

VIBRATIONAL FREQUENCIES OF DICHLORODIFLUOROMETHANE USING A LIE ALGEBRAIC FRAMEWORK

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This study introduces a symmetry-adapted Lie algebraic framework, a highly efficient tool for calculating vibrational frequencies in dichlorodifluoromethane (CCl_2F_2). With its C_{2v} point group symmetry, the molecule under consideration is particularly suited for this approach. By formulating carbon-hydrogen (C-H) and carbon-chlorine (C-Cl) bond structures in unitary Lie algebras, the determination of the vibrational quantum states of the molecule becomes remarkably straightforward. The Hamiltonian, including Casimir and Majorana invariant operators and fitted parameters, accurately reproduces the desired vibrational modes using fundamental and higher overtone frequencies. This approach, which compares modern and classical models, underscores the Lie algebraic techniques as efficient tools for modelling anharmonic interactions and transition dynamics on a molecular scale. Beyond its theoretical relevance, the model constructed provides a deep understanding of the vibrational aspects of molecules, a knowledge crucial for practical applications such as spectroscopic data interpretation, the design of materials with desired vibrational characteristics, or the study of molecules in complex environments. These practical applications enhance the versatility of the methodology and have enabled its successful application to molecular spectroscopy, chemical kinetics, and the design of energy-efficient materials and sensors, among other areas. This study provides experimentalists with confidence in the Lie algebraic approach and paves the way for further polyatomic molecule experiments. By significantly contributing to reducing the error margin in computational molecular physics, this methodology opens exciting possibilities for future research and development.

Keywords: Lie Algebraic Approach; Vibrational Hamiltonian; Casimir and Majorana Operators; Dichlorodifluoromethane; Anharmonic Vibrational Modes

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1. INTRODUCTION

Vibrational spectra are of great importance as they form the basis of molecular spectroscopy and are a valuable resource for depicting a molecule's structural, dynamic, and chemical aspects. The spectra are the result of the quantization of vibrational modes of molecular bonds and are valuable in understanding molecular behaviour, such as bond strength, structure, and energy interactions. These natural frequencies are associated with the vibrational spectra of molecules and serve as the basis for understanding inter and intra-molecular interaction and stability. Their accurate determination is important for various applications in science and industry, including the characterization of materials, monitoring of the environment, analysis of chemicals, and even drug design. Their prediction and analysis enable scientists to envisage the molecular properties under varied physical and chemical circumstances, which enhances the growth of both theoretical and experimental chemistry [1-3].

For a long time now, various means of computational geometry have existed to compute vibrational frequencies, each applying to scenarios and having flaws of their own. For example, the first approximation treats vibrations of molecules as harmonic oscillators, with the only caveat being a quadratic potential energy surface. This leads to having multiple overtones at one time; thus, considering anharmonic oscillations masks this model for a better chance of correctness while being overly simplistic when adjusting for vertical strength. As long as we narrow our scope to smaller molecules, there are quantum equations that allow such non-harmonics to work as expected, yet as the size of the molecule increases, so does the cost. Because of this, Ab initio seems infeasible, which leaves us with the now classical Density Functional Theory, which does have good scaling while providing correct values but does depend on the set basis chosen for the function, which raises their accuracy depending on the interactions at hand. A brute method and exact method are a popular combination because half the work done on the molecule allows for the rest to be narrowed down, so while being computationally less in demand, they still are limited [4-9].

To begin with, it must be pointed out that even though they are helpful, conventional strategies are faced with great difficulties when applying them to complex molecular systems. Such limitations encompass the difficulties in handling anharmonic vibrations, especially in excited states, and large computationally expensive molecules. In addition, too many conventional methods have the opportunity to account for transitions between the localized and delocalized vibrational modes, which is crucial for an adequate description of the molecular dynamics. All these disadvantages justify using different approaches, which have to specify molecular vibrations at specific but not-so-high computational expenses [10-14].

The Lie algebraic approach is a viable way to cope with such shortcomings. This method applies the mathematics of Lie algebras to the task of defining molecular vibrations in a symmetry-adapted form, which has certain benefits over the standard approach. The vibrational Hamiltonian, which encapsulates the energy of the molecules in terms of their vibrations, is written in the form of operators that include the system's characteristics regarding its vibrational aspects. These operators include Casimir operators that explain symmetry relations between the states of vibration and Majorana operators that describe an anharmonic relation between the vibration modes. The parameters connected with these operators are fitted to the experimental data, and the results obtained are used to predict the molecular vibrational characteristics. Unlike the conventional approaches, the Lie Algebraic approach automatically includes some anharmonicity and, therefore, is much more applicable when predicting higher overtones and the detail of molecular vibrations is required. In this case, the method primarily benefits from using the symmetry of molecules to substantially simplify and reduce the number of variables and operations required to perform a deep analysis of the Hamiltonian vibrational function. Lie algebraic model provides accurate, efficient calculations of molecular spectroscopic information that account for vibrational modes that are localized and delocalized. This model has applications that range from complex systems to diatomic molecules and encompasses all in between, thus proving to be quite versatile. Furthermore, this model alleviates the problems faced by traditional models that are primarily computational, such as dealing with nuclear and computational costs, which enhances its use for molecular spectroscopy [15-19].

This study calculates the vibrational frequencies of dichlorodifluoromethane using an integrated Lie algebraic approach. The vibrational spectrum of dichlorodifluoromethane helps assess computational methods due to its frequency range, making the molecule of both industrial and environmental significance. The molecule possesses overlapping stretching and bending vibrational modes and belongs to the C_{2v} symmetry point group, which validates the use of the Lie algebraic framework. The parameters of symmetry-adapted operators used in a molecule's vibrational Hamiltonian are adjusted to reduce the difference between theoretical predictions and experimental observations. This study has displayed that the system can accurately forecast the fundamental and higher over-tone frequencies while dealing with non-linear interactions.

The results of this research point out the benefits of utilizing the Lie algebraic approach compared to typical approaches. The approach's capability of accounting for anharmonic effects, cutting down the computation required, and conforming to the symmetry properties of molecules indicates that it has prospects for broader use in molecular spectroscopy. Apart from providing a thorough treatment of dichlorodifluoromethane's vibrational characteristics, this study also demonstrates the ability of the theory to deal with sophisticated molecular systems. The results demonstrate how the Lie algebraic approach fills in the important voids in vibrational analysis and provides an inexpensive and efficient substitute for the conventional computational methods.

The main goals of this study are to assess the shortcomings of the available approaches in estimating vibrational frequencies and display the inherent advantages of this Lie algebraic framework. Using dichlorodifluoromethane as an illustration, the present work seeks to validate the relevance of the method in dealing with problems on anharmonicity and offering further savings on computation time. It also targets bringing the foundations towards using the Lie algebraic technique on a larger scale and more complicated molecular structures, which can further enhance molecular spectroscopy methods. This study's results improve the vibrational dynamics of the molecule under investigation, dichlorodifluoromethane, and foster the use of such symmetry-adapted methods in studying molecular vibrations in other fields.

2. LIE ALGEBRAIC HAMILTONIAN FOR VIBRATIONAL ANALYSIS OF CCl_2F_2

The tetrahedral molecule known as Freon-12 or Dichlorodifluoromethane has a carbon atom which is bonded two each of two atoms, chlorine and two atoms of fluorine. It possesses C_{2v} symmetry which enables the vibrational modes to be divided into four unique symmetry species (A_1 , A_2 , B_1 , B_2). The components of A_1 include symmetric stretching and bending, the component of B_1 is asymmetric stretching whereas the component of B_2 is asymmetric bending that is oriented perpendicular to the molecular plane. Such symmetry classification aids in conducting vibrational analysis by estimating IR and Raman activity, besides classifying the molecular into other spectroscopic properties. Employing the Lie algebraic framework, this symmetry is applied to derive the vibrational Hamiltonian which describes in a good approximation both harmonic and anharmonic molecular interactions.

The vibrational Hamiltonian for CCl_2F_2 is expressed as [20-22]:

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

where E_0 represents the zero-point energy, $A_i, A_{ij}, \lambda_{ij}$ are algebraic parameters, C_i are Casimir operators for individual vibrational modes, C_{ij} represent coupled vibrational modes, and M_{ij} are Majorana operators capturing cross-mode interactions.

Casimir operators C_i quantify the anharmonicity of single vibrational modes with eigenvalues given by:

$$-4(N_i v_i - v_i^2) \quad (2)$$

where N_i is the vibron number, and v_i is the vibrational quantum number. For coupled modes, the operator C_{ij} has diagonal matrix elements:

$$\langle N_i, v_i; N_j, v_j | C_{ij} | N_i, v_i; N_j, v_j \rangle = 4 \left[(v_i + v_j)^2 - (v_i + v_j)(N_i + N_j) \right]. \quad (3)$$

The Majorana operator M_{ij} includes both diagonal and off-diagonal terms, representing energy exchange between coupled vibrational modes:

$$\langle N_i, v_i; N_j, v_j | M_{ij} | N_i, v_i; N_j, v_j \rangle = (N_i v_j + N_j v_i - 2v_i v_j). \quad (4)$$

Off-diagonal elements for vibrational transitions are given by:

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

The vibron numbers N_i , which quantify the anharmonicity of each bond, are calculated as:

$$N_i = \frac{(\omega_e)_i}{(\omega_e x_e)_i} - 1, \quad i = 1, 2, 3, 4, \quad (6)$$

where ω_e is the harmonic frequency, and $\omega_e x_e$ is the anharmonic constant obtained from spectroscopic data [23].

The initial estimates for algebraic parameters $A_i, A_{ij}, \lambda_{ij}$ are derived using fundamental vibrational energy relations. For the symmetric and asymmetric stretching modes:

$$\left. \begin{aligned} E^{C-F}(v = 1) &= -4A_1(N_1 - 1) \\ E^{C-Cl}(v = 1) &= -4A_2(N_2 - 1) \end{aligned} \right\} \quad (7)$$

The coupling parameters are estimated as:

$$\left. \begin{aligned} \lambda_{ij}^{C-F} &= \frac{|E^{C-F}(\text{Symmetric Stretch}) - E^{C-F}(\text{Asymmetric Stretch})|}{3N_1} \\ \lambda_{ij}^{C-Cl} &= \frac{|E^{C-Cl}(\text{Symmetric Stretch}) - E^{C-Cl}(\text{Asymmetric Stretch})|}{3N_2} \end{aligned} \right\} \quad (8)$$

Applying the least square numerical regression improves the parameters, in this way reducing the difference between computed and experimental frequencies. The Hamiltonian includes both the C-Cl bond and C-F bond contributions:

$$H = H^{C-F} + H^{C-Cl}, \quad (9)$$

where:

$$\left. \begin{aligned} H^{C-Cl} &= E_0^{C-Cl} + A_1 C_1 + A_2 C_2 + A_{12} C_{12} + \lambda_{12} M_{12} \\ H^{C-F} &= E_0^{C-F} + A_3 C_3 + A_4 C_4 + A_{34} C_{34} + \lambda_{34} M_{34} \end{aligned} \right\} \quad (10)$$

This model considers the bending and stretching vibrations of C-Cl and C-F bonds, and it portrays the vibration spectrum of CCl_2F_2 even more accurately. From the invariance group C_{2v} and the symmetry adapted operator's aid, the Lie algebraic model provides close estimates of the resonant and harmonic frequencies which makes it highly effective in analysing the molecular dynamics and the spectroscopic characteristics of the halogenated hydrocarbons.

3. RESULTS AND DISCUSSIONS

The vibrational Hamiltonian parameters were obtained by fitting to the fundamental vibrational frequency data of CCl_2F_2 , in order to determine a set of parameters such that the U(2) Lie algebraic approach for predicting the vibrational frequencies of CCl_2F_2 could be applied []. The fitted parameters are as follows:

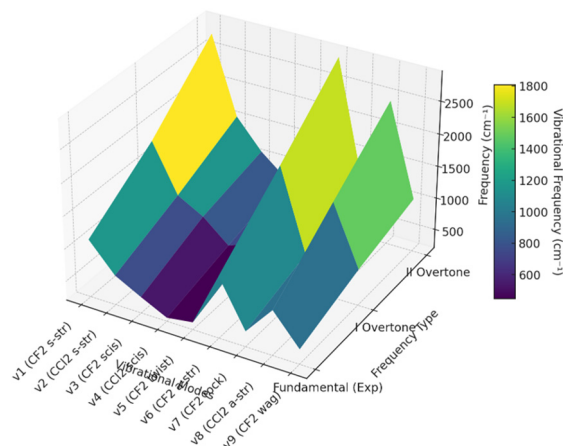
$$N_{C-F} = 118, N_{C-Cl} = 160, A_i^{C-F} = -2.35, A_i^{C-Cl} = -1.04, A_{ij}^{C-F} = 6.38, A_{ij}^{C-Cl} = 3.26, \lambda_{ij}^{C-F} = -0.16, \lambda_{ij}^{C-Cl} = -0.48$$

Table 1 below provides a comprehensive summary of the vibrational frequencies, symmetry species, and the corresponding vibrational modes within the molecule. These results highlight the distribution of vibrational energy across different modes, offering a detailed understanding of the molecular dynamics.

Further, these quantities are expressed graphically in the Figure which depicts the vibrational frequencies alongside specific symmetry species and modes graphs. This bi-presentation both integrates and enhances an analysis of the CCl_2F_2 vibrational behavior and deepens the understanding of the U(2) Lie algebraic framework effectiveness in capturing the molecular vibrational characteristics.

Table 1. Vibrational frequencies (in cm^{-1}) for CCl_2F_2

| Vibrational Mode | Symmetry Species | Fundamental | | I overtone | II overtone |
|---------------------------------|------------------|-------------------|------------|------------|-------------|
| | | Experimental [24] | Calculated | | |
| ν_1 (CF_2 s-str) | A_1 | 1101 | 1092.27 | 1822.31 | 2761.22 |
| ν_2 (CCl_2 s-str) | A_1 | 667 | 669.14 | 1086.80 | 1561.11 |
| ν_3 (CF_2 scis) | A_1 | 458 | 451.03 | 867.67 | 1109.37 |
| ν_4 (CCl_2 scis) | A_1 | 262 | 255.61 | 527.83 | 783.99 |
| ν_5 (CF_2 twist) | A_2 | 322 | 334.00 | 681.88 | 997.94 |
| ν_6 (CF_2 a-str) | B_1 | 1159 | 1136.38 | 2005.03 | 2900.55 |
| ν_7 (CF_2 rock) | B_1 | 446 | 432.77 | 753.32 | 1087.07 |
| ν_8 (CCl_2 a-str) | B_1 | 902 | 900.29 | 1683.37 | 2446.42 |
| ν_9 (CF_2 wag) | B_2 | 437 | 424.20 | 769.53 | 1033.30 |

**Figure.** Vibrational Frequencies Representation for CCl_2F_2

4. CONCLUSIONS

The findings of this paper demonstrate that the Lie algebraic framework applied in this research is a precise and accurate method for estimating the vibrational frequencies of CCl_2F_2 . The framework succeeds in calculating the fundamental frequencies close to the experimental value, resulting in a Root Mean Square (RMS) of 11.39 cm^{-1} , further illustrating the model's efficiency in accounting for anharmonic interactions. Both computational savings and flexibility substantiate it, and it works well for vibrational fundamental and overtone modes. The vibrational dynamics of the system have been successfully captured, which opens up new possibilities for using the framework and the associated techniques for broader applications like molecular dynamics and spectroscopy. This will be done by applying the developed method to more complex systems while ensuring that this work focuses on developing procedural integration with modern computational approaches.

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КОЛИВАЛЬНІ ЧАСТОТИ ДИХЛОРИДФОРМЕТАНУ З ВИКОРИСТАННЯМ АЛГЕБРАІЧНОГО ПІДХОДУ ЛІ

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У цьому дослідженні представлено симетрійно-адаптований підхід Лі, високоефективний інструмент для розрахунку коливальних частот у дихлоридформетані (CCl_2F_2). Завдяки своїй точковій груповій симетрії C_{2v} , молекула, що розглядається, особливо підходить для цього підходу. Формулюючи структури зв'язків вуглець-водень (C-H) та вуглець-хлор (C-Cl) в унітарних алгебрах Лі, визначення коливальних квантових станів молекули стає надзвичайно простим. Гамільтоніан, включаючи інваріантні оператори Казимира та Майорани та підібрані параметри, точно відтворює бажані коливальні моди, використовуючи фундаментальні та вищі обертонові частоти. Цей підхід, який порівнює сучасні та класичні моделі, підкреслює алгебраїчні методи Лі як ефективні інструменти для моделювання ангармонічних взаємодій та динаміки переходів на молекулярному рівні. Окрім своєї теоретичної значущості, побудована модель забезпечує глибоке розуміння коливальних аспектів молекул, знання, що є критично важливим для практичних застосувань, таких як інтерпретація спектроскопічних даних, проектування матеріалів з бажаними коливальними характеристиками або вивчення молекул у складних середовищах. Ці практичні застосування підвищують універсальність методології та дозволили її успішно застосувати до молекулярної спектроскопії, хімічної кінетики та проектування енергоефективних матеріалів та сенсорів, серед інших галузей. Це дослідження надає експериментаторам впевненість у алгебраїчному підході Лі та прокладає шлях для подальших експериментів з поліатомними молекулами. Роблячи значний внесок у зменшення допустимої похибки в обчислювальній молекулярній фізиці, ця методологія відкриває захопливі можливості для майбутніх досліджень та розробок.

Ключові слова: алгебраїчний підхід Лі; коливальний гамільтоніан; оператори Казимира та Майорани; дихлоридформетан; ангармонічні коливальні моди