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ORIENTAL JOURNAL OF CHEMISTRY
An International Open Access, Peer Reviewed Research Journal

www.orientjchem.org

ISSN: 0970-020 X
CODEN: OJCHEG
2022, Vol. 38, No.(5):
Pg. 1311-1313

Brief communication

Calculation of Vibrational Energies of AlH_2 Using U(2) Lie Algebraic Approach

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http://dx.doi.org/10.13005/ojc/380531

(Received: July 30, 2022; Accepted: October 21, 2022)

ABSTRACT

Using the U(2) Lie algebraic approach, it is determined that the vibrational energies of the aluminumdihydride (AlH_2) molecule up to the fifth overtone and reported the combinational bands up to the third harmonic.In this approach, the algebraic parameters and operators are used to represent the Hamiltonian operator to calculate the vibrational energies.

Keywords: Vibrational energies, U(2) Lie algebras, Hamiltonian operator, Aluminumdihydride

INTRODUCTION

The interpretation and analysis of the molecular spectra of molecules is a fascinating research area of molecular physics. Vibrational energies have played anvital role in both theoretical and experimental techniques due to their diverse applications. Vibrational spectra is currently undergoing an exciting period of renewed attention, fuelled by the rapid development of sophisticated experimental techniques. Due to their numerous applications in the research study of vibrational energies of molecules, one and three dimensional [U(2), U(4)] Lie algebraic approaches have grabbed the attention of a larger scientific community. With the use of these approaches, one can easily obtain the vibrational and rotational degrees of freedom in a physical problems[1]. The vibrational energies of a molecule are represented by the eigenvalues of the Hamiltonian matrix. These approaches are successful in the research study of polyatomic molecules vibrational spectra[2-7]. The vibrational and rotational energies are treated simultaneously in the U(4) Lie algebraic approach. When a molecule has more than four atoms, this approach becomes more complicated. To analyze the vibrational energies of aluminumdihydride, this limitation led us to utilize the U(2) Lie algebraic approach.

One dimensional Lie algebraic approach

A bent molecule with C_{2v} point group symmetry is aluminium dihydride.This aluminium dihydride molecule contains the symmetry species, A_1(Symmetric stretch), B_2(Antisymmetric stretch), and A_1(Bend).

For n vibrational modes, the general Hamiltonian[8-11] is

$$H = E_0 + \sum_{i=1}^{n} p_i b_i + \sum_{i<j}^{n} p_{ij} b_{ij} + \sum_{i<j}^{n} q_{ij} f_{ij} \quad (1)$$

In equation (1), b_i and b_{ij} are uncoupled and coupled bonds invariant operators, respectively, and knownas

$$\left\langle b_i \right\rangle = -4\left(N_i^{Al\text{-}O} \mathrm{v}_i - \mathrm{v}_i^2\right) \quad (2)$$

$$\left\langle N_i^{Al\text{-}O}, \mathrm{v}_i;\ N_j^{Al\text{-}O}, \mathrm{v}_j \middle| b_{ij} \middle| N_i^{Al\text{-}O}, \mathrm{v}_i;\ N_j^{Al\text{-}O}, \mathrm{v}_j \right\rangle = 4\left[\left(\mathrm{v}_i + \mathrm{v}_j\right)^2 - \left(\mathrm{v}_i + \mathrm{v}_j\right)\left(N_i^{Al\text{-}O} + N_j^{Al\text{-}O}\right)\right] \quad (3)$$

Majorana operator f_{ij} consist diagonal and non-diagonal matrix elements and it is useful to articulate the pair of local mode interactions[12].

$$\left\langle N_i^{Al\text{-}O}, \mathrm{v}_i; N_j^{Al\text{-}O}, \mathrm{v}_j \middle| f_{ij} \middle| N_i^{Al\text{-}O}, \mathrm{v}_i; N_j^{Al\text{-}O}, \mathrm{v}_j \right\rangle = \left(N_i^{Al\text{-}O}\mathrm{v}_j + N_j^{Al\text{-}O}\mathrm{v}_i - 2\mathrm{v}_i\mathrm{v}_j\right)$$

$$\left\langle N_i^{Al\text{-}O}, \mathrm{v}_i+1; N_j^{Al\text{-}O}, \mathrm{v}_j-1 \middle| f_{ij} \middle| N_i^{Al\text{-}O}, \mathrm{v}_i; N_j^{Al\text{-}O}, \mathrm{v}_j \right\rangle = -\sqrt{\left[\mathrm{v}_j\left(\mathrm{v}_i+1\right)\left(N_i^{Al\text{-}O} - \mathrm{v}_i\right)\left(N_j^{Al\text{-}O} - \mathrm{v}_j+1\right)\right]} \quad (4)$$

$$\left\langle N_i^{Al\text{-}O}, \mathrm{v}_i-1; N_j^{Al\text{-}O}, \mathrm{v}_j+1 \middle| f_{ij} \middle| N_i^{Al\text{-}O}, \mathrm{v}_i; N_j^{Al\text{-}O}, \mathrm{v}_j \right\rangle = -\sqrt{\left[\mathrm{v}_i\left(\mathrm{v}_j+1\right)\left(N_j^{Al\text{-}O} - \mathrm{v}_j\right)\left(N_i^{Al\text{-}O} - \mathrm{v}_i+1\right)\right]} \quad \ldots (4)$$

For two (Al-O) stretching vibrations of aluminumdihydride, the Hamiltonian operator written as

$$H = E_0 + p_1 b_1 + p_2 b_2 + p_{12} b_{12} + q_{12} f_{12} = \begin{bmatrix} -4p(N^{Al\text{-}O}-1) - 4p_{12}(2N^{Al\text{-}O}-1) + q_{12}N^{Al\text{-}O} & -q_{12}N^{Al\text{-}O} \\ -q_{12}N^{Al\text{-}O} & -4p(N^{Al\text{-}O}-1) - 4p_{12}(2N^{Al\text{-}O}-1) + q_{12}N^{Al\text{-}O} \end{bmatrix} \quad \ldots (5) \quad (5)$$

From spectroscopic data algebraic parameters p_1, p_2, p_{12} and q_{12} (cm^{-1}) are determined. Two bonds (Al-O) are equivalent in the aluminumdihydride. As a result, we consider p_1, $p_2 = p$ and Vibron number, $N_1^{Al\text{-}O} = N_2^{Al\text{-}O} = N^{Al\text{-}O}$ in equations (2), (3) and (4).

RESULTS AND DISCUSSION

The parameter p is determined using the energy equation (6)

$$E\left(\mathrm{v}=1\right) = -4p\left(N^{Al\text{-}O}-1\right) \quad (6)$$

and the value of q_{12} calculatedfrom the relation,

$$q_{12} = \frac{\left|E_1 - E_2\right|}{2\,N^{Al-O}} \quad (7)$$

Where, E_1, E_2 are the aluminum dihydride symmetric and antisymmetric vibrational energies, respectively. The number N_i for stretching bonds of aluminum dihydride is calculated from the relation,

$$N_i^{Al-O} = \frac{\omega_e}{\omega_e x_e} - 1,\ i = 1,\ 2.$$

Where, $\omega_e^{Al\text{-}O}$(=1682.37474), $\omega_e x_e^{Al\text{-}O}$ =(29.05098) are correspondingly, vibrational harmonic and anharmonic spectroscopic constants[13].

The Lie algebraic approach is utilized to compute the vibrational energies of aluminium dihydride (in higher overtones and combinational bands), as indicated in the Tables (1), (2) and (3).

Table 1: Vib. frequencies in fundamental mode (in cm^{-1})

Vib. Mode	Symmetry	Experimental#	Computed
ν_1 (Symmetric stretch)	A_1	1788	1788.38
ν_2 (bend)	A_1	760	758.7162
ν_3 (antisymmetric stretch)	B_1	1828.6	1827.9732

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Table 2: Vib. frequencies (overtone) (in cm^{-1})

Overtone	Symmetric stretch (A_1)	Vib. mode Bend(A_1)	Antisymmetric stretch(B_1)
1	$2\nu_1$(3563.761)	$2\nu_2$(1509.995)	$2\nu_3$(3644.028)
2	$3\nu_1$(5335.594)	$3\nu_2$(2237.022)	$3\nu_3$(5429.990)
3	$4\nu_1$(7091.096)	$4\nu_2$(2921.258)	$4\nu_3$(7258.733)
4	$5\nu_1$(8826.294)	$5\nu_2$(3620.721)	$5\nu_3$(8089.413)
5	$6\nu_1$(10622.643)	$6\nu_2$(4430.447)	$6\nu_3$(9758.083)

Table 3: Combinational frequencies (in cm^{-1})

Combinational Band	Computed	Combinational Band	Computed
$\nu_1+\nu_2$	2542.075	$2\nu_1+\nu_2$	4317.456
$\nu_1+\nu_3$	3615.685	$\nu_2+2\nu_2$	2258.336
$\nu_2+\nu_3$	2580.668	$\nu_2+2\nu_3$	4397.723
$\nu_1+2\nu_1$	5352.473	$2\nu_1+\nu_3$	5391.066
$\nu_1+2\nu_2$	3293.354	$\nu_3+2\nu_2$	3331.947
$\nu_1+2\nu_3$	5432.740	$\nu_3+2\nu_3$	5471.333

Table 4: Parameters

$N^{Al\text{-}O}$(stretch)	58
$N^{Al\text{-}O}$(stretch)	38
p(stretch)	-7.9275
p(bend)	-5.1351
p_{12}(stretch)	0.0415
p_{13}(bend)	-1.2968
p_{12}(stretch)	0.3327

CONCLUSION

We compared the examined data which was in the Table 1 with the calculated fundamental vibrational energies of the aluminumdihydride.

Vibrational energies up to the harmonic level six and combinational bands upto the harmonic level three were described using the one dimensional [U(2)] Lie algebraic approach in Tables 2 and 3.

ACKNOWLEDGMENT

The author, J. Vijayasekhar, would like to thank GITAM(Deemed to be University), Visakhapatnam, India, for providing financial assistance of this study under GITAM: Research Seed Grants.

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