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SPECTROSCOPIC MODELLING OF PCl_5 AND $SbCl_5$ VIBRATIONS VIA LIE ALGEBRAIC HAMILTONIAN WITH CASIMIR AND MAJORANA OPERATORS

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Abstract. The vibrational spectra of phosphorus pentachloride (PCl_5) and antimony pentachloride ($SbCl_5$), both with D_{3h} point group symmetry, are accurately calculated using a symmetry-adapted Lie algebraic framework. This study focuses on computing the fundamental frequencies, overtones up to the second order, and combination bands using a vibrational Hamiltonian constructed from Casimir and Majorana operators, which include both harmonic and anharmonic terms. The predicted frequencies, which are in excellent quantitative agreement with experimental data, not only validate the predictions but also demonstrate the method's high accuracy in replicating the complex spectroscopic phenomena of high-symmetry molecules. These results also provide a deeper understanding of the molecular structure and atmospheric behavior of PCl_5 and $SbCl_5$, emphasizing their roles in optical absorption and scattering processes. The findings presented here also underscore the potential of the Lie algebraic method in advancing molecular spectroscopy and solving problems in atmospheric chemistry and environmental science, inspiring hope for future research in the field.

Keywords: Lie algebraic framework, vibrational Hamiltonian, D_{3h} symmetry, Casimir and Majorana operators
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1. Introduction

Understanding the vibrational frequencies of molecules helps to understand their structure, spectroscopy, and dynamic properties. Their computations should also be precise, for ranges of Raman and infrared spectra are crucial to different scientific domains such as atmospheric chemistry, environmental science, materials science, and molecular physics. Of special interest in the execution of secondary processes, where they serve as catalysts, phosphorus pentachloride (PCl_5) and antimony pentachloride ($SbCl_5$), both of which belong to the D_{3h} symmetry point group, are also used for optical monitoring of atmospheric phenomena. Modelling the vibrational spectra of these compounds is particularly difficult since both anharmonic and harmonic contributions to vibrational modes, overtone, like many other combinations, need to be defined. Hence, more elaborate, theoretical, and computational methods are required to predict these complex parameters successfully.

Various methods have been developed to estimate vibrational frequencies, each with its own strengths and weaknesses. The harmonic oscillator approximation remains a useful starting point in vibrational spectroscopy. It assumes that a molecule's vibrations can be modeled with a purely harmonic potential, which works reasonably well. However, these methods do not account for anharmonic effects, which are essential for accurately determining higher-order modes (overtones and combination bands). As a result, in many cases – especially for overtones – the frequencies predicted by the harmonic oscillator approximation tend to be higher than the observed values [1-3]. Ab initio methods and Density Functional Theory (DFT) approaches are more advanced because they systematically incorporate molecular vibrations. These methods solve the Schrödinger equation for the molecule, either exactly or approximately, leading to more accurate predictions of vibrational frequencies. Realistic results can be achieved by including anharmonic effects. Unfortunately, as the size and complexity of the molecule increase, the computational cost of these calculations also grows, making them impractical for larger systems.

Furthermore, the accuracy of molecular and parametric analyses varies because of different basis sets and functionals that are preset, leading to systematic errors and affecting other molecular systems [4-8]. Often, empirical force field models are used as alternatives by parameterizing potential energy functions to predict molecular vibrations. They are useful for large-scale studies since they are computationally inexpensive. However, the parameterized system must have comprehensive information features for the data to be dependable, making the model ineffective for that system. A common issue with force field models is their failure to reproduce certain anharmonic effects, which hampers the prediction of higher-order vibrational spectra [9-11]. Especially for more atoms in highly symmetric molecules, matrix and normal mode methods are frequently used to analyze vibrational frequency patterns. These methods involve eigenvalue and eigenvector analysis of the molecules' force constant matrices to determine vibration frequencies and normal modes. However, these approaches also face limitations common to all methods, such as the increased computational resources needed for larger molecular systems and the neglect of anisotropy effects despite their high accuracy [12-14].

To overcome these challenges, the Lie algebraic approach emerges as a flexible method for studying molecular vibrational modes. From this technique, a vibrational Hamiltonian, which encompasses all relevant vibrations, and the U(2) Lie algebraic operator can be constructed. The Lie algebraic method is self-consistent and accurate for many molecular systems, especially highly symmetric ones, because it does not limit the basis set or require extensive experimental data. Using this approach improves the accuracy of higher-order anharmonic descriptions, which is essential for precise modeling of vibrational spectra. Unlike other methods that focus on simplifications and corrections based on experimental data, the Lie algebraic method applies these adjustments independently. This feature increases the method's reliability in estimating vibrational spectra, filling gaps that other methods leave [15-21].

The Lie algebraic technique is useful because it allows the direct inclusion of molecular symmetry into the vibrational Hamiltonian. This is especially helpful for high-symmetry molecules like PCl_5 and $SbCl_5$, which are part of the D_{3h} point group. Using this approach, operators can be built to greatly decrease the time and effort needed to calculate vibrational frequencies, overtone spectra, combination bands, and more. Additionally, applying the Lie algebraic method expands the understanding of molecular dynamics since local and normal vibrational modes can be examined within the same algebra framework. Researchers in the field will likely value the efficiency of the Lie algebraic method in these areas.

The algebraic method captures the full range of complex symmetric features of PCl_5 and $SbCl_5$, such as fundamental frequencies, overtones, and combination bands. This approach demonstrates that the Lie algebraic method can resolve intricate problems in environmental science and atmospheric chemistry. It confirms the effectiveness of the Lie algebraic approach using PCl_5 and $SbCl_5$, which employs Casimir and Majorana operators. Additionally, the high accuracy of this method in reconciling experimental data enhances understanding of areas where advanced molecular spectroscopy can be useful and provides new insights into the vibrational dynamics of PCl_5 and $SbCl_5$. This example clearly shows that the broad scope of the Lie algebraic method allows significant progress in solving complex problems in the field.

2. D_{3h}-symmetry-adapted Lie algebraic framework for PCl_5 and $SbCl_5$

Interactions of vibrational modes of molecules PCl_5 and $SbCl_5$ with D_{3h} symmetry can be most easily understood through stretching and bending motions, where the mixing of harmonic and anharmonic couplings – especially within stretching interactions – is dominant. These can be further divided into axial, equatorial, and axial-equatorial couplings. Axial couplings involve first-neighbor interactions between adjacent axial bonds, such as bond pairs (1,2), (2,3), and (3,1), as well as second-neighbor interactions between non-adjacent axial bonds, like (1,3). Equatorial couplings occur among the three equatorial bonds, with stronger couplings observed among bonds that are closer together (4,5). Axial-equatorial couplings are cross-couplings with adjustable switches between axial and equatorial bonds, such as the interactions of axial bond 1 with equatorial bonds 4 and 5, and similar couplings of axial bond 2 with equatorial bonds 4 and 5. These couplings are essential for energy redistribution during vibrational motion and, therefore, are crucial. Harmonic couplings described here allow linear energy exchange without re-tuning the energy levels beyond basic vibrational modes. Anharmonic couplings are key to energy transfer between stretching and bending modes, often leading to the formation of overtones or combination bands [22, 23]. This process greatly affects the vibrational dynamics and spectroscopic properties of PCl_5 and $SbCl_5$, deepening our understanding of these compounds at the molecular level. This analysis employs a symmetry-adapted Lie algebra approach, using U(2) algebraic operators to represent the vibrational modes. This methodology results in a Hamiltonian that is both harmonic and anharmonic concerning the modes and their couplings [15, 17, 19].

A mathematical framework that defines the symmetries of a system, the Lie algebraic approach is applied in modelling molecular vibrations. Employing molecular structure and symmetry, U(2) Lie algebras are allocated to specific vibrational modes, and the adaptation of symmetry preserved D_{3h} symmetry through the analysis of the system. Three U(2) Lie algebras, $\{U_i(2): i=1,2,3\}$, are assigned to represent the three equivalent axial P-Cl or Sb-Cl bond stretching vibrations, and two U(2) Lie algebras, $\{U_i^*(2): i=4,5\}$, are introduced for the two equivalent equatorial P-Cl or Sb-Cl bond stretching vibrations. The interactions in axial bond vibrations involve first-neighbor couplings, represented as $\{U_i(2)\otimes U_j(2);(i,j)=(1,2),(2,3),(3,1)\}$, and second-neighbor couplings, represented as $\{U_i(2)\otimes U_j(2);(i,j)=(1,3)\}$. For equatorial bond vibrations, first-neighbor couplings are represented as $\{U_i^*(2)\otimes U_j^*(2);(i,j)=(4,5)\}$. Axial-equatorial couplings involve cross-interactions, represented as $\{U_i^*(2)\otimes U_j^*(2);(i,j)=(1,4),(1,5),(2,4),(2,5),(3,4),(3,5)\}$.

Here, the unitary Lie algebra $U_i(2)$ is employed to represent the dynamical symmetry associated with the *i*-th vibrational degree of freedom.

The effective vibrational Hamiltonian, considering axial and equatorial bond stretching and bending vibrations, can be written as:

Axial bond vibrations:

$$H^{(axial)} = E_0 + \sum_{i=1}^{3} A_i^{(axial)} C_i + \sum_{i<j}^{3} A_{ij}^{(axial)} C_{ij} + \sum_{i<j}^{3} k_{ij} \lambda_{ij}^{(axial)} M_{ij} \; . \tag{1}$$

Equatorial bond vibrations:

$$H^{(equatorial)} = E_0 + \sum_{i=4}^{5} A_i^{(equatorial)} C_i + A_{45} C_{45} + k_{45} \lambda_{ij}^{(equatorial)} M_{45} \; . \tag{2}$$

Axial-equatorial couplings:

$$H^{(axial-equatorial)} = \sum_{i=1}^{3} \sum_{j=4}^{5} \left(A_{ij} C_{ij} + \lambda_{ij} M_{ij} \right). \tag{3}$$

In Eqs. (1) to (3), the zero-point energy, E_0, represents the vibrational energy of the molecule in its ground state, where all vibrational quantum numbers ($v_i = 0$) are zero. This term reflects the quantum mechanical principle that even at absolute zero temperature, bonds retain vibrational energy due to zero-point motion [19].

The term $A_i C_i$ describes the energy contribution of the fundamental vibrational mode of bond *i*. The Casimir operator, C_i, models anharmonicity and is defined as [15, 17]:

$$C_i = -4\left(N_i v_i - v_i^2\right). \tag{4}$$

Where $N_i = \dfrac{\omega_e}{\omega_e \chi_e} - 1$ is the vibron number, representing the maximum number of bound states for the Morse potential of bond *i*, and v_i is the vibrational quantum number. Here, $\omega_e, \omega_e \chi_e$ are the harmonic and anharmonic spectroscopic constants, respectively, of the axial and equatorial bonds in the diatomic molecule. These constants are determined using the procedure provided in reference [24].

The parameter A_i quantifies the fundamental vibrational energy of bond *i* and is estimated as [15, 17]:

$$A_i = -\frac{E^{fundamnetal}}{4\left(N_i - 1\right)}, \tag{5}$$

where $E^{fundamnetal}$ is the energy of the first vibrational state.

The term $A_{ij} C_{ij}$ represents harmonic interactions between vibrational modes *i* and *j*. The two-mode Casimir operator, C_{ij}, accounts for energy redistribution and is expressed as [15, 17]:

$$N_i, v_i; N_j, v_j \left| C_{ij} \right| N_i, v_i; N_j, v_j = 4\left(v_i + v_j\right)\left(v_i + v_j - N_i - N_j\right). \tag{6}$$

The parameter A_{ij} quantifies the coupling strength, where positive values indicate constructive coupling and negative values indicate destructive coupling.

The term $k_{ij}\lambda_{ij}M_{ij}$ captures anharmonic interactions between modes *i* and *j*. The Majorana operator, M_{ij}, mediates quantum transitions between states, defined as [15-17]:

$$\left.\begin{aligned}
&\left\langle N_i,v_i;N_j,v_j\middle|M_{ij}\middle|N_i,v_i;N_j,v_j\right\rangle = v_iN_j + v_jN_i - 2v_iv_j\\
&\left\langle N_i,v_i+1;N_j,v_j-1\middle|M_{ij}\middle|N_i,v_i;N_j,v_j\right\rangle = -\left[v_j\left(v_i+1\right)\left(N_i-v_i\right)\left(N_j-v_j+1\right)\right]^{1/2}\\
&\left\langle N_i,v_i-1;N_j,v_j+1\middle|M_{ij}\middle|N_i,v_i;N_j,v_j\right\rangle = -\left[v_i\left(v_j+1\right)\left(N_j-v_j\right)\left(N_i-v_i+1\right)\right]^{1/2}
\end{aligned}\right\} . \qquad (7)$$

The symmetry coefficient k_{ij} specifies the type of interaction (e.g., first-neighbor, second-neighbor coupling), while λ_{ij} is the anharmonic coupling strength, derived as [15]:

$$\lambda_{ij} = \frac{\left|E_s - E_{as}\right|}{mN}, \qquad (8)$$

where E_s and E_{as} are symmetric and antisymmetric combination band energies, and *m* is the interaction order.

The bending Hamiltonian, $H^{(bend)}$, captures the energy associated with angular distortions between bonds. It is expressed as:

$$H^{(bend)} = \sum_k b_k\theta_k + \sum_{k<l} b_{kl}g_{kl}. \qquad (9)$$

The term $b_k\theta_k$ accounts for the vibrational energy associated with bending mode *k*. The operator θ_k represents angular deformations, and b_k quantifies the fundamental bending frequency of mode *k* and the term $b_{kl}\,g_{kl}$ captures the interactions between bending modes *k* and *l*, where g_{kl} describes energy redistribution between these modes. The parameter b_{kl} quantifies the coupling strength.

The vibrational Hamiltonian parameters, A_i (single-mode contributions), b_k , λ_{ij} (anharmonic coupling strengths), and b_{kl} are derived and optimized using least-squares regression fitting based on the observed data [25]. This approach ensures the calculated vibrational frequencies align closely with experimental spectroscopic data. The initial guesses for A_{ij} are taken as zero because the two-mode interactions are generally weaker compared to single-mode contributions and anharmonic couplings. Their values are refined during the optimization process.

3. Results and discussion

PCl_5 and $SbCl_5$ exhibit trigonal bipyramidal geometries, characterized by the D_{3h} point group symmetry. The molecular structure consists of two axial bonds perpendicular to a trigonal plane formed by three equatorial bonds. Due to increased electron repulsion, the axial bonds are longer and weaker than the equatorial bonds, resulting in distinct vibrational features. The vibrational modes are classified under the D_{3h} irreducible representations as: $2A_1' + 2A_2'' + 3E' + E''$. A_1' modes correspond to symmetric stretching of axial and equatorial bonds, A_2'' modes describe out-of-plane distortions, E' modes represent degenerate in-plane stretching and bending of equatorial bonds, and E'' modes correspond to degenerate out-of-plane bending vibrations involving axial-equatorial interactions [22, 23]. In the gaseous phase, axial stretching frequencies typically occur in the lower range due to the weaker nature of the axial bonds, while the stronger equatorial bonds exhibit higher stretching frequencies. In the solid phase, these vibrational frequencies may shift or split, influenced by crystal packing and intermolecular interactions, further affecting their spectroscopic signatures.

In Table 1, the optimized algebraic parameters, as well as the vibron numbers, are provided. This permits accurate calculations of the moleculae vibration, thus avoiding the drawbacks caused by the traditional harmonic oscillator and the empirical force field methods. The Hamiltonian parameters were fitted with the experimental data [25] to match the known frequencies. These include single-mode vibrational energies, anharmonic coupling strengths, and symmetry coefficients for the axial and equatorial bonds. Such parameters highlight the intricate distributions of the energies in the fundamental and higher vibrational modes.

Table 1. Optimized parameters (in cm^{-1}, except *N*): U(2) Lie algebraic vibrational Hamiltonian for D_{3h} symmetry PCl_5 and $SbCl_5$.

Parameters	**PCl_5**	**$SbCl_5$**
$\omega_e, \omega_e\chi_e$ (axial)	593, 99	516, 79.5
$\omega_e, \omega_e\chi_e$ (equatorial)	580.38, 5.69	405.96, 3.98
$N^{(axial)}$	5	6
$N^{(equatorial)}$	100	102
$A_i^{(axial)}$	23.029	-15.424
$A_i^{(equatorial)}$	-1.192	-0.968
$A_{ij}^{(axial)}$	-0.295	-1.033
$A_{ij}^{(equatorial)}$	1.443	0.883
$\lambda_{ij}^{(axial)}$	8.291	6.227
$\lambda_{ij}^{(equatorial)}$	0.323	1.885
$N^{(bend)}$	52	54
b_k	-0.965	-0.599
b_{kl}	1.285	0.911

The fundamental frequencies for PCl_5 and $SbCl_5$, alongside their experimental PCl_5 and $SbCl_5$ data, are shown in Table 2. These outcomes not only confirm but also underscore the precision of the Lie algebraic method in estimating symmetric and asymmetric stretch and bend vibrations. For PCl_5, the root-mean-square (RMS) deviation between experimental and calculated frequencies is 9.35 cm^{-1}. For $SbCl_5$, the estimated RMS deviation is 9.29 cm^{-1}, leading to an impressive level of accuracy.

Tables 3 and 4 illustrate the first and second overtones of the two compounds and their combination bands. The results show that the overtones exhibit nonlinear shifts in energy due to the significant influence of anharmonicity, thereby reinforcing the crucial need to include anharmonicity in the vibrational Hamiltonian. These are termed combination bands, resulting from the interaction of the fundamental and overtone modes, and provide vital information on cross-mode interactions.

D_{3h} symmetry allows for the straightforward and clear representation of vibrational modes using symmetry-adapted operators. Axial-equatorial couplings, represented by Casimir and Majorana operators, depict the change in energy of vibration modes. The coupling strength is indicated by the amount of energy exchanged during bending and stretching vibrations. The accurate prediction of vibrational frequencies, overtones, and combination bands obtained demonstrates the application of the Lie algebraic framework to problems in spectroscopy.

Table 2. Predicted fundamental vibrational frequencies (in cm^{-1}) for PCl_5 and $SbCl_5$ using the U(2) Lie algebraic vibrational Hamiltonian: comparison with experimental observations, mode assignments, and symmetry species (irreducible representations).

Vibrational mode	**Symmetry species**	**Experimental** [25]	**Calculated**
	PCl_5		
ν_1 (PCl_3 s-str)	A_1'	395	389.2
ν_2 (PCl_2 s-str)	A_1'	370	365.2
ν_3 (PCl_2 as-str)	A_2''	465	456.4
ν_4 (PCl_3 op-deform)	A_2''	299	287.04
ν_5 (PCl_3 deg-str)	E'	592	578.32
ν_6 (PCl_3 deg-deform)	E'	273	262.08
ν_7 (PCl bend)	E'	100	96.81
ν_8 (PCl bend)	E''	261	250.56
	$SbCl_5$		
ν_1 ($SbCl_3$ s-str)	A_1'	357	342.72
ν_2 ($SbCl_2$ s-str)	A_1'	307	294.72
ν_3 ($SbCl_2$ as-str)	A_2''	384	378.64
ν_4 (PCl_3 op-deform)	A_2''	154	147.84
ν_5 ($SbCl_3$ deg-str)	E'	398	385.08
ν_6 ($SbCl_3$ deg-deform)	E'	177	169.92
ν_7 (SbCl bend)	E'	72	69.12
ν_8 (SbCl bend)	E''	165	158.4

Notation: s-str = symmetric stretch, as-str = asymmetric stretch, deg-str = degenerate stretch, deg-deform = degenerate deformation, bend = bending vibration.

Table 3. First and second overtone vibrational frequencies (in cm^{-1}) of PCl_5 and $SbCl_5$ predicted by the U(2) Lie algebraic vibrational Hamiltonian: vibrational modes and symmetry species details.

Vibrational mode	**Calculated**	**Vibrational mode**	**Calculated**
1	2	3	4
	PCl_5		
$2\nu_1$ (PCl_3 s-str)	750.816	$3\nu_1$ (PCl_3 s-str)	1167.225
$2\nu_2$ (PCl_2 s-str)	703.296	$3\nu_2$ (PCl_2 s-str)	1093.35
$2\nu_3$ (PCl_2 as-str)	883.872	$3\nu_3$ (PCl_2 as-str)	1374.075
$2\nu_4$ (PCl_3 op-deform)	568.3392	$3\nu_4$ (PCl_3 op-deform)	883.545

1	2	3	4
$2\nu_5$ (PCl_3 deg-str)	1125.2736	$3\nu_5$ (PCl_3 deg-str)	1749.36
$2\nu_6$ (PCl_3 deg-deform)	518.9184	$3\nu_6$ (PCl_3 deg-deform)	806.715
$2\nu_7$ (PCl bend)	190.08	$3\nu_7$ (PCl bend)	295.5
$2\nu_8$ (PCl bend)	496.1088	$3\nu_8$ (PCl bend)	771.255
		$SbCl_5$	
$2\nu_1$ ($SbCl_3$ s-str)	678.5856	$3\nu_1$ ($SbCl_3$ s-str)	1007.5968
$2\nu_2$ ($SbCl_2$ s-str)	583.5456	$3\nu_2$ ($SbCl_2$ s-str)	866.4768
$2\nu_3$ ($SbCl_2$ as-str)	729.9072	$3\nu_3$ ($SbCl_2$ as-str)	1083.8016
$2\nu_4$ (PCl_3 op-deform)	292.7232	$3\nu_4$ (PCl_3 op-deform)	434.6496
$2\nu_5$ ($SbCl_3$ deg-str)	756.5184	$3\nu_5$ ($SbCl_3$ deg-str)	1123.3152
$2\nu_6$ ($SbCl_3$ deg-deform)	336.4416	$3\nu_6$ ($SbCl_3$ deg-deform)	499.5648
$2\nu_7$ (SbCl bend)	136.8576	$3\nu_7$ (SbCl bend)	203.2128
$2\nu_8$ (SbCl bend)	313.632	$3\nu_8$ (SbCl bend)	465.696

Table 4. Vibrational Frequencies (in cm^{-1}) of the combination bands of PCl_5 and $SbCl_5$ predicted by the U(2) Lie algebraic vibrational Hamiltonian: combination vibrational modes from fundamental, first, and second overtones in stretching modes

Combination bands	**PCl_5**	**$SbCl_5$**
$\nu_1 + 2\nu_1$	1137.6	1028.16
$\nu_2 + 2\nu_2$	1065.6	884.16
$\nu_1 + 3\nu_1$	1516.8	1370.88
$\nu_2 + 3\nu_2$	1420.8	1178.88
$2\nu_1 + 3\nu_1$	1896	1713.6
$2\nu_2 + 3\nu_2$	1776	1473.6
$\nu_1 + \nu_2$	760.813	639.64
$2\nu_1 + \nu_2$	1150.013	982.36
$\nu_1 + 2\nu_2$	1126.013	934.36
$\nu_1 + 3\nu_2$	1491.213	1229.08
$3\nu_1 + \nu_2$	1539.213	1325.08

4. Conclusions

This study successfully applied a symmetry-adapted Lie algebraic framework to analyze the vibrational spectra of PCl_5 and $SbCl_5$, both exhibiting D_{3h} symmetry. By constructing a vibrational Hamiltonian with Casimir and Majorana operators, the approach captured harmonic and anharmonic interactions with high accuracy. The computed vibrational frequencies, including fundamentals, overtones, and combination bands, showed excellent agreement with experimental data, with RMS deviations of 9.35 cm^{-1} for PCl_5 and 9.29 cm^{-1} for $SbCl_5$.

The results demonstrate the effectiveness and accuracy of modeling vibrational dynamics in high-symmetry molecules and overcoming the limitations of traditional methods without incurring high computational costs. Additionally, the research emphasizes the potential of the Lie algebraic approach in molecular spectroscopy and, by extension, in atmospheric chemistry or environmental science. Future work could expand the application of this method to more complex molecular systems and spectroscopic challenges while deepening our understanding of molecular vibrational phenomena.

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Анотація*. Коливальні спектри пентахлориду фосфору (PCl_5) та пентахлориду сурми ($SbCl_5$) з симетрією точкової групи D_{3h}, розраховані з високою точністю за допомогою адаптованої до симетрії алгебри Лі. Це дослідження зосереджено на обчисленні основних частот, обертонів до другого порядку та комбінаційних смуг за допомогою коливального гамільтоніана, побудованого операторами Казимира та Майорани, з включенням гармонічних та ангармонічних членів. Передбачені частоти, які добре узгоджуються з експериментальними даними, не тільки підтверджують передбачення, але й демонструють високу точність методу у відтворенні складних спектроскопічних молекулярних явищ з високою симетрією. Ці результати також забезпечують глибше розуміння молекулярної структури та поведінки PCl_5 та $SbCl_5$ в атмосфері, підкреслюючи їхню роль в процесах оптичного поглинання та розсіювання. Представлені результати також підкреслюють потенціал алгебричного методу Лі в розвитку молекулярної спектроскопії та вирішенні проблем в атмосферній хімії та науці про навколишнє середовище, вселяючи надію на майбутні дослідження в цій галузі.*

Ключові слова*: алгебраїчна система Лі, коливальний гамільтоніан, D_{3h}-симетрія, оператори Казимира та Майорани*