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ANALYZING CYCLOBUTANE: A VIBRATIONAL HAMILTONIAN APPROACH USING DYNAMICAL U(2) LIE ALGEBRAS

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ABSTRACT. This study uses a one-dimensional Lie algebraic framework, precisely adapted to the symmetry of molecules, to investigate the vibrational frequencies of cyclobutane. A vibrational Hamiltonian is also constructed using one-dimensional Morse oscillators, preserving the D_{2d} point group symmetry for each molecule. The analysis compares the calculated fundamental vibrational frequencies with the observed experimental frequencies, resulting in a root mean square deviation of 0.886 cm^{-1}. The result highlights the exceptional precision of the U(2) Lie algebraic Hamiltonian in accurately predicting the vibrational frequencies and their combination bands at the sub-cm^{-1} level of precision. Specifically, this computational approach has the potential to achieve these results with lower computational costs compared to traditional theoretical approaches. The broader implications of our study suggest that the U(2) Lie algebraic framework can be effectively applied to a wide range of molecular systems, offering significant advantages in fields such as material science, drug design, and environmental monitoring by providing precise and efficient vibrational spectral analyses.

KEY WORDS: Vibrational Hamiltonian, Vibrational frequencies, Morse oscillator, Cyclobutane, Lie algebraic method

INTRODUCTION

Molecular spectroscopy is essential in understanding the complex interactions between molecules and electromagnetic radiation, providing valuable information about molecular structure and properties. Infrared and Raman spectroscopy are highly effective methods for analyzing molecules, offering various techniques. These techniques provide insights into the vibrational modes of molecules, allowing us to analyze molecular structures and determine essential functional groups. With the advancement of modern molecular spectroscopy, there is a greater demand for reliable theoretical methods to improve our understanding of new experimental techniques, especially those used to study the more complex vibrational modes in polyatomic molecules [1].

Traditionally, two conventional theoretical frameworks have been used to study polyatomic molecules and their ro-vibration spectra. The first approach is the Dunham expansion, which comprises a sequence of expansions in rotation-vibration quantum numbers to determine energy levels [2]. Despite its historical significance, this approach has certain constraints. It does not quickly produce operator matrix elements because it is not directly connected to the wave functions of individual states. Additionally, the Dunham expansion necessitates many parameters when addressing complex polyatomic molecules. Optimizing these parameters using extensive experimental databases may become impractical [3].

A more efficient alternative to the Dunham expansion is to solve the Schrödinger equation using potentials. This approach, which depends on advancements in ab initio techniques and the computation of Hamiltonian operator matrix elements using existing wave functions, provides improved precision. Nevertheless, difficulties arise when dealing with larger molecules and highly excited energy levels, frequently associated with the computational complexities of differentiation and integration [4, 5].

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An increasingly appealing third alternative is an approach based on one-dimensional symmetry-adapted Lie algebra. This method addresses various challenges encountered by traditional theoretical frameworks [6]. Innovative studies conducted by Iachello *et al.* first employed the U(2) Lie algebraic method to analyze the vibrational spectra of small molecules [7, 8]. This method has since expanded to include the analysis of higher overtone rotation-vibration spectra in medium-sized molecules [9-13]. The Lie algebraic framework offers a more efficient method for calculating the vibrational spectra, yielding a substantial computational reduction and higher precision compared to other conventional approaches [14-16]. Primary theoretical investigations [17-20] have focused on the fundamental vibrational spectra of cyclobutane, emphasizing its significant importance.

Our study's primary objective is to develop a vibrational Hamiltonian for cyclobutane using the one-dimensional dynamical U(2) Lie algebra framework. We aim to determine the vibrational frequencies at both the fundamental level and for higher overtone and combination bands precisely. This novel approach addresses significant inconsistencies found in spectra obtained from previous studies that predominantly relied on ab initio or semi-empirical methods [21, 22]. We hypothesize that the U(2) Lie algebra framework will provide more accurate and computationally efficient results for the vibrational spectra of cyclobutane than traditional methods. Our research questions focus on evaluating the precision of the U(2) Lie algebraic method in determining the fundamental and overtone vibrational frequencies of cyclobutane compared to conventional techniques.

Our findings demonstrate that the U(2) Lie algebraic approach yields higher precision and requires significantly fewer computational resources than traditional methods such as the Dunham expansion and ab initio calculations. This method's ability to handle complex vibrational modes with fewer parameters highlights its superiority and potential for broader applications in molecular spectroscopy.

The broader implications of our study lie in the enhanced accuracy and efficiency of the U(2) Lie algebraic method, which can be applied to other polyatomic molecules with complex vibrational spectra. This advancement can improve our understanding of molecular structures and dynamics, potentially benefiting various fields such as material science, chemistry, and pharmaceuticals [23, 24].

STRUCTURE OF CYCLOBUTANE

Cyclobutane plays a crucial role in organic chemistry, as it is a fundamental precursor for synthesizing more complex organic compounds, particularly those with cyclic structures. The molecular structure of cyclobutane allows for the study of its complex characteristics using infrared spectroscopy and Raman spectra techniques, which provide an incredible number of vibrational modes. The vibrational properties of cyclobutane are complex and varied, involving a variety of modes that exhibit the characteristics of its atoms and bonds. The spectra prominently exhibit the symmetric and asymmetric stretching vibrations of the carbon-hydrogen (C-H) bonds, illustrating these molecular interactions. In addition, the spectra indicate dynamic characteristics resulting from the vibrations of the C-H bonds, which are observed as bending modes. These modes provide valuable insights into the complex molecular properties of cyclobutane. Nevertheless, the vibrational modes present in cyclobutane exceed these fundamental vibrations. This structure part offers more complex molecular characteristics, such as ring puckering and twisting. The vibrational behavior of the cyclobutane ring is enhanced by these modes, which involve the deformation of the ring itself, providing complexity and depth. Now, let us delve deeper into the molecular structure of cyclobutene. The cycloalkane with the molecular formula C_4H_8 consists of a closed ring with four carbon atoms, each stably bound to two hydrogen atoms. The carbon-carbon bonds undergo fusion by forming single bonds within this molecular coordination. This establishes a planar molecular structure characterized by bond angles of approximately 90 degrees. As the study of symmetry progresses, the classification of cyclobutane into the D_{2d} point group becomes apparent. This point group encompasses symmetry species (irreducible representations), namely A_1, A_2, B_1, B_2, and E. Cyclobutane exhibits 23 normal vibrational modes within its symmetrical structure, indicating the complicated interactions among its constituent atoms and bonds. A closer examination of the molecular vibrations reveals the presence of eight C-H bonds and four C-C bonds, each playing a unique role in the vibrational spectra of cyclobutane. When spectroscopic techniques probe this unassuming molecular structure, they reveal a fascinating vibrational structure. It demonstrates the complexity within molecular spectroscopy's seemingly modest constituents.

U(2) LIE ALGEBRAIC VIBRATIONAL HAMILTONIAN OF CYCLOBUTANE

Eight identical U(2) Lie algebras, denoted as $\{U_i(2): i = 1, 2, 3, 4, 5, 6, 7, 8\}$, have been proposed to represent the eight C-H stretching bonds. Additionally, four identical U(2) Lie algebras, $\{U_i^*\,(2): i = 1, 2, 3, 4\}$, have been introduced to characterize the four C-C stretching bonds corresponding to the structure of cyclobutane.

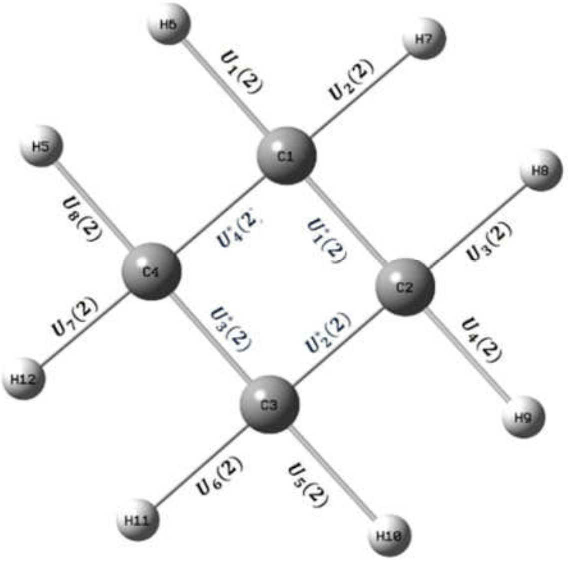

Figure 1. The structure of cyclobutane, coupled with the bond-wise assignment of eight identical U(2) Lie algebras, $U_1(2)$ to $U_8(2)$, represent the C-H stretching vibrations. Additionally, four identical U(2) Lie algebras, $U_1^*(2)$ to $U_4^*(2)$, are assigned to represent the C-C stretching vibrations.

The following are the interactions that occur between C-H bond stretching vibrations:

Interaction 1: First-neighbor couplings

$$\{U_i(2) \otimes U_j(2); (i,j) = (1,2), (2,3), (3,4), (4,5), (5,6), (6,7), (7,8), (1,8)\}$$

Interaction 2: Second-neighbor couplings

$$\{U_i(2) \otimes U_j(2); (i,j) = (1,3), (2,4), (3,5), (4,6), (5,7), (6,8), (1,7), (2,8)\}$$

Interaction 3: Third-neighbor couplings

$$\{U_i(2) \otimes U_j(2); (i,j) = (1,4),(2,5),(3,6),(4,7),(5,8),(1,6),(2,7),(3,8)\}$$

Interaction 4: Forth-neighbor couplings

$$\{U_i(2) \otimes U_j(2); (i,j) = (1,5),(2,6),(3,6),(3,7),(4,8)\}$$

The interactions among C-C bond stretching vibrations are:

Interaction 1: First-neighbor couplings

$$\{U_i^*(2) \otimes U_j^*(2); (i,j) = (1,2),(2,3),(3,4),(1,4)\}$$

Interaction 2: Second-neighbor couplings

$$\{U_i^*(2) \otimes U_j^*(2); (i,j) = (1,3),(2,4)`\}$$

Now, construct the vibrational Hamiltonian operator that maintains the D_{2d} symmetry of the molecule. Since all C-H bonds in the molecule are equivalent, the effective Hamiltonian for C-H stretching vibrations in cyclobutene is:

$$H^{C-H} = E_0 + \sum_{i=1}^{n=8} A_i^{C-H} C_i + \sum_{i<j}^{n=8} A_{ij}^{C-H} C_{ij} + \sum_{i<j}^{n=8} (k_{ij}^1 + k_{ij}^2 + k_{ij}^3 + k_{ij}^4) \lambda_{ij}^{C-H} M_{ij} \qquad (1)$$

with symmetry adapted 1st, 2nd, 3rd and 4th neighbor couplings coefficients as

$$k_{ij}^1 = 1, (i,j) = (1,2),(2,3),(3,4),(4,5),(5,6),(6,7),(7,8),(1,8)$$

$$k_{ij}^1 = 0, (i,j) = (1,3),(2,4),(3,5),(4,6),(5,7),(6,8),(1,7),(2,8)$$

$$k_{ij}^1 = 0, (i,j) = (1,4),(2,5),(3,6),(4,7),(5,8),(1,6),(2,7),(3,8)$$

$$k_{ij}^1 = 0, (i,j) = (1,5),(2,6),(3,6),(3,7),(4,8)$$

$$k_{ij}^2 = 0, (i,j) = (1,2),(2,3),(3,4),(4,5),(5,6),(6,7),(7,8),(1,8)$$

$$k_{ij}^2 = 1, (i,j) = (1,3),(2,4),(3,5),(4,6),(5,7),(6,8),(1,7),(2,8)$$

$$k_{ij}^2 = 0, (i,j) = (1,4),(2,5),(3,6),(4,7),(5,8),(1,6),(2,7),(3,8)$$

$$k_{ij}^2 = 0, (i,j) = (1,5),(2,6),(3,6),(3,7),(4,8)$$

$$k_{ij}^3 = 0, (i,j) = (1,2),(2,3),(3,4),(4,5),(5,6),(6,7),(7,8),(1,8)$$

$$k_{ij}^3 = 0, (i,j) = (1,3),(2,4),(3,5),(4,6),(5,7),(6,8),(1,7),(2,8)$$

$$k_{ij}^3 = 1, (i,j) = (1,4),(2,5),(3,6),(4,7),(5,8),(1,6),(2,7),(3,8)$$

$$k_{ij}^3 = 0, (i,j) = (1,5),(2,6),(3,6),(3,7),(4,8)$$

$$k_{ij}^4 = 0, (i,j) = (1,2),(2,3),(3,4),(4,5),(5,6),(6,7),(7,8),(1,8)$$

$$k_{ij}^4 = 0, (i,j) = (1,3),(2,4),(3,5),(4,6),(5,7),(6,8),(1,7),(2,8)$$

$$k_{ij}^4 = 0, (i,j) = (1,4),(2,5),(3,6),(4,7),(5,8),(1,6),(2,7),(3,8)$$

$$k_{ij}^4 = 1, (i,j) = (1,5),(2,6),(3,6),(3,7),(4,8)$$

In the same way, the effective vibrational Hamiltonian for the C-C stretching vibrations of cyclobutene can be written as

$$H^{C-C} = E_0 + \sum_{i=1}^{n=4} A_i^{C-C} C_i + \sum_{i<j}^{n=4} A_{ij}^{C-C} C_{ij} + \sum_{i<j}^{n=4} (l_{ij}^1 + l_{ij}^2)\, \lambda_{ij}^{C-C} M_{ij} \qquad (2)$$

with symmetry adapted 1st, 2nd neighbor couplings coefficients as

$$l_{ij}^1 = 1, (i,j) = (1,2), (2,3), (3,4), (1,4)$$

$$l_{ij}^1 = 0, (i,j) = (1,3), (2,4)$$

$$l_{ij}^2 = 0, (i,j) = (1,2), (2,3), (3,4), (1,4)$$

$$l_{ij}^2 = 1, (i,j) = (1,3), (2,4)$$

Here, E_0 is the eigenvalue of the Schrodinger equation corresponding to the electronic ground state of the bond vibrations; this eigenvalue will act as the zero references for all the excitations [13]. The second term of the vibrational Hamiltonian corresponds to the energy states of *n* independent, anharmonic oscillators. Each oscillator is linked to a specific local vibrational mode and is described by the Casimir operator C_i of the U(2) Lie algebra. The third term addresses the cross-anharmonic interactions between different local oscillators, utilizing the two-body Casimir operator C_{ij}, which represents the interactions between modes i and *j*. The last term involves anharmonic, off-diagonal interactions between pairs of local oscillators, characterized by the Majorana operator M_{ij}. $A_i, A_{ij}, \lambda_{ij}$ are the algebraic parameters; C_i, C_{ij} represent the Casimir (invariant) operators of the associated Lie algebras. Majorana (invariant) operators, M_{ij}, are related to coupling schemes involving Lie algebras of the *n* interacting one-dimensional Morse oscillators. The spectroscopic data is used for determining the algebraic parameters, and the following expressions are used to determine the algebraic operators:

$$\langle C_i \rangle = -4(N_i v_i - v_i^2) \qquad (3)$$

$$\langle N_i, v_i; N_j, v_j | C_{ij} | N_i, v_i; N_j, v_j \rangle = 4(v_i + v_j)(v_i + v_j - N_i - N_j) \qquad (4)$$

$$\left.\begin{array}{r} \langle N_i, v_i; N_j, v_j | M_{ij} | N_i, v_i; N_j, v_j \rangle = v_i N_j + v_j N_i - 2 v_i v_j \\ \langle N_i, v_i + 1; N_j, v_j - 1 | M_{ij} | N_i, v_i; N_j, v_j \rangle = -[v_j (v_i + 1)(N_i - v_i)(N_j - v_j + 1]^{1/2} \\ \langle N_i, v_i - 1; N_j, v_j + 1 | M_{ij} | N_i, v_i; N_j, v_j \rangle = -[v_i (v_j + 1)(N_j - v_j)(N_i - v_i + 1]^{1/2} \end{array}\right\} \qquad (5)$$

where v_i, v_j are the vibrational quantum numbers. The Casimir operator C_{ij} is diagonal in v_i and v_j, and the Majorana operator, M_{ij}, in contrast, transfers one vibrational quantum from bond *i* to the bond *j*.

The following mathematical expressions for the matrix elements $\langle C_i \rangle, \langle C_{ij} \rangle, \langle M_{ij} \rangle$ describe the fundamental vibrations,

$$\langle C_i \rangle = -4(N-1), \langle C_{ij} \rangle = -4(2N-1), \langle M_{ij} \rangle = \begin{cases} -N \ (i \neq j) \\ \ N \ (i = j) \end{cases} \qquad (6)$$

The following relation gives the vibron number *N*, corresponding to the maximum number of bound states of the Morse potential in each vibrating bond species [15],

$$N = \frac{\omega_e}{\omega_e \chi_e} - 1 \qquad (7)$$

where $\omega_e = 2860.7508\ (\mathrm{C-H}), 1855.0663\ (\mathrm{C-C})$ and $\omega_e\chi_e = 64.387\ (\mathrm{C-H})$, $13.6007\ (\mathrm{C-C})$ are the spectroscopic constants of the respective bonds determined from experimental data of diatomic molecules [25, 26, 27].

The initial guess for A_i^{C-H}, A_i^{C-C} are obtained from the energy expression for single-oscillator fundamental mode,

$E^{C-H} = -4A_i^{C-H}(N^{C-H}-1), E^{C-C} = -4A_i^{C-C}(N^{C-C}-1)$ as

$$A_i^{C-H} = -\frac{E^{C-H}}{4(N^{C-H}-1)}, A_i^{C-C} = -\frac{E^{C-C}}{4(N^{C-C}-1)} \qquad (8)$$

The initial guesses for $\lambda_{ij}^{C-H}, \lambda_{ij}^{C-C}$ are obtained by the relations,

$$\lambda_{ij}^{C-H} = \frac{|E_s^{C-H} - E_{as}^{C-H}|}{6N^{C-H}},\ \lambda_{ij}^{C-C} = \frac{|E_s^{C-C} - E_{as}^{C-C}|}{2N^{C-C}} \qquad (9)$$

Here, E_s and E_{as} are the different energies corresponding to symmetric and antisymmetric combination of the two local modes. The values of parameters, $A_i^{C-H}, A_i^{C-C}, \lambda_{ij}^{C-H}$ and λ_{ij}^{C-C} are optimized by least-square regression fitting, starting from the initial guesses as given by equations (8) and (9). The initial guesses for $A_{ij}^{C-H}, A_{ij}^{C-C}$ are taken as zero.

RESULTS

This study employed symmetry-adapted dynamical U(2) Lie algebras to construct a vibrational Hamiltonian for cyclobutane. The optimized algebraic parameters and vibron numbers are comprehensively shown in Table 1. Our calculations have yielded a comprehensive representation of the fundamental, first overtone, and their combination bands, which are presented in Tables 2, 3, and 4.

Table 1. Optimized fitting parameters: U(2) Lie algebraic vibrational Hamiltonian for D_{2d} symmetry cyclobutane.

Parameters	Value
N^{C-H} *(C-H stretching)*	44
N^{C-C} *(C-C stretching)*	136
A_i^{C-H} *(C-H stretching)*	-15.8078
A_i^{C-C} *(C-C stretching)*	-1.7582
A_{ij}^{C-H} *(C-H stretching)*	1.4817
A_{ij}^{C-C} *(C-C stretching)*	0.1492
λ_{ij}^{C-H} *(C-H stretching)*	2.0921,
λ_{ij}^{C-C} *(C-C stretching)*	0.0514
N (bending)	26
A_i *(bending)*	-11.5733
A_{ij} *(bending)*	0.7283
λ_{ij} *(bending)*	3.4967

Table 2. Predicted fundamental vibrational frequencies (in cm^{-1}) for cyclobutane using the U(2) Lie algebraic vibrational Hamiltonian, together with experimental observations, mode assignments, and symmetry species (irreducible representations).

Vibrational mode	Symmetry species	Experimental [28]	Calculated
v_1 *(CH_2 s-str)*	A_1	2895	2895.3328
v_2 *(CH_2 scis)*	A_1	1443	1443.2752
v_3 *(CH_2 scis)*	A_1	1001	1001.6640
v_4 *(CH_2 a-str)*	A_1	2975	2975.2312
v_5 *(CH_2 rock)*	A_1	741	740.8023
v_6 *(ring puck)*	A_1	197	196.4120
v_7 *(CH_2 wag)*	A_2	1260	1261.5139
v_8 *(CH_2 twist)*	A_2	1257	1256.7816
v_9 *(CH_2 wag)*	B_1	1219	1219.8067
v_{10} *(Ring deform)*	B_1	926	927.1403
v_{11} *(CH_2 twist)*	B_1	1222	1221.7160
v_{12} *(CH_2 s-str)*	B_2	2893	2892.3441
v_{13} *(CH_2 scis)*	B_2	1443	1442.5139
v_{14} *(Ring deform)*	B_2	1001	1002.8071
v_{15} *(CH_2 a-str)*	B_2	2987	2986.4107
v_{16} *(CH_2 rock)*	B_2	627	626.9212
v_{17} *(CH_2 a-str)*	E	2952	2953.2273
v_{18} *(CH_2 twist)*	E	1223	1222.4693
v_{19} *(CH_2 rock)*	E	749	748.3305
v_{20} *(CH_2 s-str)*	E	2887	2888.5371
v_{21} *(CH_2 scis)*	E	1447	1446.2840
v_{22} *(CH_2 wag)*	E	1257	1257.9781
v_{23} *(Ring deform)*	E	898	899.7773

Table 3. The first overtone vibrational frequencies (in cm^{-1}) of cyclobutane, as anticipated by the U(2) Lie algebraic vibrational Hamiltonian, are presented together with details about vibrational modes and symmetry species.

Vibrational mode	Symmetry species	Calculated
$2v_1$ *(CH_2 s-str)*	A_1	5673.0755
$2v_2$ *(CH_2 scis)*	A_1	2765.6914
$2v_3$ *(CH_2 scis)*	A_1	1985.1109
$2v_4$ *(CH_2 a-str)*	A_1	5793.5742
$2v_5$ *(CH_2 rock)*	A_1	1326.0063
$2v_6$ *(ring puck)*	A_1	343.9843
$2v_7$ *(CH_2 wag)*	A_2	2428.4403
$2v_8$ *(CH_2 twist)*	A_2	2437.3634
$2v_9$ *(CH_2 wag)*	B_1	2289.1770
$2v_{10}$ *(Ring deform)*	B_1	1676.8535
$2v_{11}$ *(CH_2 twist)*	B_1	2380.3163
$2v_{12}$ *(CH_2 s-str)*	B_2	5569.8128
$2v_{13}$ *(CH_2 scis)*	B_2	2706.7340
$2v_{14}$ *(Ring deform)*	B_2	1989.5054
$2v_{15}$ *(CH_2 a-str)*	B_2	5825.1040
$2v_{16}$ *(CH_2 rock)*	B_2	1152.7771
$2v_{17}$ *(CH_2 a-str)*	E	5829.1959
$2v_{18}$ *(CH_2 twist)*	E	2274.2430
$2v_{19}$ *(CH_2 rock)*	E	1343.0852
$2v_{20}$ *(CH_2 s-str)*	E	5577.6613
$2v_{21}$ *(CH_2 scis)*	E	2704.6355
$2v_{22}$ *(CH_2 wag)*	E	2388.3027
$2v_{23}$ *(Ring deform)*	E	1632.1314

Table 4. The frequencies of the combination bands of cyclobutane, as anticipated by the U(2) Lie algebraic vibrational Hamiltonian, refer to the collective vibrational modes resulting from the combination of the fundamental and first overtone.

Vibrational mode	Calculated	Vibrational mode	Calculated
$v_1 + v_{12}$	5799.5305	$2v_1 + 2v_{12}$	11254.7419
$v_1 + v_{20}$	5795.7235	$2v_1 + 2v_{20}$	11262.5904
$v_{12} + v_{20}$	5792.5687	$2v_{12} + 2v_{20}$	11159.3277
$v_4 + v_{15}$	5973.4955	$2v_4 + 2v_{15}$	11630.5318
$v_4 + v_{17}$	5940.3121	$2v_4 + 2v_{17}$	11634.6237
$v_{15} + v_{17}$	5951.4916	$2v_{15} + 2v_{17}$	11654.2999
$v_1 + 2v_{12}$	8476.9992	$2v_1 + v_{12}$	8577.2732
$v_1 + 2v_{20}$	8484.8477	$2v_1 + v_{20}$	8573.4662
$v_{12} + 2v_{20}$	8481.8590	$2v_{12} + v_{20}$	8470.2035
$v_4 + 2v_{15}$	8812.1888	$2v_4 + v_{15}$	8791.8385
$v_4 + 2v_{17}$	8885.9088	$2v_4 + v_{17}$	8758.6551
$v_{15} + 2v_{17}$	8827.4602	$2v_{15} + v_{17}$	8790.1849

CONCLUSIONS

This study utilizes the one-dimensional Lie algebraic model's powerful capabilities to reveal cyclobutane's vibrational frequencies. The robust theoretical framework allowed us to compute molecules' vibrational frequencies accurately. The outcomes of our endeavors showcased the exceptional precision of the U(2) Lie algebraic Hamiltonian model. The model exhibits remarkable accuracy, as evidenced by a root mean square deviation of 0.886 cm^{-1} for analysing the 23 fundamental vibrational modes. The level of precision achieved in vibrational spectroscopy is impressive, showcasing the effectiveness of the U(2) Lie algebraic method in accurately capturing the fundamental characteristics of molecular vibrations.

Moreover, our results provide insight into an essential component of this research endeavor: the effectiveness of our proposed approach in accurately predicting higher-order overtones and combination bands. This remarkable outcome demonstrates the adaptability and reliability of the U(2) Lie algebraic model. It overcomes the limitations of fundamental vibrations to explain more complex vibrational modes. Our study proves that the U(2) Lie algebraic model effectively captures vibrational frequencies with a high degree of accuracy comparable to spectroscopy. This includes predicting primary vibrational frequencies and accurately determining first-overtone frequencies and their corresponding combination bands. The statement highlights theoretical models' efficacy in deciphering molecular spectroscopy's vibrational frequencies, equipping researchers with essential tools for understanding the characteristics of atoms and bonds within molecules.

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