan potential for AlBr and All molecules eq. (7) is used for the ground state by depending on dissociation energy, bond length, spectroscopic constants in table 1, and here are the results of Deng-Fan potential for these molecules in figure (3,4).



The calculations of these molecules appeared the maximum value of Deng-Fan potential is at ( $r = 1.2 \text{ \AA}$ ) that mean there are similarity in the behavior of this curve comparing with Morse potential for these molecules at all values of ( $r$ ).. At bond length ( $r = r_e$ ), the potential equal (zero), the dissociation happen after that because the diatomic molecule dissociate when the value of ( $r$ ) increase to determinate limit.

**Conclusions:**

The potential curves of AlBr and All molecules by using Morse function for ground state is agreement rather than with results Deng-Fan potential and the important notice that bond length ( $r$ ) with spectroscopic constants have an effect upon values of the potential. In general all values of potentials in beginning be high and decrease with increasing bond length and after ( $r=r_e$ ) be increasing in the values with increasing values of ( $r$ ). Dissociation energies for these molecules for ground state very convergence with experimental dissociation energies.

**References:**

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