

ISSN 2278 -134X

Original Article

Study of effect the rotation on Morse potential of the ground state of diatomic AlF, AlCl, AlBr and AlI molecules

Adil Nameh Ayyash

Department of Physics, College of Science, University of Anbar, Anbar, Iraq.

E-mail: adil_nameh78@yahoo.com

Phone No. 009647903251427

Received 27 April 2015; accepted 26 April 2015

Abstract

The Morse and effective potential has been calculated for ground states of the Aluminum halides (AlF, AlCl, AlBr and AlI) molecules by using computer model, for the rotational quantum number $J = 150$. It has been found that the values of the rotation effective potential has larger values than that of Morse potential. A calculation of the rotation energies has been carried out for ground states. It was found that the rotation potential of the ground states for these molecules decrease with increasing the internuclear distance (r).

© 2015 Universal Research Publications. All rights reserved

Keywords: AlF, AlCl, AlBr and AlI molecules, ground state, Morse potential.

1. Introduction:

Spectroscopic investigations on the diatomic halides of aluminum have been the subject of much interest for a long time and the Aluminum monohalides play an important role in all fields. A potential energy curve is a graphical representation of the change in potential energy of the molecule as a function of the distribution 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 spectra [1]. The ground state of all Aluminum monohalides is of the $^1\Sigma^+$ similar to other diatomic molecules formed by IIIA group elements (e.g., B, Ga, and In) with halogens (e.g., F, Cl, Br, and I). Naturally to compute the turning points of various vibrational levels the accurate spectroscopic constants are required. The empirical potential functions also require these molecular constants [2].

In 1976, rotational analysis of the $A^3\Pi-X^1\Sigma^+$ transition of AlF was studied by Kopp et al [3]. In 1989, the $A^3\Pi-X^1\Sigma^+$ transition of AlCl was studied by Mahieu et al [4]. And the rotational analysis of the 0-0 band of the $A^3\Pi-X^1\Sigma^+$ transition of AlCl was studied by Saksena et al [5]. In 1990, rotational analysis of the $A^3\Pi-X^1\Sigma^+$ transition of AlI was studied by Mahieu et al [6]. In 1996, the $A^1\Pi-X^1\Sigma^+$ transition of AlBr was studied by Fleming et al [7]. Recently comparison of RKR and Hulbert-Hirschfelder, extended Rudberg potential energy curves of ground states of diatomic aluminum halides molecules reported

by Londheet al [8]. The rotation effect on Morse potential for some diatomic molecules was studied by Al-Amiedy et al [9]. In the present work the spectroscopic constants of ground state $X^1\Sigma$ of AlF, AlCl, AlBr and AlI are used.

2. Theory:

The electronic state is represented, usually, by a potential curve which refers to position and values of energy for this state depending upon the internuclear distance r (bond length), where the potential is a function of the distance between the two atoms of this molecule according to a different electronic transitions. The Morse potential functions, which almost verify an experimental potential curve used in work is given by [10]:

$$U_{morse} = D_e \left(1 - e^{\beta(r-r_e)} \right)^2 \dots\dots\dots(1)$$

where D_e is a spectral dissociation energy, r_e is the equilibrium distance between two atoms, and β is a constant for each electronic state of molecule under investigation, which is related to the value of bending profile of potential curve and is given by :

$$\beta = \sqrt{\frac{8\pi^2 \mu (\omega_e \chi_e) c}{h}} \dots\dots\dots(2)$$

where μ is the reduced mass of molecule, c the velocity of light in vacuum and h Planck's constant. The effective potential U_{eff} equals Morse potential adding to centrifugal contribution of rotation [10], i.e:

$$U_{\text{eff.}} = U_{\text{morse}} + U_{\text{rot}} \dots \dots \dots (3)$$

$$U_{\text{rot}} = \frac{h}{8\pi^2 \mu r^2 c} J(J+1) \dots \dots \dots (4)$$

where r is the bond length and J the rotational quantum number.

3. Results and discussion:

In the present work, the calculations of the Morse potential and effect rotation on this potential at rotational quantum number $J=150$ for aluminummonohalides molecules (AlF , AlCl , AlBr and AlI) are presented by using computer model and by depended on spectroscopic constants for ground state $X^1\Sigma^+$ for these molecules as shown in table (1).

Where μ : reduce mass (a.m.u.), ω_e : the fundamental vibration frequency (cm^{-1}), $\omega_e x_e$: the anharmonicity constant (cm^{-1}), B_e : the rotational constant at equilibrium bond length (cm^{-1}), r_e : equilibrium bond length of the molecule (\AA) and α_e : the vibration – rotation interaction constant (cm^{-1}).

By using equation (4), U_{rot} for all aluminum halides is calculated and figure (1) shows the relation between rotation potential and internuclear distance, which appear that rotation potential is decrease with increasing (r) and maximum values for AlF but minimum values for AlI at rotation quantum number equal 150, that is due to the fact the constants of the AlF molecule are several orders of magnitude larger than that for the other molecules (AlCl , AlBr and AlI).

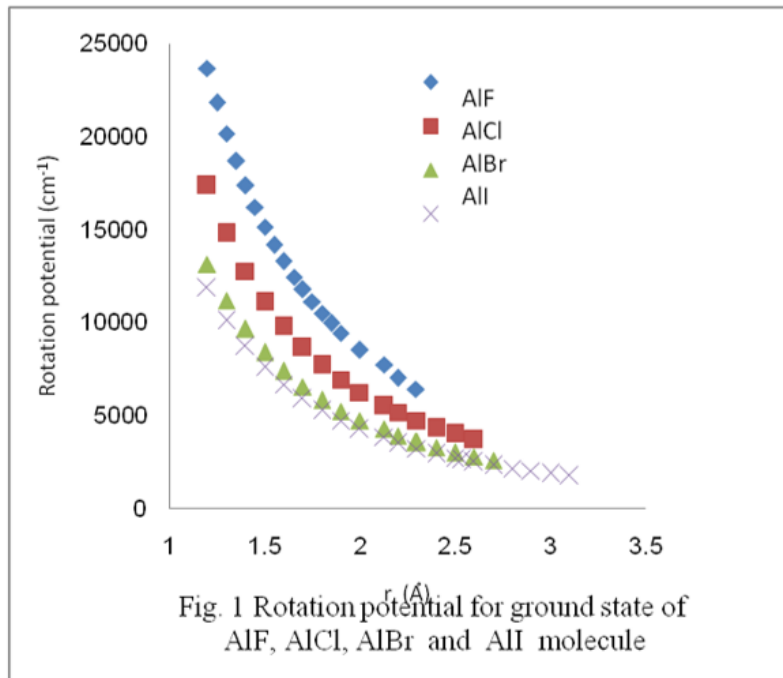


Fig. 1 Rotation potential for ground state of AlF , AlCl , AlBr and AlI molecule

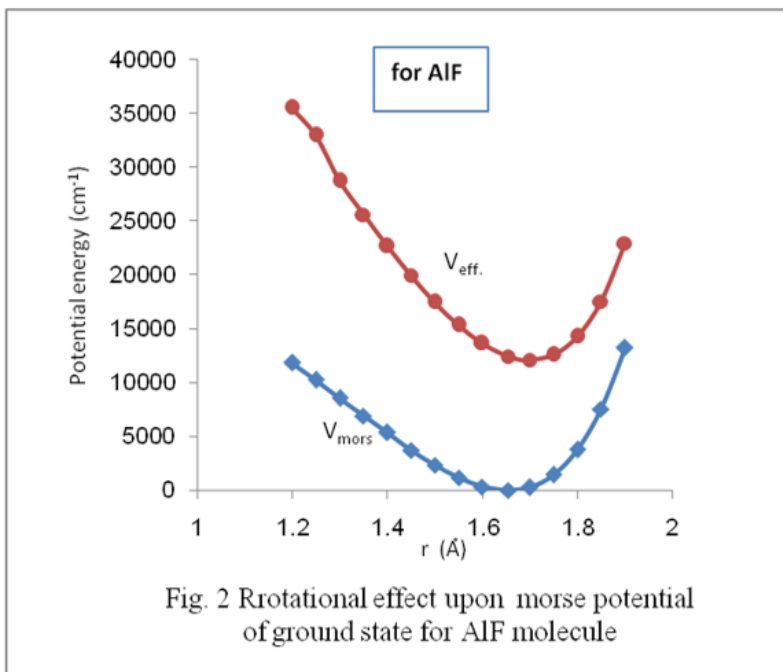


Fig. 2 Rotational effect upon morse potential of ground state for AlF molecule

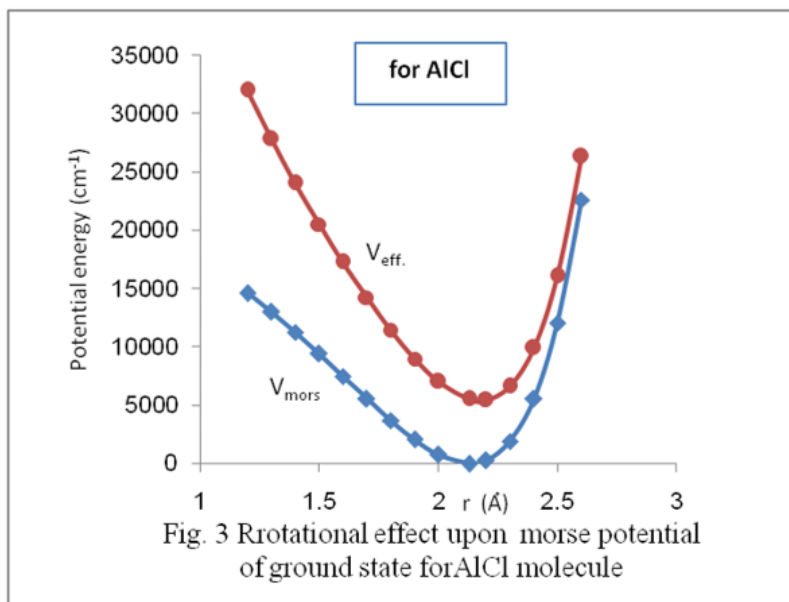


Fig. 3 Rotational effect upon morse potential of ground state for AlCl molecule

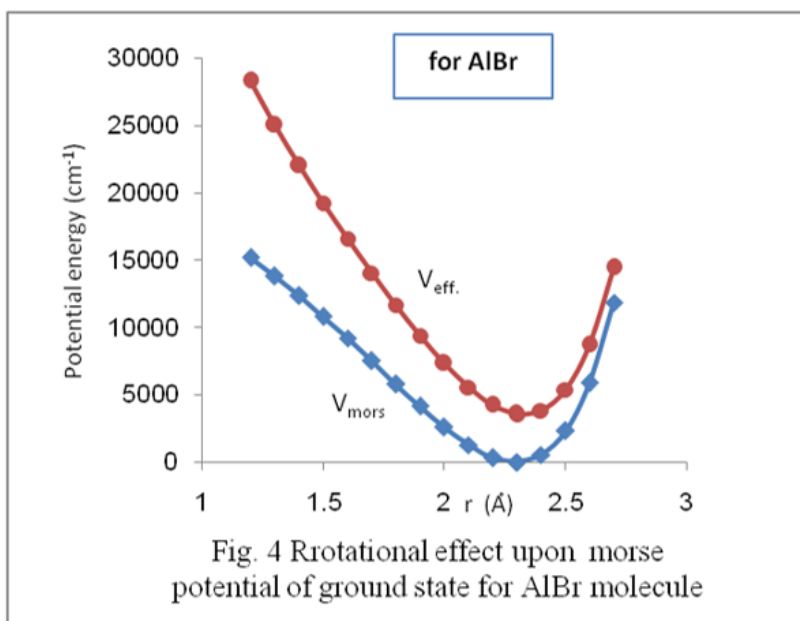


Fig. 4 Rotational effect upon morse potential of ground state for AlBr molecule

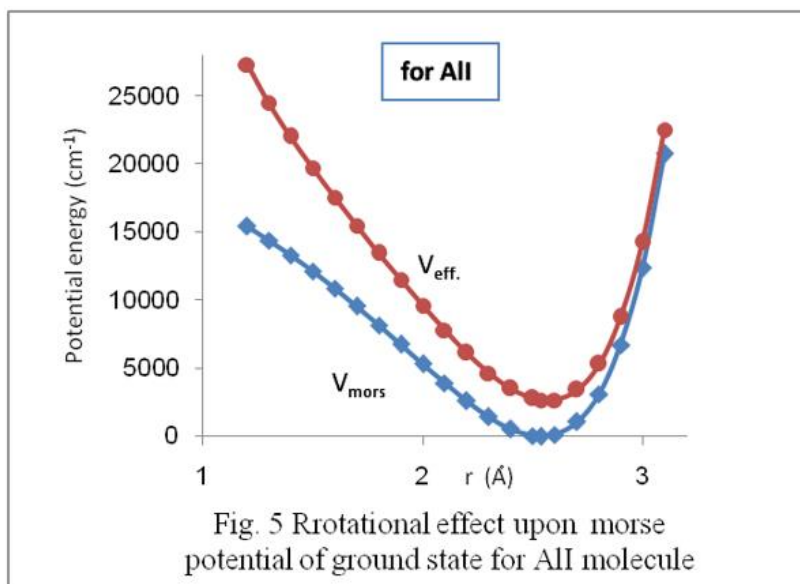


Fig. 5 Rotational effect upon morse potential of ground state for AlI molecule

Table 1. Spectroscopic constants of Aluminum halides of ground state measured in cm^{-1} , μ in a. m. u. and r_e in (\AA) [1,3,4,5,6,7]

molecule	Spectroscopic constants of ground state						
	μ	ω_e	$\omega_e X_e$	r_e	B_e	α_e	D_e
AIF	11.1484	802.26	4.77	1.6544	0.5524	0.0049	33732
AlCl	15.2301	481.4	2.037	2.1303	0.2439	0.0016	28442
AlBr	20.1070	378.10	1.307	2.2948	0.1591	0.0008	27337
AlI	22.2505	316.1	1	2.5371	0.1176	0.0005	24980

Table 2. Results of morse and effective potential after rotation effect for ground state of AIF molecule.

$r \times 10^{-8} \text{cm}$	For AIF molecule	
	$U_m (\text{cm}^{-1})$ AIF	$U_{\text{eff.}} (\text{cm}^{-1})$ AIF
1.2	11881.03	35571.13
1.25	10246.82	32979.61
1.3	8582.85	28768.49
1.35	6916.76	25634.86
1.4	5385.85	22690.82
1.45	3739.47	19964.79
1.5	2342.15	17503.81
1.55	1177.33	15376.6
1.6	352.03	13677.71
1.6544	0	12463.74
1.7	301.45	12105.51
1.75	1466.31	12605.49
1.8	3770.14	14299.07
1.85	7554.51	17522
1.9	13245.33	22950.52

Table 3. Results of morse and effective potential after rotation effect for ground state of AlCl molecule.

$r \times 10^{-8} \text{cm}$	For AlCl molecule	
	$U_m (\text{cm}^{-1})$ AlCl	$U_{\text{eff.}} (\text{cm}^{-1})$ AlCl
1.2	14626.31	32017.85
1.3	12996.85	27815.67
1.4	11248.71	24026.17
1.5	9401.5	20532.08
1.6	7489.18	17271.92
1.7	5565.72	14231.4
1.8	3712.7	11442.27
1.9	2049.67	8987.01
2	747.36	7008.31
2.13	0	5518.47
2.2	280.02	5454.36
2.3	1908.24	6642.42
2.4	5557.83	9905.71
2.5	12079.24	16086.25
2.6	22620.14	26324.84

Table 4. Results of morse and effective potential after rotation effect for ground state of AlBr molecule.

$r \times 10^{-8} \text{cm}$	For AlBr molecule	
	$U_m (\text{cm}^{-1}) \text{ AlBr}$	$U_{\text{eff.}} (\text{cm}^{-1}) \text{ AlBr}$
1.2	15193.55	28354.71
1.3	13843.8	25058.04
1.4	12390.19	22059.61
1.5	10840.46	19263.6
1.6	9209.47	16612.62
1.7	7521.93	14079.74
1.8	5815.93	11665.33
1.9	4147.6	9397.48
2	2597.15	7335.37
2.1	1276.85	5574.37
2.2	341.37	4257.04
2.2948	0	3598.87
2.3	1.1625	3583.78
2.4	539.93	3830.22
2.5	2337.23	5369.56
2.6	5897.71	8701.27
2.7	11888.97	14488.7

Table 5. Results of morse and effective potential after rotation effect for ground state of AlI molecule.

$r \times 10^{-8} \text{cm}$	For AlI molecule	
	$U_m (\text{cm}^{-1}) \text{ AlI}$	$U_{\text{eff.}} (\text{cm}^{-1}) \text{ AlI}$
1.2	15406.83	27283.98
1.3	14396.77	24516.94
1.4	13304.27	22030.34
1.5	12129.84	19731.21
1.6	10876.77	17557.66
1.7	9552.17	15470.19
1.8	8168.36	13447.09
1.9	6744.61	11482.31
2	5309.4	9585.17
2.1	3903.28	7781.53
2.2	2582.65	6116.34
2.3	1424.43	4657.52
2.4	532.15	3501.43
2.5	43.63	2780.12
2.5371	0	2657.04
2.6	140.77	2670.81
2.7	1061.91	3408.01
2.8	3117.95	5299.46
2.9	6711.71	8745.37
3	12363.79	14263.63
3.1	20744.8	22524.51

By using equations (1 and 4), U_{morse} and $U_{\text{eff.}}$ for all aluminum halides is calculated and tables (2,3,4 and 5) and figures (2,3,4 and 5) show the results of morse potential and effective potential after rotation effect for ground states for (AlF, AlBr, AlCl and AlI) molecules. It is evident that the rotation has a large effect on the potential. Also it obvious that the morse and the rotation effect have larger values due to the value of rotational quantum number and

rotation energy. All values of morse potential at (r_e) are equal zero for all molecules. Our results for potential before effect the rotation was in agreement with another researcher by using different potential function [8].

4. Conclusions:

The first main conclusion from this work that there is inverse relation between the rotation potential and internuclear distance, therefore rotation potential decrease

with increasing (r) and the second main conclusion is the rotation has a large effect on the morse potential and the effective potential has large values due to the value of rotational quantum number in rotation energy.

5. References:

1. G. Hertzberg, Spectra of diatomic molecules, Van Nostrand Reinhold Company, New York, (1950).
2. S.K. Mishra, Raj. K. S. Yadav, S. B. Rai, and V. B. Singh, J. Phys. Chem. Ref. Data. 33(2) 453 (2004).
3. Kopp, Lindgren, and Malmberg, Phys. Scr., 14 (1976) 170-174.
4. E. Mahieu, I. Dubois, and H. Bredohl, J. Mol. Spectrosc. 134 (1989) 317-328.
5. M. D. Saksena, D. S. Dixit, Mahavir Singh, J. Mol. Spectrosc., 187 (1989)1-5.
6. Mahieu, Dubois, and Bredohl, J. Mol. Spectrosc. 143 (1990) 359-365.
7. P. E. Fleming and C. W. Mathews, J. Mol. Spectrosc. 175 (1996) 31-36.
8. C. T. Londhe, N. H. Mhaske, S. H. Behere, IJETCAS 12-310 (2013)1-4.
9. D.H. Al-Amiedy, B.T. Chiad, Z.A. saleh, Atti Fond. G. Ronchi, 62, (2007)197-202.
10. G. GAYDON, Dissociation energies and Spectra of Diatomic Molecules, (Chapman andHall, 1968).

Source of support: Nil; Conflict of interest: None declared