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VIBRATIONAL IR SPECTRA
OF SOLID CARBON MONOXIDE

The vibrational energy levels of solid carbon monoxide are calculated, by considering a local Hamiltonian with the Morse potential with the use of the U(2) algebra. Each bond of the molecule is changed by a corresponding Lie algebra, and, finally, the local Hamiltonian is constructed with the help of interacting Casimir and Majorana operators. Only the fundamental infrared stretching modes of vibration of solid carbon monoxide are then calculated, by using that Hamiltonian, and are compared with the experimental results.

K e y w o r d s: vibrational spectra, Lie algebra, solid carbon monoxide.

1. Introduction

Recently, the molecular spectroscopy has undergone an exciting change. In terms of a quantitative change, the better initial state preparation, improved light sources, specially designed pumping schemes, and more sensitive detection techniques are providing the ever improved resolution and a wider range of accessible final states. Regarding a qualitative change, a closer view suggests that not only better results, but also new ideas are forthcoming.

The study of excited vibrational states of polyatomic molecules has been one of the most interesting advanced topics in the field of molecular spectra in the theoretical, as well as experimental, background in the recent past due to the development and the introduction of new laser techniques. In 1979, the introduction of the algebraic approach to the molecular spectra by Wulfman fetched a revolutionary change in the theoretical field (the algebraic approach to a Morse oscillator) to study the vibrational states of molecules [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]. This new model seems to offer a specific complementary technique to the traditional approaches used in molecular spectroscopy. The Vibron model was originally developed for diatomic and triatomic molecules [3], and, thus, the $U(4)$ Lie algebra can be used to calculate the

stretching and vibrational excitations of polyatomic molecules. But the $U(4)$ model becomes complicated, when the number of atoms in a molecule becomes more than four. On the other hand, the $U(2)$ model introduced by Wulfman and Levine [1] is found to be successful in explaining the stretching vibrations of polyatomic molecules such as tetrahedral, octahedral, and benzene-like molecules. The brief review and the research work done with the algebraic models up to the year 2000 and its outlook and perception in the first decade of the 21st century was presented by Iachello and Oss [4]. Recently, it was found that the Lie algebraic method [5–17] was extremely successful and accurate in calculating the vibrational frequencies of polyatomic molecules as compared with the other methods such as the Dunham expansion and the potential approach method reported earlier [4].

After the introduction of Lie algebras at the end of the nineteenth century by Lie, they became much more familiar and popularized in the field of physics only in the recent past. This Lie algebra is the unitary algebra $U(n+1)$. Hence, one can formulate quantum mechanics in n dimensions in terms of the unitary algebra $U(n+1)$. In this work, we concentrate on the Lie algebraic techniques for solid carbon monoxide. This Lie algebraic model does not involve rotational motions. Nonetheless, it can be used to obtain a complete picture of the vibrational behavior of complex situations, falling even beyond the possibilities of a three-dimensional approach. We will see how this simple model can account for anharmonic cou-

plings between local modes (both stretching and non-degenerate bending vibrations), anharmonic (Fermi) resonances, symmetry adaption of wave functions, and some other important aspects of molecular spectroscopy.

The molecule of solid carbon monoxide considered in this theoretical work has the D_{5h} point group symmetry. The symmetry is an extremely important concept in the development of scientific knowledge. The beauty of symmetry rests in its connection to a possible invariance in a physical system. Such invariance leads directly to conserved quantities, which allow one in a quantum mechanical framework to observe specific degeneracies in the energy spectrum and to introduce a meaningful labeling scheme for the corresponding eigenstates.

Till date, few extensive experimental studies of the vibrational spectra of solid carbon monoxide were reported [18], which comes forward to analyze the study of vibrational spectra of solid carbon monoxide with its different energy bands [18]. By using the one-dimensional $U(2)$ algebraic model, we calculate the stretching vibrational energies of solid carbon monoxide, which is an excellent alternative mathematical treatment for the determination of the energy bands of solid carbon monoxide from the spectroscopic point of view.

The advantage of the algebraic models, as compared to the Dunham models is that the models need typically fewer parameters to obtain the same level of accuracy. The algebraic models also provide a simultaneous description of bending and stretching modes. Finally, the models produce not only energies, but also wave functions (similar to that of the potential approach). Hence, they can be used to compute other observables. The algebraic models are particularly useful for large molecules, where a few number of parameters play a major role. Our purpose here is to show that the model can be brought to the spectroscopy accuracy. Further, the species studied in this work is of interest due to its importance not only in human life, but also in scientific researches.

2. Review of the Theory

Recently, the algebraic method has been introduced as a computational tool for the analysis and the interpretation of experimental rotational-vibrational spectra of large and medium-size molecules. This method has been used extensively in chemical physics and molecular physics. This method is based on the idea of dynamical symmetry, which, in turn, is expressed in the language of Lie algebras.

In connection with molecular spectroscopy, the dynamical symmetries explored in this work constitute a big step forward over a conventional use of symmetry arguments, especially those concerning the description and classification of energy spectra denoting specific degeneracy patterns. The dynamical symmetries contain within themselves both the degeneracy aspects of a physical system and the complete machinery for describing the transitions among different states. All these tasks can be carried out in the extremely compact and convenient framework of Lie groups and Lie algebras. The use of the dynamical symmetry, a very powerful technique related to a dynamical group, leads to a conveniently simple form of the second-quantized Hamiltonian operator. The most important steps leading to the formulation of a dynamical symmetry have been presented. This formulation should be thought as a very efficient specialized version of the usual second-quantized realization of a quantum problem. In such realization, (1) the wave equation is replaced by an algebraic equation, (2) the wave functions are replaced with a Fock space, and (3) the most general algebraic expansion in terms of the (boson) creation-annihilation operators is restricted to invariant or Casimir operators of subalgebras of the dynamical algebra. Such ultimate algebraic structure turns out to be, for n-dimensional problems, the Lie algebra $U(n+1)$. These three steps constitute the basic components for the definition of the dynamical symmetry realization of the Hamiltonian operator.

Thus, by applying Lie algebraic techniques, we obtain an effective Hamiltonian operator that conveniently describes the rotational-vibrational degrees of freedom of the physical system [19]. The algebraic methods are formulated in such a way that they contain the same physical information of both *ab initio* theories (based on the solution of the Schrödinger equation) and of semiempirical approaches (with the use of phenomenological expansions in powers of appropriate quantum numbers). However, by employing the powerful method of group theory, the results can be obtained in a more rapid straightforward way [20]. In Lie algebraic approaches, $U(4)$ and $U(2)$ algebraic models have been extensively used. The $U(4)$ model deals with the rotation and the vibration simul-

taneously, but it becomes quite complicated, when the number of atoms in a molecule are more than four. The $U(2)$ model was particularly successful in explaining the stretching vibrations of polyatomic molecules such as benzene-like, octahedral, and icosahedral molecules. Here, we use the $U(2)$ algebraic model to study the higher excited vibrations of solid carbon monoxide.

For introducing the $U(2)$ algebraic model, we use the isomorphism of the Lie algebra of $U(2)$ with that of a one-dimensional Morse oscillator. The most appealing feature of the Morse potential is that one can solve the associated Schrödinger equation in an exact way for one-dimensional problems or in a quasiexact way for two- or three-dimensional problems, the error often being smaller than 1 part in 10^8–10^{10} (for zero angular momentum). Such an approximation comes from the fact that analytical solutions can be achieved only under the constraint that $V(r) \rightarrow \infty$, as $r \rightarrow 0$. Such a condition is only approximately fulfilled by the Morse potential [19].

The eigenstates of the one-dimensional Schrödinger equation, $h\psi = \epsilon\psi$ with the Morse potential [21],

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

which can be put into one-to-one correspondence with the representations of $U(2) \supset O(2)$ characterized by the quantum numbers $|N, m\rangle$ with the provision that one takes only the positive branch of m, i.e. $m = N, N-2, ..., 1$ or 0 for $N =$ odd or even (N being an integer). The Morse Hamiltonian corresponds in the $U(2)$ basis to a simple Hamiltonian $h = \epsilon_0 + AC$ where C is the invariant operator of $O(2)$ with eigenvalues $m^2 - N^2$.

The eigenvalues of h are

$$\epsilon = \epsilon_0 + A(m^2 - N^2), \qquad (2)$$

where $m = N, N - 2, ..., 1$ or 0 (N being an integer), and A is the normalization constant. Introducing the vibrational quantum number $v = \frac{(N-m)}{2}$, Eq. (2) can be rewritten as

$$\epsilon = \epsilon_0 - 4A(Nv - v^2), \qquad (3)$$

where $v = 0, 1, ..., \frac{N}{2}$ or $\frac{N-1}{2}$ (for N even or odd, respectively). The values of ϵ_0, A, N are given in terms of μ, D, α, by using the relations

$$\epsilon_0 = -D, \quad -4AN = h\alpha \left(\frac{2D}{\mu}\right)^{1/2}, \quad 4A = -\frac{h^2\alpha^2}{2\mu}.$$

One can verify that these are the eigenvalues of the Morse oscillator.

Now, we consider a molecule with n bonds. In the algebraic model, each bond is replaced by an algebra with the Hamiltonian $h_i = \epsilon_{0i} + A_i C_i$ [22], where C_i is the invariant operator with eigenvalues $-4(N_i\nu_i - \nu_i^2)$. The bonds interact through a bond-bond interaction. Two types of interaction are usually considered in terms of two operators C_{ij} and M_{ij}, called the Casimir and Majorana operators, respectively. The Casimir operator has only the diagonal matrix elements, whereas the Majorana operators have both diagonal and off-diagonal matrix elements. They are invariant operators of the combined algebras $O_{ij}(2)$ and $U_{ij}(2)$ in the group lattice. Their physical meaning can be seen from the matrix elements given by Eq. (5) and Eq. (6).

The algebraic model Hamiltonian under consideration has the following form [19]:

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

In Eq. (4), C_i is an invariant operator with eigenvalues $4(\nu_i^2 - N_i\nu_i)$, and the operator C_{ij} is diagonal with matrix elements

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

while the operator M_{ij} has both diagonal and off-diagonal matrix elements

$$\langle N_i, \nu_i; N_j, \nu_j | M_{ij} | N_i, \nu_i; N_j, \nu_j \rangle =$$
$$= (N_i\nu_j + N_j\nu_i - 2\nu_i\nu_j),$$
$$\langle N_i, \nu_i + 1; N_j, \nu_j - 1 | M_{ij} | N_i, \nu_i; N_j, \nu_j \rangle =$$
$$= -[\nu_j(\nu_i + 1)(N_i - \nu_i)(N_j - \nu_j + 1)]^{1/2},$$
$$\langle N_i, \nu_i - 1; N_j, \nu_j + 1 | M_{ij} | N_i, \nu_i; N_j, \nu_j \rangle =$$
$$= -[\nu_i(\nu_j + 1)(N_j - \nu_j)(N_i - \nu_i + 1)]^{1/2}. \qquad (6)$$

Equation (6) is a generalization of the two-bond model to n bonds [20].

The role of the Majorana operators M_{ij} is to introduce off-diagonal couplings between pairs of local modes. In the simplest case of equivalent interacting bonds, the Majorana operator naturally leads to a solution for symmetrized coupled modes, in which the invariance of the Hamiltonian operator, under bond exchange, is explicitly taken into account. A rather

appealing feature of this algebraic model is that such a symmetrizing property of the Majorana operator, actually quite a trivial one for two equal bonds, can readily be extended to any molecular geometry, even a very complex one. The key point is that the basic information characterizing the specific molecular geometry can easily be incorporated by introducing the proper linear combinations of Majorana operators.

In the purely local limit of N oscillators, these oscillators are somehow correlated with one another through the C_{ij} operators, which account for (diagonal) cross-anharmonicities represented by the equation

$$C_{ij} = C_i - N_{ij} \left(\frac{C_i}{N_i} + \frac{C_j}{N_j} \right), \tag{7}$$

where $N_{ij} = N_i + N_j$. Furthermore, following Eq. (7), it should be noted that, from C_i, one basically

subtracts the terms arising from uncoupled single-oscillator contributions. In the special case of a pair of equivalent oscillators i and $j (N_i = N_j)$, the above equation can be replaced by the following matrix elements

$$\langle \nu_i \nu_j | C_{ij} | \nu_i \nu_j \rangle = -4(\nu_i - \nu_j)^2, \tag{8}$$

i.e., the matrix elements do not depend on $N_i(N_j)$. As a result, C_{ij} will account for different contributions throughout different polyads and within the same polyad. The most important aspect of C_{ij} is the dependence of its matrix elements on the product $\nu_i \nu_j$.

The simplest basis to diagonalize the Hamiltonian is characterized by the local mode chain representation [12]:

$$
\begin{array}{ccccccc}
U^{(1)}(2) \otimes U^{(2)}(2) \otimes U^{(3)}(2) \otimes & \supset & SO^{(1)}(2) \otimes SO^{(2)}(2) \otimes & SO^{(3)}(2) & \supset SO(2) \\
\downarrow \quad\quad \downarrow \quad\quad \downarrow & & \downarrow \quad\quad\quad \downarrow & \downarrow & \downarrow \\
|[N_1], \quad [N_2], \quad [N_3]; & & \nu_1, \quad\quad \nu_2, & \nu_3; & V \rangle,
\end{array} \tag{9}
$$

where, below each group, we have indicated the eigenvalues that label their irreducible representations. Explicitly this basis is given by

$$[N_1], [N_2], [N_3]; \nu_1 \nu_2 \nu_3 \rangle = [N_1]; \nu_1 \rangle | [N_2]; \nu_2 \rangle | [N_3]; \nu_3 \rangle, \tag{10}$$

where $\left| [N]; \nu \right\rangle = \sqrt{\frac{(N-\nu)!}{N!\nu!}} (J_-)^{\nu_i} \left| [N]; 0 \right\rangle.$

Here, N is the total number of bosons fixed by the potential shape, ν corresponds to the number of quanta in the oscillator, and J is the angular momentum operator (has both raising J_+ and lowering J_- components connecting different energy states) in $U(2)$ algebra. The quantum numbers ν_i correspond to the number of quanta in each oscillator, while V is the total vibrational quantum number given by

$$V = \sum_{i=1}^{\infty} \nu_i. \tag{11}$$

For a particular polyad, the total vibrational quantum number is always conserved. The inclusion of M_{ij} in the local Hamiltonian operator cannot affect the conservation rule. In Eq. (4), C_i is an invariant operator of uncoupled bond with eigenvalues

$4(\nu_i^2 - N_i\nu_i)$, and the operators C_{ij} for coupled bonds are diagonal with matrix elements given in Eqs. (5) and (6).

3. Results and Discussion

In this work, we use the algebraic parameters A, A', λ, λ', and the Vibron number N to study the vibrational spectra of solid carbon monoxide molecules. Considering the common coupled and uncoupled bond-bond interaction in the molecular configuration in the case of solid carbon monoxide, as well as the Majorana couplings, the number of algebraic parameters are reduced to four on the basis of the symmetry of the molecules. In this regard, one should note that this is the unique beauty of the algebraic model, where one needs only a few parameters to describe the vibrational spectra of a molecule with a good accuracy.

The values of Vibron number (N) can be determined by the relation

$$N_i = \frac{\omega_e}{\omega_e x_e} - 2 \quad (i = 1, 2, 3, ...), \tag{12}$$

where ω_e and $\omega_e x_e$ are the spectroscopic constants.

For a solid carbon monoxide molecule in the stretching mode, we can have the values of ω_e and $\omega_e x_e$ for the CO bond from the works by Nakamoto [23] and by Huber and Herzberg [24]. Using the values of ω_e and $\omega_e x_e$ for the bond C-O, we can have the initial guess for the value of Vibron number N. It may be noted here that, in the algebraic approach, there is a provision to change (not more than $\pm 20\%$) the the value of N to get better results. This is equivalent to change the single-bond anharmonicity according to a specific molecular environment, in which it can be slightly different.

To obtain a starting guess for the parameter A, we use the expression for the single-oscillator fundamen-tal mode, which reads

$$E(\nu = 1) = -4A(N - 1). \tag{13}$$

Using Eq. (13), $\overline{A}$ can be obtained as

$$\overline{A} = \frac{\overline{E}}{4(1 - N)}, \tag{14}$$

where $\overline{A}$ and $\overline{E}$ are the average values of the algebraic parameters A and E.

We will obtain the initial guess for λ by $\overline{E}$ used in Eq. (14), where the role of λ is to split the initially degenerate local modes. Such an estimate follows from the consideration of the simple Hamiltonian matrix structure

$$\begin{pmatrix} -4A(N - 1) - 4A'(2N - 1) + \lambda N & -\lambda N \\ -\lambda N & -4A(N - 1) - 4A'(2N - 1) + \lambda N \end{pmatrix}. \tag{15}$$

We easily find that

$$\lambda = \frac{E_3 - E_1}{2N}, \tag{16}$$

$$\lambda' = \frac{E_2 - E_1}{6N}. \tag{17}$$

To have better results, a numerical fitting procedure (in a least-square sense) is required to obtain the parameters A, A', λ, and λ' starting from the values, as given by Eqs. (14), (16), and (17). The initial guess for A' may be taken as zero.

The data in Table 2 are taken from the experimental observations [18], which show a good agreement with the algebraic calculations, whereas Table 1 shows the fitting algebraic parameters to study the vibrational spectra of solid carbon monoxide.

Table 1. **Fitting parameters* of solid carbon monoxide**

Vibron number	Stretching parameters		
N	A	λ	λ'
88	–6.0	0.135	0.0072

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

Table 2. **Experimental and calculated energies (cm^{-1}) of solid carbon monoxide**

Normal level	I Reference [18]	II This study
ν_1	2088.4	2090.21
ν_2	2092.2	2090.69
ν_3	2112.3	2113.99
ν_4	2138.1	2136.62
ν_5	...	2156.43
ν_6	...	2167.98
ν_7	2182.0	2179.09
ν_8	2197.0	2195.08
ν_9	2208.0	2203.19
ν_{10}	...	2208.45
ν_{11}	2222.0	2214.07

4. Conclusion

The algebraic model presented here is a model of coupled one-dimensional Morse oscillators describing the C–O stretching vibrations of a molecule of solid carbon monoxide. By using this algebraic model, one can avoid the complicated integrations in the solution of coupled differential Schrödinger equations. For the C–O stretching interbond interactions, this model can be used in a simple straightforward way, and the reliable calculation of the stretching bonds can

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be explained in terms of the above fitting parameters. In this paper, we have presented only a few modes of vibrations of solid carbon monoxide, which are in good agreement with the experimental values [18]. Apart from those, we calculate few hitherto unknown values, which were not observed experimentally. We hope for that, with the further advancement of the $U(2)$ model, the higher order modes of vibrations of solid carbon monoxide can be also explained with good accuracy, by considering the bent vibrations of molecules along with the stretch vibrations.

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КОЛИВАЛЬНІ ІНФРАЧЕРВОНІ СПЕКТРИ
ТВЕРДОТІЛЬНОГО МОНООКИСУ ВУГЛЕЦЮ

Р е з ю м е

Розраховані коливальні рівні енергії твердотільного монооксиду вуглецю на основі локального гамільтоніана з використанням потенціалу Морзе і $U(2)$ алгебри. Кожен зв'язок молекули змінюється оператором відповідної Лі алгебри, і локальний гамільтоніан будується за допомогою взаємодіючих операторів Казимира і Майорана. Проведено порівняння розрахованих основних інфрачервоних поздовжніх мод з експериментом.