

Vibrational spectra of oxygen and nitrogen-bridged iron octaethylporphyrin dimers by an U(2) algebraic technique

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ABSTRACT

Using U(2) algebraic model Hamiltonian the resonance Raman spectra of Oxygen bridged iron porphyrin dimers (OEPFe)₂O and (OEPFe)₂N calculated for selected some vibrational modes. Using this model the Hamiltonian so constructed, we have calculated vibrational energy levels of (OEPFe)₂O and (OEPFe)₂N accurately.

Keywords: Vibrational Spectra; Lie Algebra; Octaethylporphyrin

1. INTRODUCTION

The structural and electronic properties of a number of metalloporphyrins and heme proteins have been elucidated with resonance Raman (RR) spectroscopy [1,2]. Vibrational spectra of metalloporphyrins are necessary not only to assign resonance Raman lines of hemoproteins but also to study the excited electronic states of metalloporphyrins with the vibronic interactions. Last two decades, few group members have done experimental and theoretical work on metalloporphyrins [3,4]. Vibrational assignments of the resonance Raman spectra of various metalloporphyrins have been extensively studied by several groups [5-8]. Recently, an algebraic approach has been proposed for the study of bio-molecular spectroscopy [9-10]. In the algebraic approach, the vibrational Hamiltonian is expanded in terms of certain operators in Lie algebra; U(4) in the full three-dimensional approach and U(2) in the simpler one-dimensional approach [11-26].

In the present paper, we have calculated the in-plane

fundamental and combinational vibrational frequencies of Oxygen-bridged iron porphyrin dimers at various wavelengths using U(2) algebraic approach.

2. THEORY: U(2) ALGEBRAIC APPROACH

In constructing this model, we use the isomorphism of the Lie algebra of U(2) with that of the one-dimensional Morse oscillator [27]. The eigen states of the one-dimensional Schrodinger equation, $h\psi = E\psi$, with a Morse potential [28]

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

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. $m = N, N-2, \dots, 1$ or 0 for $N = \text{odd}$ or even ($N = \text{integer}$). The Morse Hamiltonian (1) corresponds in the U(2) basis to a simple Hamiltonian, $h = E_0 + AC$, where C is the invariant operator of $O(2)$, with eigen values $(m^2 - N^2)$.

$$\text{The eigen values of } h \text{ are } E = E_0 + A(m^2 - N^2) \quad (2)$$

$$M = N, N-2, \dots, 1 \text{ or } 0 \text{ (} N = \text{integer)}.$$

Introducing the vibrational quantum number $\nu = (N - m)/2$, Eq.2 can be rewritten as

$$E = E_0 - 4A(N\nu - \nu^2), \nu = 0, 1, \dots, N/2 \quad (3)$$

or $N-1/2$ ($N = \text{even or odd}$)

The values of E_0 , A , and N are given in terms of μ , D , and α by $E_0 = -D$, $-4AN = \hbar\alpha(2D/\mu)^{1/2}$, $4A = -\hbar^2\alpha^2/2\mu$. One can immediately verify that these are the eigen values of the Morse oscillator.

Now, consider a molecule with n bonds. In the algebraic model [29], each bond i is replaced by an algebra (here $U_i(2)$), with Hamiltonian $h_i = \epsilon_{0i} + A_i C_i$, where C_i is the invariant operator of $O_i(2)$ with eigen values $-4(N_i v_i - v_i^2)$. The bonds interact with a bond-bond interaction. Two types of interaction are usually considered [29], which we denote by C_{ij} and M_{ij} , are called Casimir and Majorana interactions respectively.

The algebraic model Hamiltonian we consider is thus

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

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

$$\begin{aligned} & \langle N_i, v_i; N_j, v_j | C_{ij} | N_i, v_i; N_j, v_j \rangle \\ & = 4 \left[(v_i + v_i^2) - (v_i + v_j)(N_i + N_j) \right] \end{aligned} \quad (5)$$

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

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

Eq.6 is a generalization of the two-bond model of Ref. [28] to n bonds.

2.1. Symmetry-Adapted Operators

In polyatomic molecules, the geometric point group symmetry of the molecule plays an important role. States must transform according to representations of the point symmetry group. In the absence of the Majorana operators M_{ij} , states are degenerate. The introduction of the Majorana operators has two effects:

1) It splits the degeneracy's of figure and (2) in addition it generates states with the appropriate transformation properties under the point group. In order to achieve this result the λ_{ij} must be chosen in an appropriate way that reflects the geometric symmetry of the molecule. The total Majorana operator

$$S = \sum_{i<j}^n M_{ij} \quad (11)$$

is divided into subsets reflecting the symmetry of the

molecule

$$S = S' + S'' + \dots \quad (12)$$

The operators S' , S'' , \dots are the symmetry-adapted operators. The construction of the symmetry-adapted operators of any molecule becomes clear in the following sections where the cases of Metalloporphyrins (D_{4h}) discussed.

2.2. Sample: Vibrational Analysis of Metalloporphyrins

As an example of the use of an algebraic method we analyze the stretching/bending vibrations of different Metalloporphyrins. We number the bonds as shown in **Figure 1**. Each bond, i , is characterized by its Vibron number N_i , and parameter A_i . The Casimir part of the interbond interactions is characterized by parameter A_{ij} . For the Majorana part we can have, the view of symmetry of the molecule, two possible types of couplings:

Different Porphyrins are obtained by specific substitution at X or 1 to 8 positions.

By inspection of the **Figure 1**, one can see that two types of interactions in Metalloporphyrins:

- 1) First-neighbor couplings (Adjacent interactions);
- 2) Second-neighbor couplings (Opposite interactions).

The symmetry-adapted operators of Metalloporphyrins with symmetry D_{4h} are those corresponding to these two couplings, that is,

$$S' = \sum_{i<j}^n c'_{ij} M_{ij}, \quad S'' = \sum_{i<j}^n c''_{ij} M_{ij}, \quad (13)$$

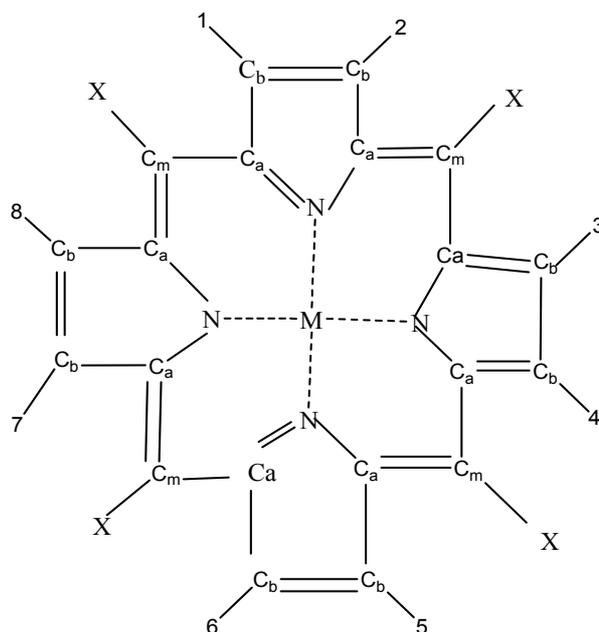


Figure 1. The structure of metalloporphyrins.

with

$$\begin{aligned} c'_{12} &= c'_{23} = c'_{34} = c'_{45} = \dots = 1, \\ c'_{13} &= c'_{24} = c'_{35} = c'_{46} = \dots = 0, \\ c''_{12} &= c''_{23} = c''_{34} = c''_{45} = \dots = 0, \\ c''_{13} &= c''_{24} = c''_{35} = c''_{46} = \dots = 1. \end{aligned}$$

The total Majorana operator S is the sum

$$S = S' + S'' \quad (14)$$

Diagonalization of S produces states that carry representations of S , the group of permutations of objects, while diagonalization of the other operators produces states that transform according to the representations A_{1g} , A_{2g} , B_{1g} , B_{2g} , E_{1u} of D_{4h} .

2.3. Local to Normal Transition: The Locality Parameter (ξ)

The local-to-normal transition is governed by the dimensionless locality parameter (ξ). The local-to-normal transition can be studied [10] for polyatomic molecules,

for which the Hamiltonian is

$$H = A_i C_i + A_{ij} C_{ij} + \lambda_{ij} M_{ij} \quad (18)$$

For these molecules, the locality parameters [9] are

$$\xi_i = (2/\pi) \tan^{-1} \left[8\lambda_{ij} / (A_i + A_{ij}) \right], i, j = 1, 2, 3, \dots \quad (19)$$

corresponding to the two bonds. A global locality parameter for XYZ molecules can be defined as the geometric mean

$$\xi = (|\xi_1 \xi_2|)^{1/2} \quad (20)$$

Locality parameters of this metalloporphyrins are given in the results and discussions. With this definition, due to Child and Halonen [9,10], local-mode molecules are near to the $\xi = 0$ limit, normal mode molecules have $\xi \rightarrow 1$.

3. RESULTS & DISCUSSIONS

As an example, we report in the **Table 1** & **Table 2**, the results of fundamental and combinational vibrational

Table 1. Resonance Raman bands (cm^{-1}) of OEPFeCl, (OEPFe)₂O and (OEPFe)₂N assignable to in-plane skeletal modes.

Symmetry	no ^a	OEPFeCl		(OEPFe) ₂ O		(OEPFe) ₂ N	
		Exp ^(b)	Calc	Exp ^(b)	Calc	Exp ^(b)	Calc
A_{1g}	ν_2	1582	1581.89	1583	1584.73	1590	1591.86
	ν_3	1494	1492.01	1495	1494.28	1513	1515.76
	ν_4	1376	1377.34	1377	1375.36	1378	1378.83
	$\nu_5 + \nu_9$	1256	1256.82	1258	1258.91	1261	1259.10
	$\nu_6 + \nu_8$	1136	1137.09	1136	1136.24	1138	1138.56
	$\nu_5 + \nu_9$	1024	1021.36	1023	1024.82	1023	1025.82
	$\nu_{32} + \nu_{35}$	961	963.86	963	965.78	-	966.49
	$\nu_{33} + \nu_{35}$	732	728.01	733	735.99	733	731.87
	ν_7	676	678.92	668	668.02	668	665.05
	ν_8	-	343.30	345	346.92	335	336.27
B_{1g}	ν_{10}	1628	1627.91	1627	1626.09	1647	1647.02
	ν_{13}	1210	1212.36	1211	1212.28	1212	1212.34
	ν_{16}	752	753.81	753	754.91	753	754.68
	ν_{19}	1565	1566.03	1559	1560.04	1572	1567.78
A_{2g}	ν_{20}	1390	1389.61	1388	1389.73	1390	1389.01
	ν_{21}	1311	1312.73	1315	1316.01	1312	1315.78
	ν_{22}	1125	1126.37	1129	1127.81	1132	1135.04
	ν_{29}	1404	1405.36	1403	1400.85	1405	1406.63
B_{2g}	ν_{30}	1156	1157.92	1159	1162.47	1159	1159.82
		$\Delta(\text{r.m.s}) = 11.40 \text{ cm}^{-1}$		$\Delta(\text{r.m.s}) = 16.24 \text{ cm}^{-1}$		$\Delta(\text{r.m.s}) = 11.22 \text{ cm}^{-1}$	

^aSkeletal mode numbering follows Kitagawa *et al.* [30]; ^bExperimental data follow David F. Bocian *et al.* [31]. The values of the algebraic parameters are used in calculation of Octaethylporphyrin dimmers at 4067 Å. $A = -2.3084 \text{ cm}^{-1}$, $A' = -1.0576 \text{ cm}^{-1}$, $\lambda = 0.2397 \text{ cm}^{-1}$, $\lambda' = 0.0192 \text{ cm}^{-1}$.

Table 2. Resonance Raman bands (cm^{-1}) of (OEPFeCl), (OEPFe)₂O and (OEPFe)₂N at $\lambda = 5208 \text{ \AA}$, $\lambda = 5682 \text{ \AA}$, and $\lambda = 5145 \text{ \AA}$ respectively.

Symmetry	no ^a	OEPFeCl ($\lambda = 5208 \text{ \AA}$)		(OEPFe) ₂ O ($\lambda = 5682 \text{ \AA}$)		(OEPFe) ₂ N ($\lambda = 5145 \text{ \AA}$)		
		Exp ^(b)	Calc	Exp ^(b)	Calc	Exp ^(b)	Calc	
<i>A</i> _{1g}	ν_8	1628	1630.97	1627	1630.28	1647	1648.20	
	ν_{16}	752	750.09	753	755.87	753	755.30	
	ν_{19}	1566	1566.03	1559	1560.04	1572	1567.78	
	ν_{20}	1390	1389.61	1388	1389.73	1390	1389.01	
	ν_{21}	1311	1312.73	1315	1316.01	1312	1315.78	
	ν_{22}	1125	1126.37	1129	1127.81	1132	1135.04	
	ν_{29}	1404	1405.36	1403	1400.85	1405	1406.63	
	ν_{30}	1156	1157.92	1159	1162.47	1159	1159.82	
			$\Delta(\text{r.m.s}) = 7.08 \text{ cm}^{-1}$		$\Delta(\text{r.m.s}) = 8.76 \text{ cm}^{-1}$		$\Delta(\text{r.m.s}) = 7.56 \text{ cm}^{-1}$	

^aSkeletal mode numbering follows Kitagawa *et al.* [30]; ^bExperimental data follow David F. Bocian *et al.* [31]. The values of the algebraic parameters are used in calculation of Octaethylporphyrin dimmers at 4067 \AA . $A = -1.368 \text{ cm}^{-1}$, $A' = -0.2096 \text{ cm}^{-1}$, $\lambda = 0.792 \text{ cm}^{-1}$, $\lambda' = 0.0320 \text{ cm}^{-1}$.

frequencies of OEPFeCl, (OEPFe)₂O and (OEPFe)₂N at 4067 \AA and at different wavelengths ($\lambda = 5208 \text{ \AA}$, $\lambda = 5682 \text{ \AA}$, and $\lambda = 5145 \text{ \AA}$) of Octaethyl dimers respectively. Here, we have used U(2) algebraic model to study the resonance Raman spectra of Octaethyl dimmers molecules with fewer algebraic parameters *i.e.* A , A' , λ , λ' and N (Vibron number).

The values of vibron number can be determined [10] by the relation

$$N_i = \frac{\omega_e}{\omega_e x_e} - 1, (i = 1, 2)$$

where ω_e and $\omega_e x_e$ are the spectroscopic constants of diatomic molecules of stretching and bending interactions of molecules considered. The Vibron number N between the diatomic molecules C-H & C-C are ≈ 44 and ≈ 140 respectively. This numerical value must be seen as initial guess; depending on the specific molecular structure, one can expect changes in such an estimate, which, however, should not be larger than $\pm 20\%$ of the original value (Eq.6). Using the established norms the Vibron numbers N and other algebraic parameters A , A' , λ , λ' are determined.

From the view of group theory, the molecule of (OEPFeCl), (OEPFe)₂O & (OEPFe)₂N takes a square planar structure with the D_{4h} symmetry point group. Molecular vibrations of metalloporphyrins are classified into the in-plane and out of plane modes. For Octaethyl dimmers of D_{4h} structure assuming the peripheral ethyl group is point mass the in-plane vibrations of Octaethyl dimmers are factorized into 35 gerade and 18 ungerade. Out of planes are factorized into 8 gerade and 18 ungerade modes. The A_{2u} and E_u modes are IR active where the A_{1g} , B_{1g} , A_{2g} , B_{2g} & E_g modes are Raman ac-

tive in an ordinary sense.

4. CONCLUSIONS

In the study of Resonance Raman spectra of Octaethyl dimers, we have applied one dimensional algebraic model *i.e.* U(2) Vibron model. In this study we reported RMS deviation and the locality parameter (ξ) for Oxygen and Nitrogen-Bridged Iron Octaethylporphyrin dimmers of in-plane skeletal modes at $\lambda = 4067 \text{ \AA}$ and also for OEPFeCl at $\lambda = 5208 \text{ \AA}$, (OEPFe)₂O at $\lambda = 5682 \text{ \AA}$, and for (OEPFe)₂N at $\lambda = 5145 \text{ \AA}$ respectively.

In this study we reported the vibrations of Oxygen and Nitrogen-Bridged Iron Octaethylporphyrin dimmers are in accurate agreement with experimental data.

In this study the resonance Raman spectra of OEPFeCl, (OEPFe)₂O and (OEPFe)₂N for in-plane skeletal modes at $\lambda = 4067 \text{ \AA}$ (Table 1), we obtain the RMS deviation *i.e.* $\Delta(\text{r.m.s})$ as 11.40 cm^{-1} , 16.24 cm^{-1} , 11.22 cm^{-1} and the locality parameters are $\xi_1 = 0.0231$, $\xi_2 = 0.0234$, $\xi_3 = 0.0232$ respectively.

In this study the resonance Raman spectra of OEPFeCl for in-plane skeletal modes at $\lambda = 4067 \text{ \AA}$ (Table 2), we obtain the RMS deviation *i.e.* $\Delta(\text{r.m.s})$ as 7.08 cm^{-1} and the locality parameter (ξ) = 0.0014.

In this study the resonance Raman spectra of (OEPFe)₂O for in-plane skeletal modes at $\lambda = 4067 \text{ \AA}$ (table 1), we obtain the RMS deviation *i.e.* $\Delta(\text{r.m.s})$ as 8.76 cm^{-1} and the locality parameter (ξ) = 0.0019.

In this study the resonance Raman spectra of (OEPFe)₂N for in-plane skeletal modes at $\lambda = 4067 \text{ \AA}$ (Table 1), we obtain the RMS deviation *i.e.* $\Delta(\text{r.m.s})$ as 7.56 cm^{-1} and the locality parameter (ξ) = 0.0017.

The locality parameter of Oxygen and Nitrogen-

bridged Iron Octatehyloporphyrin dimmers at various wavelengths confirms that highly local mode behavior. Therefore, here the Hamiltonian mode is obviously the local Hamiltonian mode.

Hence, one may conclude that the algebraic local Hamiltonian mode fits well with the Oxygen and Nitrogen-bridged Iron Octatehyloporphyrin dimmers at various wavelengths. Therefore the higher excited states and combinational bands are calculated using algebraic local Hamiltonian mode with sufficient experimental data.

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