

HIGHER OVERTONE VIBRATIONAL FREQUENCIES OF CYCLOBUTANE-D8 USING LIE ALGEBRAIC FRAMEWORK

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This research study employs a Lie algebraic framework to investigate the second and third overtone vibrational frequencies and their combination bands in cyclobutane-d8 (C₄D₈). The application of this framework ensures the preservation of the point symmetry group D_{2d}, characterized by the symmetry species A₁, A₂, B₁, B₂, and E. The analysis encompasses 23 normal vibrational modes within the molecular structure of cyclobutane-d8. Our study extensively explores the vibrational spectra, elucidating the intricate interactions among these vibrational modes. Preserving molecular symmetry allows for a deeper understanding of vibrational interactions, offering valuable insights into spectroscopy. The research enhances the comprehension of molecular structure and its applications in various fields, providing a detailed view of higher energy levels and complex vibrational transitions in cyclobutane-d8.

Keywords: Hamiltonian operator; Lie algebraic framework; Vibrational Spectra; Morse oscillator; Cyclobutane-d8

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1. INTRODUCTION

The vibrational frequencies of molecules represent the specific frequencies at which atoms within a molecule vibrate, with atoms connected by chemical bonds acting like springs, allowing oscillation. Each vibrational mode corresponds to a unique oscillation frequency, offering valuable insights into molecular structure, bonding, and dynamic behavior. Experimental techniques such as infrared and Raman spectroscopy are commonly utilized to determine these frequencies associated with bond stretching and bending, influenced by factors like bond strength, atomic mass, and molecular symmetry. Understanding vibrational frequencies is pivotal in diverse scientific fields, including chemistry, physics, and biology, contributing to molecular spectroscopy, quantum chemistry, and molecular dynamics investigations. Various theoretical approaches are employed to determine vibrational frequencies, each with distinct principles. The harmonic oscillator model, as the simplest, assumes molecular vibrations as harmonic oscillators, approximating the potential energy surface near equilibrium and calculating frequencies as multiples of the harmonic oscillator frequency. Anharmonic methods extend beyond this model, considering deviations and utilizing quantum chemistry methods like vibrational configuration interaction and vibrational coupled cluster to include anharmonic effects [1-4]. Density functional theory approximates electronic structure based on electron density [5-7]. Ab initio methods, including Hartree-Fock theory and post-Hartree-Fock methods, offer accurate electronic structure information but demand computational intensity. Semi-empirical methods balance accuracy and computational efficiency, and force field methods use empirical potential energy functions parameterized for molecular dynamics simulations. Coupled mode approaches consider vibrational excitations as coupled modes, while group theory and symmetry considerations exploit molecular symmetry [8-13]. Each method involves trade-offs between computational efficiency and accuracy, emphasizing consideration of the specific molecule under study. Combining methods and validating against experimental data enhances overall reliability.

Introducing the symmetry-adapted Lie algebraic method for polyatomic molecules seeks to improve outcomes and address limitations found in traditional theoretical approaches [14, 15]. This innovative method strives to overcome constraints by modifying and integrating existing theoretical frameworks with the foundational principles of Lie algebras. Built upon Lie algebra principles, this method emerges as a potent theoretical approach within quantum chemistry. Particularly effective for symmetric molecules, it streamlines the analysis of vibrational motion by systematically simplifying vibrational degrees of freedom [16-20]. Its utility extends to both quantum chemistry and spectroscopy, offering valuable insights into vibrational modes and significantly contributing to interpreting experimental spectra. This research study emphasizes the analysis of second and third overtone vibrational frequencies and their combination bands in cyclobutane-d8 of point group D_{2d} with the symmetry species A₁, A₂, B₁, B₂, E. The investigation uses the symmetry-adapted Lie algebraic method and is motivated by various factors with potential implications for practical uses. Studying these higher energy levels yields an intricate understanding of molecular oscillations, particularly in response to changes in molecular environments. The practical significance of this research spans various fields, such as spectroscopy, material and chemical engineering, environmental monitoring, and isotopic studies. It not only contributes to theoretical knowledge but also leads to practical advancements in these areas.

2. SYMMETRY-ADAPTED LIE ALGEBRAIC METHOD

The vibrational Hamiltonian (H), formulated within the framework of the Lie algebraic method, is expressed in terms of Casimir and Majorana operators, establishing a systematic foundation for analysing vibrational modes [15]. In this framework, the construction of the Hamiltonian is centred around operators that commute with it, forming a Lie algebra and ensuring compatibility with molecular symmetry, thereby systematically addressing vibrational degrees of freedom. Casimir operators, acting as invariants within the Lie algebra, are pivotal in identifying constants of motion within the vibrational system. These operators play a crucial role in systematically simplifying the vibrational Hamiltonian, significantly enhancing computational efficiency, particularly in studying symmetric molecules. Majorana operators, intricately connected to coupling schemes involving Lie algebras of interacting one-dimensional Morse oscillators, are instrumental in the diagonalization process of the vibrational Hamiltonian [16, 18]. The relationships between Majorana operators and the Lie algebraic framework aid in simplifying and diagonalizing the Hamiltonian, facilitating a more accessible analysis of vibrational modes. Expressed in terms of Casimir and Majorana operators, the vibrational Hamiltonian ensures a systematic treatment of vibrational degrees of freedom. It provides valuable insights into the symmetries and dynamics governing molecular vibrations. This approach contributes to a profound understanding of molecular structure and enhances the interpretability of experimental spectra, such as those obtained through techniques like infrared and Raman spectroscopy. Incorporating Casimir and Majorana operators in the vibrational Hamiltonian associated with the Lie algebraic method represents a powerful and efficient approach to studying molecular vibrations within the quantum mechanical framework [14, 17].

The vibrational Hamiltonians governing the C-D and C-C stretching vibrations in Cyclobutene-d8, used to calculate the vibrational frequencies, are represented as follows [21]:

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

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

with symmetry adapted neighbor couplings coefficients as

$$k_{ij}^1 = \begin{cases} 1, (i, j) = (1,2), (2,3), (3,4), (4,5), (5,6), (6,7), (7,8), (1,8) \\ 0, \text{ otherwise} \end{cases}$$

$$k_{ij}^2 = \begin{cases} 1, (i, j) = (1,3), (2,4), (3,5), (4,6), (5,7), (6,8), (1,7), (2,8) \\ 0, \text{ otherwise} \end{cases}$$

$$k_{ij}^3 = \begin{cases} 1, (i, j) = (1,4), (2,5), (3,6), (4,7), (5,8), (1,6), (2,7), (3,8) \\ 0, \text{ otherwise} \end{cases}$$

$$k_{ij}^4 = \begin{cases} 1, (i, j) = (1,5), (2,6), (3,6), (3,7), (4,8) \\ 0, \text{ otherwise} \end{cases}$$

$$l_{ij}^1 = \begin{cases} 1, (i, j) = (1,2), (2,3), (3,4), (1,4) \\ 0, \text{ otherwise} \end{cases}$$

$$l_{ij}^2 = \begin{cases} 1, (i, j) = (1,3), (2,4) \\ 0, \text{ otherwise} \end{cases}$$

In this context, $A_i, A_{ij}, \lambda_{ij}$ denote the algebraic parameters, while C_i and C_{ij} represent the Casimir (invariant) operators associated with the respective Lie algebras. Majorana (invariant) operators M_{ij} are intricately connected to coupling schemes incorporating Lie algebras of n interacting one-dimensional Morse oscillators. Utilizing spectroscopic data facilitates the determination of algebraic parameters, and the following expressions are applied to compute the algebraic operators:

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

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

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

The following relationship provides the dimensionless vibronic number N , corresponding to the maximum bound states for each vibrating bond species within the Morse potential. The equation is expressed as follows:

$$N = \frac{\omega_e}{\omega_e \chi_e} - 1. \quad (6)$$

Here, ω_e and $\omega_e \chi_e$ represent the spectroscopic constants for the specific bonds and these constants are determined based on experimental data from diatomic molecules [22, 23]. The vibrational quantum numbers are denoted by v_i and v_j of the different bonds i and j respectively.

The initial estimates for A_i are derived from the energy expression for the single-oscillator fundamental mode:

$$E(v = 1) = -4A_i(N - 1). \quad (7)$$

Similarly, the initial approximations for λ_{ij} are determined through the following relations:

$$\lambda'_{ij} = \frac{|E'_s - E'_{as}|}{6N'}, \lambda''_{ij} = \frac{|E''_s - E''_{as}|}{2N''}. \quad (8)$$

Here, E'_s and E'_{as} represent the symmetric and asymmetric energies for the C-D stretching vibrations, while E''_s and E''_{as} denote the corresponding energies for the C-C stretching vibrations. The optimization of parameter values is achieved through a least-square regression fitting process, commencing with the initial estimates provided by equations (7) and (8). In this iterative procedure, the initial guesses for A_{ij} are set to zero.

3. RESULTS AND DISCUSSIONS

Within the Lie algebraic framework, Table 1 shows the optimized values for the algebraic parameters and vibron numbers that are part of the vibrational Hamiltonian. According to the reference [21], these specific parameters were used.

Table 1. Optimized parameters

Parameters	Value
N' (C-D stretching), N'' (C-C stretching)	60, 136
A_i' (C-D stretching), A_i'' (C-C stretching)	-9.2076, -1.2807
A_{ij}' (C-D stretching), A_{ij}'' (C-C stretching)	1.0112, 0.1542
λ_{ij}' (C-D stretching), λ_{ij}'' (C-C stretching)	0.3277, 0.8848
N (bending)	36
A_i (bending)	-6.4142
A_{ij} (bending)	0.4952
λ_{ij} (bending)	1.3449

The presented table (Table 2) showcases the calculated second and third overtone vibrational frequencies, along with their combination bands, for various vibrational modes of C_4D_8 (cyclobutane-d8) in wave numbers (cm^{-1}), utilizing the Lie algebraic method. A thorough study of the molecular vibrations and their interactions in cyclobutane-d8 provides significant insights into its vibrational spectroscopy. By identifying vibrational modes according to their symmetry species (A_1 , A_2 , B_1 , B_2 , and E), one can identify essential modes such as symmetric stretching (s-str), asymmetric stretching (a-str), scissoring (scis), rocking (rock), wagging (wag), twisting (twist), and ring deformation (ring deform). The vibrational modes v_{17} (CD_2 a-str), v_{15} (CD_2 a-str) and v_4 (CD_2 a-str) indicate higher frequencies, indicating strong molecular vibrations. Including combination bands, such as $v_4 + v_{17}$ and $v_{15} + v_{17}$, introduces higher frequencies that play a crucial role in the complex vibrational transitions of the molecule. The derived frequencies, which are essential for interpreting experimental spectra acquired via infrared and Raman spectroscopy, highlight the practical utility of this research. The identified combination bands significantly contribute to interpreting experimental spectra, enhancing our comprehension of the molecule's vibrational characteristics. Including second and third harmonic frequencies yields valuable information about higher energy levels, enabling a thorough comprehension of the vibrational structure of cyclobutane-d8.

Table 2. Vibrational frequencies of C_4D_8 (cm^{-1})

Vibrational mode	Symmetry species	II overtone	III overtone
v_1 (CD_2 s-str)	A_1	5835	8087
v_2 (CD_2 scis)	A_1	2967	4132
v_3 (CD_2 scis)	A_1	2188	3304
v_4 (CD_2 a-str)	A_1	6014	8328
v_5 (CD_2 rock)	A_1	1532	2360
v_6 (ring puck)	A_1	420	512
v_7 (CD_2 wag)	A_2	2791	3625
v_8 (CD_2 twist)	A_2	2497	3230
v_9 (CD_2 wag)	B_1	2910	4121
v_{10} (Ring deform)	B_1	1865	2647
v_{11} (CD_2 twist)	B_1	2205	3346
v_{12} (CD_2 s-str)	B_2	5879	8223

Vibrational mode	Symmetry species	II overtone	III overtone
ν_{13} (CD ₂ scis)	B ₂	2724	3867
ν_{14} (Ring deform)	B ₂	2597	3529
ν_{15} (CD ₂ a-str)	B ₂	6315	8614
ν_{16} (CD ₂ rock)	B ₂	1215	1786
ν_{17} (CD ₂ a-str)	E	6533	8540
ν_{18} (CD ₂ twist)	E	2671	3644
ν_{19} (CD ₂ rock)	E	1415	2120
ν_{20} (CD ₂ s-str)	E	5845	8106
ν_{21} (CD ₂ scis)	E	3063	4184
ν_{22} (CD ₂ wag)	E	2750	3798
ν_{23} (Ring deform)	E	1789	2513
$\nu_{1+} \nu_{12}$		11716	16312
$\nu_{1+} \nu_{20}$		11682	16195
$\nu_{12+} \nu_{20}$		11726	16331
$\nu_{4+} \nu_{15}$		12331	16744
$\nu_{4+} \nu_{17}$		12549	16870
$\nu_{15+} \nu_{17}$		12850	17156

4. CONCLUSION

The second and third overtone vibrational frequencies and combination bands in cyclobutane-d₈ have been investigated using the symmetry-adapted Lie algebraic method in this study. Our study has highlighted the complex interactions among 23 normal vibrational modes while preserving the D_{2d} point symmetry group. Utilizing Casimir and Majorana operators, the Lie algebraic framework has accelerated computations while fostering a profound understanding of the dynamics of molecular vibrations. A thorough comprehension of the molecular structure of Cyclobutene-d₈ has been attained by evaluating the vibrational Hamiltonians for C-D and C-C stretching vibrations with Casimir and Majorana operators. Our representation was enhanced, and our understanding of molecular dynamics was improved by including symmetry-adapted neighbor coupling coefficients. The presentation of calculated second and third overtone vibrational frequencies and significant combination bands simplifies understanding of experimental spectra from various fields. The research holds practical implications, as evidenced by our results. The robust theoretical approach known as the symmetry-adapted Lie algebraic method excels in studying symmetric molecules by systematically simplifying vibrational degrees of freedom. Its value extends beyond improving computational efficiency and provides invaluable information about how molecular structures function.

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REFERENCES

- [1] C.W. Bauschlicher, and S.R. Langhoff, "The calculation of accurate harmonic frequencies of large molecules: the polycyclic aromatic hydrocarbons, a case study," *Spectrochim. Acta A*, **53**(8), 1225-1240 (1997). [https://doi.org/10.1016/S1386-1425\(97\)00022-X](https://doi.org/10.1016/S1386-1425(97)00022-X)
- [2] V. Špirko, and W.P. Kraemer, "Anharmonic potential function and effective geometries for the NH₃ molecule," *J. Mol. Spectrosc.* **133**(2), 331-344 (1989). [https://doi.org/10.1016/0022-2852\(89\)90196-3](https://doi.org/10.1016/0022-2852(89)90196-3)
- [3] S. Brodersen, and J.-E. Lolck, "Calculation of rotation-vibrational energies directly from an anharmonic potential function," *J. Mol. Spectrosc.* **126**(2), 405-426 (1987). [https://doi.org/10.1016/0022-2852\(87\)90246-3](https://doi.org/10.1016/0022-2852(87)90246-3)
- [4] P.T. Panek, A.A. Hoeske, and C.R. Jacob, "On the choice of coordinates in anharmonic theoretical vibrational spectroscopy: Harmonic vs. anharmonic coupling in vibrational configuration interaction," *J. Chem. Phys.* **150**(5), 054107 (2019). <https://doi.org/10.1063/1.5083186>
- [5] E.E. Porchelvi, and S. Muthu, "Vibrational spectra, molecular structure, natural bond orbital, first-order hyperpolarizability, thermodynamic analysis and normal coordinate analysis of Salicylaldehyde p-methylphenylthiosemicarbazone by density functional method," *Spectrochim. Acta A*, **134**, 453-464 (2015). <https://doi.org/10.1016/j.saa.2014.06.018>
- [6] B. Karthikeyana, K. Sakthiraj, and P. Senthilkumar, "Investigation of Indium Trihydride Molecule and Its Clusters Using Density Functional Theory for Semiconductor Application," *Acta Phys. Pol. A*, **139**(1), 14-19 (2021). <https://doi.org/10.12693/APhysPolA.139.14>
- [7] N.e Mardirossian, and M. Head-Gordon, "Thirty years of density functional theory in computational chemistry: an overview and extensive assessment of 200 density functionals," *Mol. Phys.* **115**(19), 2315-2372 (2017). <https://doi.org/10.1080/00268976.2017.1333644>
- [8] L. Lapinski, H. Rostkowska, M.J. Nowak, J.S. Kwiatkowski, and J. Leszczyński, "Infrared spectra of thioracils: experimental matrix isolation and ab initio Hartree-Fock, post-Hartree-Fock and density functional theory studies," *Vib. Spectrosc.* **13**(1), 23-40 (1996). [https://doi.org/10.1016/0924-2031\(96\)00026-4](https://doi.org/10.1016/0924-2031(96)00026-4)

- [9] P. Echenique, and J.L. Alonso, "A mathematical and computational review of Hartree–Fock SCF methods in quantum chemistry," *Mol. Phys.* **105**(23-24), 3057-3098 (2007). <https://doi.org/10.1080/00268970701757875>
- [10] H. Ghalla, N. Rezik, A. Michta, B. Oujia, and H.T. Flakus, "Theoretical modeling of infrared spectra of the hydrogen and deuterium bond in aspirin crystal," *Spectrochim. Acta A*, **75**(1), 37-47 (2010). <https://doi.org/10.1016/j.saa.2009.09.029>
- [11] W. Li, Z. Ni, and S. Li, "Cluster-in-molecule local correlation method for post-Hartree–Fock calculations of large systems," *Mol. Phys.* **114**(9), 1447-1460 (2016). <https://doi.org/10.1080/00268976.2016.1139755>
- [12] R. Venkatraman, J.S. Kwiatkowski, G. Bakalarski, and J. Leszczynski, "Molecular structure and IR spectra of bromomethanes by DFT and post-Hartree-Fock MP2 and CCSD(T) calculations," *Mol. Phys.* **98**(6), 371-386 (2000). <https://doi.org/10.1080/00268970009483302>
- [13] K.B. Beć, J. Grabska, and C.W. Huck, "Current and future research directions in computer-aided near-infrared spectroscopy: A perspective," *Spectrochim. Acta A*, **254**, 119625 (2021). <https://doi.org/10.1016/j.saa.2021.119625>
- [14] F. Iachello, and R.D. Levine, *Algebraic theory of molecules*, (Oxford University Press, Oxford, 1995).
- [15] V. Jaliparthi, and M.R. Balla, "Vibrational Hamiltonian of Tetrachloro-, Tetrafluoro-, and Mono- Silanes Using U(2) Lie Algebras," *Spectrochim. Acta A*, **264**, 120289 (2022). <https://doi.org/10.1016/j.saa.2021.120289>
- [16] M.R. Balla, and V. Jaliparthi, "Vibrational Hamiltonian of Naphthalene (C₁₀H₈) Using Dynamical U(2) Lie Algebras," *Polycycl. Aromat. Compd.* **42**(7), 4684-4699 (2022). <https://doi.org/10.1080/10406638.2021.1901126>
- [17] S. Oss, "Algebraic models in molecular spectroscopy," in: *Advances in Chemical Physics: New Methods in Computational Quantum Mechanics*, vol. 93, edited by I. Prigogine, and S.A. Rice (John Wiley & Sons, Inc. 1996). pp.455-649. <https://doi.org/10.1002/9780470141526.ch8>
- [18] M.R. Balla, and V. Jaliparthi, "Vibrational Hamiltonian of Methylene Chloride Using U(2) Lie Algebra," *Mol. Phys.*, **115**, e1828634 (2021). <https://doi.org/10.1080/00268976.2020.1828634>
- [19] V. Jaliparthi, "Vibrational Energies of Silylene, Difluorosilylene and Dichlorosilylene, Using U(2) Lie Algebraic Model," *Ukr. J. Phys. Opt.* **23**(3), 126-132 (2022). <https://doi.org/10.3116/16091833/23/3/126/2022>
- [20] M.R. Balla, S. Venigalla, and V. Jaliparthi, "Calculation of Vibrational Frequencies of Sulfur Dioxide by Lie Algebraic Framework," *Acta Phys. Pol. A*, **140**(2), 138-140 (2021). <https://doi.org/10.12693/APhysPolA.140.138>
- [21] J. Vijayasekhar, P. Suneetha, and K. Lavanya, "Vibrational spectra of cyclobutane-d8 using symmetry-adapted one-dimensional Lie algebraic framework," *Ukr. J. Phys. Opt.* **24**, 193-199 (2023). <https://doi.org/10.3116/16091833/24/3/193/2023>
- [22] K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A: Theory and Applications in Inorganic Chemistry*, (Wiley, New York, 2009).
- [23] K.P. Huber, and G. Herzberg, *Molecular Spectra and Molecular Structure. IV: Constants of Diatomic Molecules*, (Van Nostrand Reinhold, New York, 1979).

ДОСЛІДЖЕННЯ ВИЩИХ ОБЕРТОНІВ КОЛИВАЛЬНИХ ЧАСТОТ ЦИКЛОБУТАНУ-D8 З ВИКОРИСТАННЯМ АЛГЕБРИ ЛІ

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У цьому дослідницькому дослідженні використовується алгебраїчна структура Лі для дослідження частот коливань другого та третього обертонів та їхніх комбінованих смуг у циклобутані-d8 (C₄D₈). Застосування цього каркасу забезпечує збереження точкової групи симетрії D_{2d}, що характеризується видами симетрії A₁, A₂, B₁, B₂ та E. Аналіз охоплює 23 нормальні коливальні моди в молекулярній структурі циклобутану-d8. Наше дослідження широко досліджує вібраційні спектри, з'ясовуючи складну взаємодію між цими вібраційними модами. Збереження молекулярної симетрії дозволяє глибше зрозуміти вібраційні взаємодії, пропонуючи цінну інформацію про спектроскопію. Дослідження покращує розуміння молекулярної структури та її застосування в різних областях, забезпечуючи детальне уявлення про вищі енергетичні рівні та складні коливальні переходи в циклобутані-d8.

Ключові слова: оператор Гамільтона; алгебра Лі; коливальні спектри; осцилятор Морзе; циклобутан-d8