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EXPLORING CYCLOHEXANE VIBRATIONAL DYNAMICS THROUGH A LIE ALGEBRAIC HAMILTONIAN FRAMEWORK

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Abstract. This study explores the anharmonic local mode vibrational frequencies of the cyclohexane (C_6H_{12}) molecule, classified under the D_{3d} point group, up to the second overtone. We use a vibrational Hamiltonian model based on U(2) Lie algebras. Our Lie algebraic method is characterized by integrating minimized algebraic parameters precisely adapted for cyclohexane. This process involves substituting each bond in the molecule with a corresponding Lie algebra, leading to the development of a Hamiltonian that includes interacting operators. Through this detailed analysis, we illuminate the anharmonic vibrational behavior of cyclohexane, providing significant insights into its molecular dynamics within a framework that respects symmetry adaptation.

Keywords: vibrational frequencies, Lie algebraic framework, U(2) Lie algebras, cyclohexane, anharmonic vibrations, D_{3d} point group
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1. Introduction

Studying the vibrational spectra of molecules represents a formidable challenge in contemporary mathematical physics research. The advent of advanced experimental techniques capable of generating higher vibrational excitations in polyatomic molecules necessitates robust theoretical methodologies for accurate interpretation. Traditionally, two theoretical frameworks have been employed to analyze the experimental data of the rovibrational spectra of polyatomic molecules. The first approach, the Dunham expansion, involves a series expansion of energy levels based on rotation-vibration quantum numbers [1]. However, this method proves less suitable for rigorous modeling due to various limitations. Firstly, it necessitates alignment with the wave functions of individual states, rendering the direct calculation of operator matrix elements unfeasible. Secondly, a substantial number of parameters are required for the Dunham expansion in the case of large polyatomic molecules, demanding an extensive experimental database for optimization, which is only occasionally practical. The second approach, a more favorable alternative to the Dunham expansion, involves solving the Schrödinger equation with potentials through enhanced ab initio methods and utilizing provided wave functions to compute the matrix elements of the Hamiltonian operator. Nonetheless, this approach encounters difficulties, particularly with larger molecules and highly excited levels, as all manipulations involve differentiation or integration [2-5]. A third and notably intriguing alternative is the Lie algebraic framework, also known as the one-dimensional symmetry-

adapted Lie algebraic method. Initially applied by Iachello F. et al. and Oss S. using the U(2) Lie algebraic method, this model demonstrated efficacy in studying the vibrational spectra of small molecules [6-8]. Subsequently, it was refined to investigate the vibration spectra of medium-sized molecules at higher overtones [9-16]. The Lie algebraic method enables the estimation of vibrational energies with reduced computational expense and heightened accuracy compared to other theoretical approaches.

Remarkably, there has yet to be any prior endeavor to calculate the vibrational frequencies of cyclohexane, including fundamental frequencies and higher overtones. Thus, this work endeavors to apply the Lie algebraic model for computing vibrational frequencies up to the second overtone.

2. Structure of cyclohexane

Cyclohexane, an unsaturated hydrocarbon molecule, plays a pivotal role in the chemical industry as a nonpolar solvent due to its versatile properties. However, its widespread usage comes with significant health and environmental risks, as it is known to be toxic to humans and animals. Inhalation of cyclohexane can lead to various symptoms, including headaches, dizziness, drowsiness, incoordination, and even euphoria. Cyclohexane is a six-membered ring hydrocarbon with the molecular formula C_6H_{12}. In its most stable conformation, the chair conformation cyclohexane adopts a three-dimensional structure belonging to the D_{3d} point group (Fig.1). This is because the chair conformation exhibits three C2 axes of rotation perpendicular to the main molecular plane and three perpendicular σ_v mirror planes. Remember that the chair conformation of cyclohexane is a dynamic structure, meaning it can interconvert between two chair forms (the "up" chair and the "down" chair) through a process known as ring flipping. Represented by the molecular formula C_6H_{12}, cyclohexane is classified as a cycloalkane. Its distinctive ring structure is a hallmark feature, with identical bonds connecting all the carbon atoms. Specifically, each carbon atom forms bonds with two other carbon atoms and two hydrogen atoms. With 18 atoms, cyclohexane qualifies as a relatively large molecule, imposing exciting challenges in its vibrational analysis.

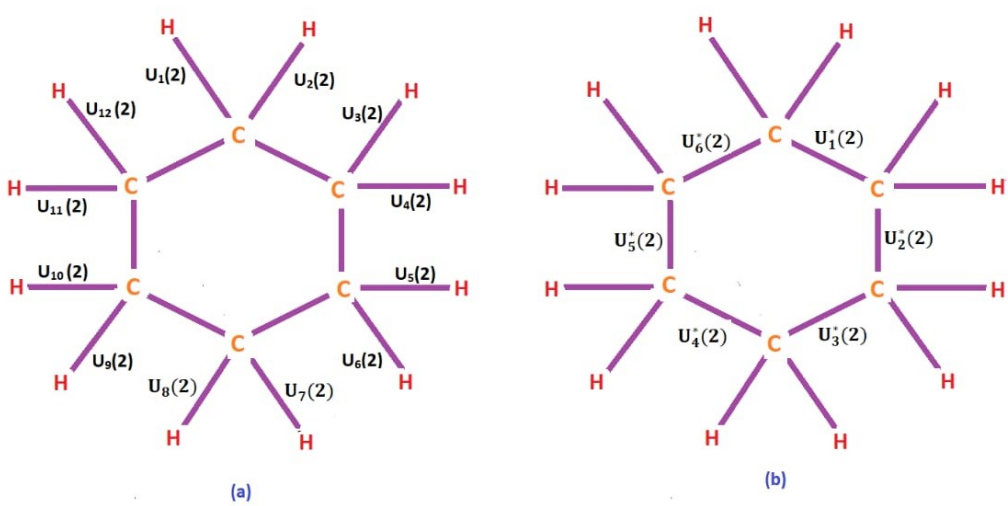

Fig. 1. Cyclohexane structure is illustrated with specific Lie algebras assigned to various bond species. (a) For the C-H bonds, the Lie algebras $U_1(2)$ through $U_{12}(2)$ are assigned; (b) for the C-C bonds, the Lie algebras $U_1^*(2)$ through $U_6^*(2)$ are designated.

Cyclohexane exhibits an impressive 48 degrees of freedom in vibrational modes. These modes can be systematically categorized into distinct groups, comprising 12 C-H stretching vibrations, 6 H-C-H bending vibrations, 6 C-C-C bending vibrations, and 18 CH_2 rocking and twisting vibrations [17, 18]. This extensive array of vibrational modes sheds light on the intricate and dynamic nature of cyclohexane's molecular structure.

3. Formulation of vibrational Hamiltonian for cyclohexane

Formulating the vibrational Hamiltonian for cyclohexane involves building a mathematical framework that accounts for the molecule's vibrational behavior. This encompasses assigning appropriate mathematical operators to represent the molecule's vibrational degrees of freedom. The resulting Hamiltonian encapsulates the interactions between these vibrational modes, comprehensively describing the molecule's vibrational spectrum [6-16]. This formulation is crucial in understanding and predicting cyclohexane's vibrational frequencies, enabling further insights into its dynamic behavior in chemical processes and reactions.

As per the structure of cyclohexane, we have introduced twelve $U_i(2)$ (i=1 to 12) Lie algebras to describe the twelve C-H stretching bonds (Fig. 1a) and six $U_i(2)$ (i=1 to 6) Lie algebras to describe the six C-C stretching bonds (Fig. 1b). The interactions among these vibrations can be effectively described by two chains of dynamical $U(2)$ Lie algebras as:

$$U_1(2)\otimes U_2(2)\otimes ...\otimes U_{12}(2)\supset O_1(2)\otimes O_2(2)\otimes ...\otimes O_{12}(2)\to C-H \text{ local coupling,}$$

$$U_1(2)\otimes U_2(2)\otimes ...\otimes U_{12}(2)\supset U(2)\supset O(2)\to C-H \text{ normal coupling,}$$

$$U_1(2)\otimes U_2(2)\otimes ...\otimes U_6(2)\supset O_1(2)\otimes O_2(2)\otimes ...\otimes O_6(2)\to C-C \text{ local coupling,}$$

$$U_1(2)\otimes U_2(2)\otimes ...\otimes U_6(2)\supset U(2)\supset O(2)\to C-C \text{ normal coupling.}$$

The interactions among the C-H bond stretching vibrations in cyclohexane are given by $\{U_k(2)\otimes U_l(2)\}$.

Interaction I (First-neighbour couplings):
$(k,l)=(1,2),(2,3),(3,4),(4,5),(5,6),(6,7),(7,8),(8,9),(9,10),(10,11),(11,12),(12,1)$.

Interaction II (Second-neighbour couplings):
$(k,l)=(1,3),(2,4),(3,5),(4,6),(5,7),(6,8),(7,9),(8,10),(9,11),(10,12),(11,1),(12,2)$.

Interaction III (Third-neighbour couplings):
$(k,l)=(1,4),(2,5),(3,6),(4,7),(5,8),(6,9),(7,10),(8,11),(9,12),(10,1),(11,2),(12,3)$.

Interaction IV (Fourth-neighbour couplings):
$(k,l)=(1,5),(2,6),(3,7),(4,8),(5,9),(6,10),(7,11),(8,12),(9,1),(10,2),(11,3),(12,4)$.

Interaction V (Fifth-neighbour couplings):
$(k,l)=(1,6),(2,7),(3,8),(4,9),(5,10),(6,11),(7,12),(8,1),(9,2),(10,3),(11,4),(12,5)$.

Interaction VI (Sixth-neighbour couplings): $(k,l)=(1,7),(2,8),(3,9),(4,10),(5,11),(6,12)$.

The interactions among the C-C bond stretching vibrations in cyclohexane are given by $\{U_p(2)\otimes U_q(2)\}$.

Interaction I (First-neighbour couplings): $(p,q)=(1,2),(2,3),(3,4),(4,5),(6,1)$.

Interaction II (Second-neighbour couplings): $(p,q)=(1,3),(2,4),(3,5),(4,6),(1,5),(2,6)$.

Interaction III (Third-neighbour couplings): $(p,q)=(1,4),(2,5),(3,6)$.

The Hamiltonian operator that preserves the D_{3d} symmetry of the cyclohexane is as follows:

$$H^{C-H}=E_0+\sum_{i=1}^{n=12}A_i^{C-H}C_i+\sum_{i<j}^{n=12}A_{ij}^{C-H}C_{ij}+\sum_{i<j}^{n=12}\lambda_{ij}^{C-H}M_{ij}, \tag{1}$$

$$H^{C-C}=E_0+\sum_{i=1}^{n=6}A_i^{C-C}C_i+\sum_{i<j}^{n=6}A_{ij}^{C-C}C_{ij}+\sum_{i<j}^{n=6}\lambda_{ij}^{C-C}M_{ij}. \tag{2}$$

Here, E_0 is the term representing the eigenvalue of the Schrodinger equation associated with the electronic ground state of the bond vibrations, which will be taken as the zero reference for all the excitations; $A_i^{C-H},A_{ij}{}^{C-H},\lambda_{ij}{}^{C-H},A_i^{C-C},A_{ij}{}^{C-C},\lambda_{ij}{}^{C-C}$ are stretching algebraic parameters; C_i,C_{ij} are the Casimir (invariant) algebraic operators of the applicable Lie algebras; and M_{ij} are the Majorana (invariant) algebraic operators connected with coupling schemes involving Lie algebras of the *n* interacting one-dimensional Morse oscillators.

For cyclohexane, the algebraic parameters are determined from the spectroscopic data, and the algebraic operators are determined from the following expressions:

$$\begin{aligned}
&\langle C_i\rangle=-4\left(N_i\mathrm{v}_i-\mathrm{v}_i^2\right),\\
&\left\langle N_i,\mathrm{v}_i;N_j,\mathrm{v}_j\middle|C_{ij}\middle|N_i,\mathrm{v}_i;N_j,\mathrm{v}_j\right\rangle=4\left[\left(\mathrm{v}_i+\mathrm{v}_j\right)^2-\left(\mathrm{v}_i+\mathrm{v}_j\right)\left(N_i+N_j\right)\right],\\
&\left\langle N_i,\mathrm{v}_i;N_j,\mathrm{v}_j\middle|M_{ij}\middle|N_i,\mathrm{v}_i;N_j,\mathrm{v}_j\right\rangle=\left(N_i\mathrm{v}_j+N_j\mathrm{v}_i-2\mathrm{v}_i\mathrm{v}_j\right),\\
&\left\langle N_i,\mathrm{v}_i+1;N_j,\mathrm{v}_j-1\middle|M_{ij}\middle|N_i,\mathrm{v}_i;N_j,\mathrm{v}_j\right\rangle=-\left[\mathrm{v}_j\left(\mathrm{v}_i+1\right)\left(N_i-\mathrm{v}_i\right)\left(N_j-\mathrm{v}_j+1\right)\right]^{1/2},\\
&\left\langle N_i,\mathrm{v}_i-1;N_j,\mathrm{v}_j+1\middle|M_{ij}\middle|N_i,\mathrm{v}_i;N_j,\mathrm{v}_j\right\rangle=-\left[\mathrm{v}_i\left(\mathrm{v}_j+1\right)\left(N_j-\mathrm{v}_j\right)\left(N_i-\mathrm{v}_i+1\right)\right]^{1/2},
\end{aligned} \tag{3}$$

where $\mathrm{v}_i,\mathrm{v}_j$ are vibrational quantum numbers of bonds *i* and *j* respectively, and N_i,N_j are vibron numbers, which correspond to the maximum number of bound states of the Morse potential in each vibrating bond species, is calculated from the relation:

$$N=\frac{\omega_e}{\omega_e x_e}-1, \tag{4}$$

where $\omega_e,\omega_e x_e$ are the spectroscopic constants of the corresponding bonds obtained from experimental data of diatomic molecules. Considering the experimental values of these constants [19, 20] for C–H (ω_e = 2860.7508 cm^{-1}, $\omega_e x_e$ = 64.4387 cm^{-1}) and C–C (ω_e = 855.0663 cm^{-1}, ω_e = 13.6007 cm^{-1}), their $N^{C\text{-}H}$ (stretching), $N^{C\text{-}C}$ (stretching), N^{sci} (bending-scissoring) and N^{rock} (bending-rocking) values for cyclohexane are fixed as 44, 136, 20 and 60, respectively [19-21].

The initial guess for the parameters A_i is obtained from the energy expression for single-oscillator fundamental mode:

$$\begin{aligned}
E_i^{C-H}(v=1)&=-4A_i^{C-H}\left(N^{C-H}-1\right),\\
E_i^{C-H}(v=1)&=-4A_i^{C-C}\left(N^{C-C}-1\right).
\end{aligned} \tag{5}$$

The initial guesses for λ_{ij} are obtained by the relations:

$$\lambda_{ij}^{C-H} = \frac{E_i^{C-H} - E_j^{C-H}}{12N^{C-H}},\ \lambda_{ij}^{C-C} = \frac{E_i^{C-C} - E_j^{C-C}}{6\,N^{C-C}}, \tag{6}$$

$$\lambda_{ij}^{sci(1)} = \frac{E(a_{2u}) - E(a_{1g})}{12N^{sci}},\ \lambda_{ij}^{sci(2)} = \frac{E(e_u) - E(e_g)}{12N^{sci}}, \tag{7}$$

$$\lambda_{ij}^{rock(1)} = \frac{E(a_{2u}) - E(a_{1g})}{4N^{rock}},\ \lambda_{ij}^{rock(2)} = \frac{E(e_u) - E(e_g)}{4N^{rock}}. \tag{8}$$

Here, $E_i^{C-H}, E_j^{C-H}, E_i^{C-C}, E_j^{C-C}$ are the different energies corresponding to symmetric and antisymmetric combination of the two local modes and $E(a_{2u})$, $E(a_{1g})$, $E(e_u)$, $E(e_g)$ represents the scissoring, rocking energies (indicated in Table 2). Here, E_i, E_j represents the symmetric and antisymmetric stretching energies, respectively. The initial guesses for A_{ij} are taken as zero. The values of algebraic parameters are optimized by least-square regression fitting, starting from the initial guesses as given by Eqs. (5) and (6).

4. Results

In Table 1, we present the fitted values of algebraic parameters and vibron numbers used within the context of the Lie algebraic framework. These parameters play a pivotal role in influencing the simulation outcomes, highlighting the importance of their meticulous optimization to ensure the model's effectiveness and accuracy. Table 2 outlines the vibrational frequencies for the fundamental, first, and second overtones, along with their symmetry species and vibrational modes within the cyclohexane molecule.

Table 1. Optimized Fitting Parameters for the U(2) Lie Algebraic Vibrational Hamiltonian in D_{3d} symmetry cyclohexane.

Algebraic Parameters	
A_i^{C-H} (stretching)	-16.8081
A_i^{C-C} (stretching)	-0.4316
$A_{i\,j}{}^{C-H}$ (stretching)	0.0073
A_{ij}^{C-C} stretching	-0.1049
λ_{ij}^{C-H} (stretching)	-0.1482
λ_{ij}^{C-C} (stretching)	0.3125
$A_i^{sci(1)}, A_i^{sci(2)}$	-19.09, -19.07
$A_i^{rock(1)}, A_i^{rock(2)}$	-4.63, -3.58
$A_{ij}^{sci(1)}, A_{ij}^{sci(2)}$	0.80, 1.46
$A_{ij}^{rock(1)}, A_{ij}^{rock(2)}$	-0.55, -0.303
$\lambda_{ij}^{sci(1)}, \lambda_{ij}^{sci(2)}$	-0.11, 0.05
$\lambda_{ij}^{rock(1)}, \lambda_{ij}^{rock(2)}$	-0.52, 0.508

Table 2. Vibrational frequencies (in cm^{-1}) for cyclohexane using the $U(2)$ Lie algebraic vibrational Hamiltonian, together with fundamental experimental observations [22], mode assignments, and symmetry species (irreducible representations).

Vibrational Mode	Symmetry Species	Fundamental Mode (Experimental)	Fundamental Mode (Calculated)	I overtone	II overtone
ν_1 (CH_2 a-str)	a_{1g}	2930	2930.28	5759.24	8689.62
ν_2 (CH_2 s-str)	a_{1g}	2852	2852.03	5672.62	8432.28
ν_3 (CH_2 scis)	a_{1g}	1465	1465.86	2598.03	3876.35
ν_4 (CH_2 rock)	a_{1g}	1157	1155.12	2151.42	3376.73
ν_5 (CC str)	a_{1g}	802	801.622	1543.22	2276.51
ν_9 (CC str)	a_{1u}	1057	1056.56	2064.70	3024.42
ν_{12} (CH_2 a-str)	a_{2u}	2915	2915.02	5761.71	8657.31
ν_{13} ((CH_2 s-str))	a_{2u}	2860	2860.00	5654.38	8471.66
ν_{14} (CH_2 scis)	a_{2u}	1437	1440.78	2523.61	4008.07
ν_{15} (CH_2 rock)	a_{2u}	1030	1036.56	1875.74	2763.30
ν_{17} ((CH_2 a-str))	e_g	2930	2928.75	5781.11	8712.56
ν_{18} ((CH_2 s-str))	e_g	2897	2901.24	5706.78	8634.73
ν_{19} (CH_2 scis)	e_g	1443	1449.60	2579.44	3972.80
ν_{22} (CC Str)	e_g	1027	1025.49	1943.44	2854.26
ν_{23} (CH_2 rock)	e_g	785	784.58	1407.69	2197.25
ν_{25} (CH_2 a-str)	e_u	2933	2832.95	5812.32	8703.00
ν_{26} (CH_2 s-str)	e_u	2863	2864.84	5624.68	8476.47
ν_{27} (CH_2 scis)	e_u	1457	1461.00	2692.10	3920.88
ν_{30} (CH_2 rock)	e_u	907	900.40	1657.71	2445.29
ν_{31} (CC str)	e_u	863	861.75	1679.00	2513.75

Notation: s-str = symmetric stretch, a-str = asymmetric stretch, scis = scissor, rock = rocking.

5. Conclusion

This study utilized an advanced computational method to predict cyclohexane's higher overtone vibrational frequencies up to the second overtone. The calculated fundamental vibrational frequencies were compared with available experimental data, revealing a consistent match. By applying a Lie algebraic framework within the vibrational Hamiltonian, we elucidated the complex vibrational dynamics of the molecule. Our results demonstrate the effectiveness of this approach in understanding cyclohexane's vibrations. The integration of experimental data with theoretical advancements bridged the gap between observation and exploration, paving the way for new scientific and technological possibilities. This study advances the understanding of vibrational dynamics and offers new avenues for exploring and applying molecular vibrations, with promising practical applications.

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Анотація*. У цьому дослідження вивчені ангармонічні локальні моди коливальних частот молекули циклогексану (C_6H_{12}), яка характеризується точковою групою D_{3d}, до другого обертону. В роботі використана модель коливального гамільтоніана на основі алгебр Лі U(2). Наш метод, який базується на алгебрах Лі, характеризується*

інтеграцією мінімізованих алгебраїчних параметрів, точно адаптованих для циклогексану. Цей процес передбачає заміну кожного зв'язку в молекулі відповідною алгеброю Лі, що приводить до отримання гамільтоніана, який включає взаємодіючі оператори. Завдяки цьому детально проаналізована ангармонічна коливальна поведінка циклогексану і висвітлена його молекулярна динаміка в рамках підходу, який враховує симетрійну адаптацію.

***Ключові слова**: коливальні частоти, алгебраїчний підхід Лі, алгебри Лі U(2), циклогексан, ангармонічні коливання, точкова група D_{3d}*