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Brief Communication

Resonance Raman Spectra of Erythrocytes: Vibron Model

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ABSTRACT

In this paper, vibrational spectra (infrared and Raman) of oxygenated and deoxynated functional erythrocytes are calculated using theoretical method "Vibron model" in the one-dimensional [U(2)] framework. The determined vibrational modes by Vibron model are compared with experimental data. It has been observed that results from the theoretical model reveal near to the exact, reliable with the experimental data.

Keywords: Lie algebras, Resonance Raman spectra, Vibron model, Erythrocytes.

INTRODUCTION

Molecular spectroscopy is a key tool for the explanation of molecular structure. The study of fundamental and higher overtones of molecule helps in better understanding of the molecular structure, which might have a great importance in medical science. This spectra is useful to analyse biological molecules for identifying diseases in near the beginning stage and also useful to compare *in vivo* experimental results. The frame of new experimental methods to identify higher vibrational excitations in polyatomic molecules requires theoretical models (example, Vibron model) for their interpretation. Vibrational spectra of molecules are analysed with the help of two well-known approaches Dunham expansion and Potential approach. The most serious drawback of these approaches is that large number of parameters required for polyatomic molecules. To overcome this difficulty, we consider the Vibron model[1,2]. In 1991, Iachello presented Vibron model in the study of spectra of molecules[3, 4, 5, 6].

Vibron model

The Vibron model (Hamiltonian) for polyatomic molecule is

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

Here (A_i, A_{ij},A_{ij}) are parameters (algebraic) and (C_i,C_{ij},M_{ij}) are algebraic operators, which are differ from molecule to molecule. Algebraic operators, C_i and C_{ij} are invariant operators associated with uncoupled and coupled bonds with diagonal matrix elements. The Majorana operator, M_{ij} associated with coupling schemes. Algebraic parameters can be determined by spectroscopic data. Algebraic operators can be determined by

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

$$\langle N_i, v_i; N_j, v_j | C_{ij} | N_i, v_i; N_j, v_j \rangle = 4\left[(v_i + v_j)^2 - (v_i + v_j)(N_i + N_j)\right] \quad (3)$$

$$\langle N_i, v_i; N_j, v_j | M_{ij} | N_i, v_i; N_j, v_j \rangle = \left(N_i v_j + N_j v_i - 2 v_i v_j\right)$$

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

$$\langle N_i, v_i-1; N_j, v_j+1 | M_{ij} | N_i, v_i; N_j, v_j \rangle = -\left[v_i(v_j+1)(N_j - v_j)(N_i - v_i + 1)\right]^{1/2}. \quad (4)$$

In above equations, $N_i, v_i (i=1,2,\ldots)$ represents Vibron and vibrational quantum numbers respectively.

The vibron number N_i for stretching bonds of molecule will be calculated by

$$N_i = \frac{\omega_e}{\omega_e x_e} - 1, i = 1,2,3,\ldots \ (N_i = N_j) \quad (5)$$

Here ω_e and $\omega_e\chi_e$ are the spectroscopic constants. The initial guess value for the parameter A_i is obtained by using the energy equation, which is known as,

$$E(v=1) = -4A_i(N_i - 1) \quad (6)$$

The first guess for A_{ij} can be taken as zero. The parameter obtained from the relation,

$$\lambda_{ij} = \frac{|E_i - E_j|}{kN} \ (k = 2,6) \quad (7)$$

RESULTS

From the group theory point of view, the molecule of oxygenated and deoxygenated erythrocytes is a square planar structure with the D_{4h} symmetry point group[8]. We considered a experimental data from high-quality Raman speectra of red blood cells in both the oxygenated and the deoxygenated states for cell at 782 nm[7].

Table 1: Vibrational spectra of erythrocytes

Symmetry Species[3]	Vibrational mode	Vibrational frequencies (cm^{-1})	
		Calculated	Experimental[7]
	oxynated erythrocytes		
B_{1g}	(C_m-H)	1305.2346	1306
E_u	(C_m-H)	1250.0429	1248
	deoxynated erythrocytes		
B_{1g}	(C_m-H)	1303.0086	1305
E_u	(C_m-H)	1244.9821	1248

Table 2: Algebraic parameters

Algebraic parameters	oxynated	deoxynated
A	-9.3485	-10.5453
λ	0.3581	0.1277
N	44	44

Values of algebraic parameters in cm^{-1}, but *N* is dimensionless

CONCLUSION

In this paper we have calculated the vibrational frequencies of oxynated and deoxynated erythrocytes for the vibrational mode (Cm-H) by Vibron model and also compared with experimental data. These calculations shows that this model is an alternative appoarch of other theoretical models like Ab initio methods.

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