



Vibrational Spectra of C_2Cl_4 Using Lie Algebraic Technique

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ABSTRACT

In this paper, we have calculated the vibrational frequencies of medium-size molecule (5-100 atoms), Tetrachloroethylene (C_2Cl_4) in fundamental mode by one dimensional unitary Lie algebraic technique. In this method, bonds C-Cl and C-C of the Tetrachloroethylene are replaced with a unitary Lie algebras and Hamiltonian expressed in terms of Casimir and Majorana invariant operators and parameters. This Hamiltonian operator describes stretching vibrations of molecule. The determined vibrational frequencies by this theoretical method are compared with experimental results. The obtained results are consistent with experimental results.

Keywords: Vibrational spectra, Lie algebraic technique, Tetrachloroethylene.

INTRODUCTION

Spectroscopy today, becomes the most accurate source of information of the spectral structure and energy calculation of molecules. There is considerable present research interest in the analysis of vibrational frequencies of molecules. The emergence of new experimental methods to detect higher vibrational excitations in polyatomic molecules require theoretical methods for their interpretation. In 1991, Iachello and Oss introduced a theoretical method, Lie algebraic method as a computational tool for the analysis and interpretation of experimental and ro-vibrational spectra of molecules. This method is based on the mathematical theory of unitary Lie algebras^{1,2}.

Lie algebraic method

The Hamiltonian operator associated with Lie algebraic method³ for n interacting bonds of molecule is

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

Where, C_i and C_{ij} are invariant operators of the uncoupled and coupled bonds respectively and are given by

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

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



and the Majorana operator M_{ij} is used to describe local mode interactions in pairs and contains both diagonal and non-diagonal matrix elements given by

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

Where, v_i, v_j are vibrational quantum numbers of bonds i and j respectively. The Vibron number N_i is calculated by

$$N_i = \frac{\omega_e}{\omega_e x_e} - 1, i = 1, 2, \dots (\omega_e \text{ and } \omega_e x_e \text{ are the spectroscopic constants}^6).$$

We consider a numerical fitting procedure to adjust the parameters A_i , λ_{ij} and A_{ij} over an experimental results of vibrational energy levels^{4,5}. The starting guess for the parameter A_i will be obtained by using the energy equation for the single-oscillator fundamental mode as

$$E(v=1) = -4A_i(N_i - 1).$$

The parameter λ_{ij} can be calculated from the relation,

$$\lambda_{ij} = \frac{|E_i - E_j|}{2N}.$$

Structure of Tetrachloroethylene

Tetrachloroethylene containing two carbon and four chlorine atoms with one (C-C) and four (C-Cl) bonds. Symmetry species of C_2Cl_4 are $A_g, A_u, B_{1g}, B_{1u}, B_{2g}, B_{2u}, B_{3u}$ (Point group, D_{2h}).

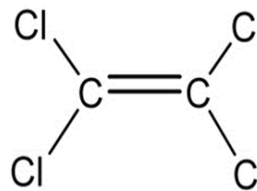


Fig.1. Tetrachloroethylene

RESULTS

Table 1. Algebraic parameters

Stretching parameters	
$N_1 = 174$ (C-C), $N_2 = 132$ (C-Cl)	
$A_1 = 9.52$, $A_2 = 8.27$ (cm^{-1})	
$A_{12} = 2.321$, $A_{13} = -1.35$ (cm^{-1})	
$\lambda_{12} = 2.321$, $\lambda_{23} = -1.35$ (cm^{-1})	

Table 2: Experimental and calculated vibrational frequencies (in cm^{-1}) of C_2Cl_4

Symmetry Species	Mode	Experimental ^{7,8}	Calculated
A_g	C-C Stretch	1571	1571.38
A_g	C-Cl ₂ Symmetric Stretch	447	446.82
B_{1g}	C-Cl ₂ Asymmetric Stretch	1000	1000.32
B_{2u}	C-Cl ₂ Asymmetric Stretch	908	997.62
B_{3u}	C-Cl ₂ Symmetric Stretch	777	776.61

CONCLUSION

In this paper we have calculated the vibrational spectra of C_2Cl_4 in fundamental mode by Lie algebraic method and also compared with available experimental results. These calculations shows that this technique is a reliable approach of other theoretical techniques like *Ab initio* methods.

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