Calculation of Vibrational Energies of AlH₂ 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 aluminum dihydride (AlH₂) 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, Aluminum dihydride

INTRODUCTION

The interpretation and analysis of the molecular spectra of molecules is a fascinating research area of molecular physics. Vibrational energies have played a vital 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 problems⁴. 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 spectra⁵-⁷. 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 aluminum dihydride, 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 is

$$H = \sum p_i^0 + \sum p_i^1 + \sum q_i f_{ij}$$

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

$$(b_i) = - 4(N_{Al-O}^1 V_i - V_i^2)$$

$$\left[ N_{Al-O}^1, V_i, N_{Al-O}^2, V_j \right] = \frac{4}{2} \left( V_i + V_j \right)^2 - \left( V_i + V_j \right) \left[ N_{Al-O}^1 + N_{Al-O}^2 \right]$$

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

$$\left[ N_{Al-O}^1, V_i, N_{Al-O}^2, V_j \right] = \frac{4}{2} \left( V_i + V_j \right)^2 - \left( V_i + V_j \right) \left[ N_{Al-O}^1 + N_{Al-O}^2 \right]$$

$$\left[ N_{Al-O}^1, V_i, N_{Al-O}^2, V_j \right] = \frac{4}{2} \left( V_i + V_j \right)^2 - \left( V_i + V_j \right) \left[ N_{Al-O}^1 + N_{Al-O}^2 \right]$$

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

$$H^{Al-O} = \sum p_i^0 + \sum p_i^1 + \sum q_i f_{ij}$$

$$\left[ \begin{array}{c} \gamma_{N_{Al-O}^1} \gamma_{N_{Al-O}^2} \gamma_{N_{Al-O}^1} \gamma_{N_{Al-O}^2} \\ \end{array} \right] = \left[ \begin{array}{c} \gamma_{N_{Al-O}^1} \gamma_{N_{Al-O}^2} \gamma_{N_{Al-O}^1} \gamma_{N_{Al-O}^2} \\ \end{array} \right]$$

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 aluminium dihydride. As a result, we consider $p_1 = p_2 = p$ and Vibron number, $N_{Al-O}^1 = N_{Al-O}^2 = N_{Al-O}$ in equations (2), (3) and (4).

RESULTS AND DISCUSSION

The parameter $p$ is determined using the energy equation

$$E(v=1) = - 4p \left( N_{Al-O}^1 - 1 \right)$$

and the value of $q_{12}$ calculated from the relation, $q_{12} = \frac{|E_1 - E_2|}{2N_{Al-O}}$

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

$$N_{Al-O}^i = \frac{\omega_{X_{Al-O}} - 1}{\omega_{X_{Al-O}}}$$

Where, $\omega_{X_{Al-O}}$ (1682.37474), $\omega_{X_{Al-O}}$ = (29.05098) are correspondingly, vibrational harmonic and anharmonic spectroscopic constants.

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$^{-1}$)

<table>
<thead>
<tr>
<th>Vib. Mode</th>
<th>Symmetry</th>
<th>Experimental</th>
<th>Computed</th>
</tr>
</thead>
<tbody>
<tr>
<td>$v_1$ (Symmetric stretch)</td>
<td>$A_1$</td>
<td>1788</td>
<td>1788.38</td>
</tr>
<tr>
<td>$v_2$ (bend)</td>
<td>$A_1$</td>
<td>760</td>
<td>758.7162</td>
</tr>
<tr>
<td>$v_3$ (antisymmetric stretch)</td>
<td>$B_1$</td>
<td>1828.6</td>
<td>1827.9732</td>
</tr>
</tbody>
</table>

*webbook.nist.gov/cgi/cbook.cgi?ID=C14457659&Units=SI&Mask=800#Electronic-Spec
Table 2: Vib. frequencies (overtone) (in cm⁻¹)

<table>
<thead>
<tr>
<th>Overtone</th>
<th>Symmetric stretch (A₁)</th>
<th>Vib. mode Bend(A₁)</th>
<th>Antisymmetric stretch(B₁)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2ν₁(3563.761)</td>
<td>2ν₁(1509.995)</td>
<td>2ν₁(3644.028)</td>
</tr>
<tr>
<td>2</td>
<td>3ν₁(5335.594)</td>
<td>3ν₁(2237.022)</td>
<td>3ν₁(5429.990)</td>
</tr>
<tr>
<td>3</td>
<td>4ν₁(7091.096)</td>
<td>4ν₁(2921.258)</td>
<td>4ν₁(7258.733)</td>
</tr>
<tr>
<td>4</td>
<td>5ν₁(8826.294)</td>
<td>5ν₁(3620.721)</td>
<td>5ν₁(8089.413)</td>
</tr>
<tr>
<td>5</td>
<td>6ν₁(10622.643)</td>
<td>6ν₁(4430.447)</td>
<td>6ν₁(9758.083)</td>
</tr>
</tbody>
</table>

Table 3: Combinational frequencies (in cm⁻¹)

<table>
<thead>
<tr>
<th>Combinational Band</th>
<th>Computed</th>
<th>Combinational Band</th>
<th>Computed</th>
</tr>
</thead>
<tbody>
<tr>
<td>ν₁+ν₂</td>
<td>2542.075</td>
<td>ν₁+ν₂</td>
<td>4317.456</td>
</tr>
<tr>
<td>ν₁+ν₃</td>
<td>3615.685</td>
<td>ν₂+ν₃</td>
<td>2258.336</td>
</tr>
<tr>
<td>ν₁+2ν₁</td>
<td>5235.473</td>
<td>ν₂+2ν₆</td>
<td>4397.723</td>
</tr>
<tr>
<td>ν₁+2ν₂</td>
<td>3293.354</td>
<td>ν₂+2ν₃</td>
<td>5391.066</td>
</tr>
<tr>
<td>ν₁+2ν₃</td>
<td>5432.740</td>
<td>ν₂+2ν₃</td>
<td>5431.947</td>
</tr>
</tbody>
</table>

Table 4: Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>N⁺⁽.RichTextBox⁾</td>
<td>58</td>
</tr>
<tr>
<td>N⁻⁽쇤⁡RichText⁡)</td>
<td>38</td>
</tr>
<tr>
<td>ρ(stretch)</td>
<td>-7.9275</td>
</tr>
<tr>
<td>ρ(bend)</td>
<td>-5.1351</td>
</tr>
<tr>
<td>ρₓ(stretch)</td>
<td>0.0415</td>
</tr>
<tr>
<td>ρₓ(bend)</td>
<td>-1.2968</td>
</tr>
<tr>
<td>ρᵧ(stretch)</td>
<td>0.3327</td>
</tr>
</tbody>
</table>

CONCLUSION

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

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.

REFERENCES