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Research Paper

VIBRATIONAL SPECTRA OF C_{80} AND ITS EPOXIDE (C_{80}-O): A LIE ALGEBRAIC STUDY

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ABSTRACT:

The U(2) algebra is used to calculate the vibrational energy levels of the fullerene C80 and its epoxide (C80-O) while taking the local Hamiltonian of Morse potential into account. Here, a corresponding Lie algebra is used to replace each of the molecule's chemical bonds, and the Hamiltonian is then written while taking the interacting Casimir and Majorana operators into account. In order to fit the findings of the semi-empirical PM3 molecular modelling technique, we computed the local mode vibrational energy levels of the fullerene C80 and its epoxide (C80-O) by building the model Hamiltonian.

Keywords: Morse potential, vibrational energy level, Lie algebra, Operators in Casimir and Majorana, C_{80}, C_{80}-O.

1. INTRODUCTION:

Since the advent of new laser techniques, one of the most interesting and developing areas in the field of molecular spectra has been the study of excited vibrational states of polyatomic molecules. A significant change in perspective in the theoretical field (the algebraic approach to Morse oscillator) to study the vibrational states of molecules was brought about in 1979 by Wulfman's introduction of the algebraic approach to molecular spectra. [1]. Two years later, in 1981, a new theoretical concept, known as Vibron model (based on *U*(4) lie algebra) to study the molecular spectra was introduced by Iachello [2]. In contrast to the conventional methods employed in molecular spectroscopy, this new model appears to provide a tangible and supplementary technique. Initially, the Vibron model was created for diatomic and triatomic molecules [3] and the stretching and vibrational excitations of polyatomic molecules can be computed using lie algebra. However, when a molecule has more than four atoms overall, the U(4) model becomes complex. However, the U(2) model, which was developed by Wulfman and Levine [1], is thought to be successful in explaining the stretching vibrations of polyatomic molecules, including tetrahedral, octahedral, and benzene-like molecules. Iachello and Oss[4] provided a succinct overview of the work done with algebraic models up until the year 2000 and the observation in the first ten years of the twenty-first century. In comparison to other techniques like Dunham expansion and the potential approach method [4], it has recently been observed that the lie algebraic method [5–6] was incredibly accurate in calculating the vibrational frequencies of polyatomic molecules. Only the quantum mechanical approach of PM3 method was discovered to examine the study of vibrational spectra of fullerene C80 & C80-O with its different energy bands [7]. To date, no noteworthy experimental research work on the vibrational spectra of C80 has been reported. In order to determine and study the energy bands of fullerene C80 & C80-O and formulate the comparison in spectroscopic point of view, we propose to obtain the stretching vibrational energies of fullerene C80 & C80-O using the 1d U(2) algebraic model.

2. THEORETICAL REVIEW:

First, a brief review of the algebraic model's theory is required. A computational tool for analysing and interpreting experimental ro-vibrational spectra of large and medium-sized molecules has recently been introduced: the algebraic method. Chemical and molecular physics have made extensive use of this technique. The foundation of this approach is the concept of dynamic symmetry, which is subsequently articulated using the language of Lie algebras. A very helpful Hamiltonian operator that explains the ro-vibrational degrees of freedom of different physical systems is obtained by using lie algebraic techniques [8]. The algebraic techniques are designed to include the same physical information as semi-empirical approaches (using phenomenological expansions in powers of suitable quantum numbers) and ab initio theories (based on the solution of Schrödinger's equation). However, the results can be obtained more quickly and easily by using the potent method of group theory [9]. The U(4) model in Lie algebraic approaches deals with both rotation and vibration simultaneously, but it gets complicated when a molecule has more than four atoms. The stretching vibrations of polyatomic molecules, including benzene-like and other octahedral molecules, were well described by the U(2) model. Thus, in this case, we examine the higher excited vibrations of fullerene C80 & C80-O using the U(2) algebraic model.

We utilise the isomorphism between the Lie algebra of U(2) and the one-dimensional Morse oscillator to introduce the U(2) algebraic model. The Schrodinger equation's (1-dimensional) Eigen states with a Morse potential are as follows:

$$h(p.x) = p_2 / 2\mu + D[1-\exp(-\alpha x)]^2 \qquad (1)$$

One-on-one communication is possible in this state with the representations of $U(2) \supset O(2)$, mainly illustrated by the quantum numbers $|N, m\rangle$ with the condition that one takes only the positive branch of *m*, i.e. *m* = N, N - 2, ...,1 or 0 for N = odd or even (N = integer). In the U (2) basis, the Morse Hamiltonian (1) is equivalent to a simple Hamiltonian. $h = \bar{C}_0 + AC$, where C is the invariant operator.

The Eigen values of *h* are $\bar{C} = \bar{C}_0 + A(m^2 - N^2), \qquad (2)$

where $m = N, N-2, \ldots\ldots\ldots\ldots 1 \text{ or } 0 \quad (N = \text{Integer})$

Presenting the new novel vibrational quantum no $\nu = (N-m)/2$, *Eq.* (2) can be rewritten as,

$$\bar{C} = \bar{C}_0 - 4A(N\nu - \nu^2), \qquad (3)$$

where, $\nu = 0,1,\ldots\ldots\ldots N/2$ or $\dfrac{N-1}{2}$ (where *N* = even or odd) .

The value of C_0, A and N are given in terms of μ, D and α by using the following relations

$$C_0 = -D, \qquad -4AN = h\alpha(2D/\mu)^{1/2}, \qquad 4A = -h^2\alpha^2/2\mu$$

It is possible to confirm that these are the Morse oscillator's Eigen values.

Now consider a molecule with n bonds. In the algebraic model, each bond i is replaced by an algebra with Hamiltonian $h_i = \bar{C}_{0i} + A_i C_i$ where C_i is the invariant operator with Eigen values $-4(N_i\nu_i - \nu_i^2)$. There is a bond–bond interaction between the bonds. The two types of interaction that are typically taken into consideration are known as Casimir and Majorana interactions, respectively, and are represented by the symbols C_{ij} and M_{ij} respectively.

The following is the form of the algebraic model Hamiltonian that we are considering [5],

$$H = E_0 + \sum_{i=1}^{n} A_i C_i + \sum_{i<j}^{n} A_{ij} C_{ij} + \sum_{i<j}^{n} \lambda_{ij} M_{ij} \qquad (4)$$

In the equation (4), C_i is an operator known as invariant operator with Eigen values $4(v_i^2 - N_i v_i)$ and the operator C_{ij} is diagonal with matrix elements.

$$\langle N_i, v_i; N_j, v_j | C_{ij} | N_i, v_i; N_j, v_j \rangle = 4[(v_i + v_j)^2 - (v_i + v_j)(N_i + N_j)] \qquad (5)$$

while the operator M_{ij} has both diagonal and non-diagonal matrix element

$$\left.\begin{aligned} &\langle N_i, v_i; N_j, v_j | M_{ij} | N_i, v_i; N_j, v_j \rangle = \langle N_i v_j + N_j v_i - 2 v_i v_j \rangle \\ &\langle N_i, v_i + 1; N_j, v_j - 1 | M_{ij} | N_i, v_i; N_j, v_j \rangle = -[v_j (v_i + 1)(N_i - v_i)(N_j - v_j + 1)]^{1/2} \\ &\langle N_i, v_i - 1; N_j + 1 | M_{ij} | N_i, v_i; N_j, v_j \rangle = -[v_i (v_j + 1)(Nj - v_j)(N_i - v_i + 1)]^{1/2} \end{aligned}\right\} \qquad (6)$$

Eq. (6) is a generalization of the two-bond model to n bonds [9].

The representation of the local mode chain characterises the simple eigen basis to diagonalise the Hamiltonian. Below each group, we have employed quantum numbers to characterise the Eigen values of the corresponding invariant operator N, which is the number of bosons associated with stretching physical modesThe quantum numbers v_i corresponds to the number of quanta in each oscillator while V is the total vibrational quantum number as given by

$$V = \sum_{i=1}^{n} v_i \qquad (7)$$

The total vibrational quantum number is always conserved for a given polyad. The conservation rule is unaffected by the inclusion of Mij in the local Hamiltonian operator. In eq. (4), C_i is the invariant operator of uncoupled bond with Eigen values $4(v_i^2 - N_i v_i)$ and the operator C_{ij} are diagonal with matrix elements for coupled bonds.

3. RESULTS AND DISCUSSION:

In this work we use four algebraic parameters *i.e.* A, A', λ, λ' & N, to know the vibrational spectra of the C_{80} molecules where N is the vibron number.

The values of the vibron no. (N) can be obtained from the relation,

$$N_i = \frac{\omega_e}{\omega_e \chi_e} - 1, \qquad (i = 1, 2 \ldots\ldots) \qquad (8)$$

where ω_e and $\omega_e \chi_e$ are the spectroscopic constants of the stretching interaction of the polyatomic molecule under consideration. This number must be regarded as an initial estimate; variations in this estimate may be expected based on the particular molecular structure, but they shouldn't exceed the initial value by $\pm$ 20% [Eq. (8)]. It should be noted that when calculating fullerene's vibrational frequencies, the value of N is not utilised as a free parameter and is maintained fixed.

We utilise the expression for the single-oscillator fundamental mode, which is provided as follows, to get a preliminary estimate for the parameter A.

$$E(v = 1) = -4A(N - 1) \qquad (9)$$

Using the relation (9), $\bar{A}$ can be obtained as, $\bar{A} = \frac{\bar{E}}{4(1-N)}$ (10)

By taking into account the relationship, one can obtain an early estimate for the parameter λ whose function it is to split the initially degenerate local modes.

$$\lambda = \frac{|E_1 - E_2|}{2N} \quad (11)$$

In order to achieve better results, anumerical fitting process (in a least-squares sense) is necessary to determine the parameters A, A' and λ starting from the values as given by Eq. (10) and Eq. (11). The Initial value for A' may be taken as zero.

Table 1 lists the fitting parameters that are used to calculate the vibrational spectra of fullerene C_{80}.

Table 1: Fitting parameters* of Fullerene C_{80}

Vibron number	Stretching parameters		
N	A	λ	λ'
140	-0.2897	0.516	-0.076

*A, λ, λ' all are in cm^{-1} and N is dimensionless.

Table 2: Experimental and calculated energies (cm^{-1}) of fullerene C_{80}

Normal level	I Ref.[10]*	II This Study	Δ (I – II)
ν_1	162.92	162.50	+0.42
ν_2	227.54	226.34	+1.20
ν_3	306.89	306.98	-0.09
ν_4	353.04	357.38	- 4.34
ν_5	393.5	391.4	+2.10

*Medhat Ibrahim, 2005.

The fitting parameters which are used in the investigation of vibrational spectra of fullerene C_{80}-O is given in Table 3.

Table 3: Fitting parameters* of Fullerene C_{80} -O (Epoxide of C_{80})

Vibron number	Stretching parameters		
N	A	λ	λ'
140	-0.3580	0.339	-0.0857

*A, λ, λ' all are in cm^{-1} whereas N is dimensionless.

Table 4: Experimental and calculated energies (cm^{-1}) of fullerene C_{80} -O (Epoxide of C_{80})

Normal level	I Ref.[10]*	II This Study	Δ (I – II)
ν_1	199.63	199.10	+0.53
ν_2	271.47	271.08	+0.39
ν_3	294.93	294.02	+0.91
ν_4	339.02	339.90	- 0.88
ν_5	373.10	374.10	-1.00

*Medhat Ibrahim, 2005.

4. CONCLUSION:

This article discusses an algebraic model of coupled 1-dimensional Morse oscillators that unfold the C-C stretching vibrations of the molecules C_{80}-O and C_{80}. One can avoid the challenging integrations in the solution of coupled differential Schrodinger equations by using this algebraic model. This model can be applied to the C-C stretching interbond interactions in a straightforward manner, and the above fitting parameters can be used to explain the stretching bonds' accurate calculation. Only a few C_{80} and C_{80}-O vibrational modes that are in good agreement with the findings of the semi-empirical PM3 molecular modelling technique were presented in this paper[10]. With the continued development of the U(2) model, it is hoped that the bent and stretch vibrations of the molecules will also be able to provide a good explanation for the higher order vibrational modes of C80 and C_{80}-O .

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