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(Brief Communication)

Vibrational Spectra of Copper Tetramesityl Porphyrin Using Vibron Model

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ABSTRACT

In this paper we calculated the fundamental level vibrational spectra of Metalloporphyrin (bio molecule) copper tetramesityl porphyrin (Cu(TMP)) using Vibron model.

Keywords: Vibrational spectra, Vibron model, Metalloporphyrins, Cu(TMP).

INTRODUCTION

Group theory is a well known tool that simplifies the process of obtaining a variety of information about molecules and their symmetries. Molecules are classified according to their symmetry properties and from that one can identify, the molecular symmetry point group. The molecular symmetry point group of metalloporphyrins is D_{4h}, which contains the principal C_n axis, n perpendicular C_2 axis, and the horizontal plane of symmetry.

I-IV are pyrrole rings; 1-8 are substituent positions. X positions are (=CH-) bridges

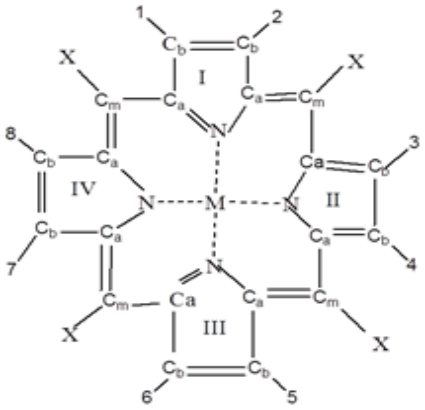

Fig.1. The strucure of metalloporphyrins

In 2008, Karumuri *et al.,* applied Vibron model for coupled anharmonic oscillators to describe the stretching vibrations of medium size molecules and calculated vibrational spectra of nickel octaethyl porphyrins for the stretching mode in Cm–H. the intervening years extended this model to calculate stretching vibrational frequencies of nickel tetraphenyl porphyrin and copper octaethyl porphyrin for different vibrational bands[1-9].

Vibron model for Metalloporphyrins

The general calculation procedure of vibrational spectra of metalloporphyrin by Vibron Model discussed here[10, 11]. The Hamiltonian for the polyatomic molecules is of the form Here vary from 1 to n for n stretching bonds and ($A_i, A_{ij}, \lambda_{ij}$) are algebraic parameters, which are determined by spectroscopic data. Where is an invariant operator (uncoupled bonds) with eigenvalues $-4(N_i v_i - v_i^2)$ diagonal matrix elements of the invariant operator C_{ij}(coupled bonds) and diagonal and non-diagonal matrix elements of Majorana operator M_{ij}obtained from the following relations,

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

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

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

$$\left\langle N_i, v_i - 1; N_j, v_j + 1 \middle| M_{ij} \middle| N_i, v_i; N_j, v_j \right\rangle = -\left[v_i\left(v_j + 1\right)\left(N_j - v_j\right)\left(N_i - v_i + 1\right)\right]^{1/2} \quad (3)$$

Where v_i(i=1,2,3,...) are vibrational quantum numbers.

The vibron number N_i(i=1,2,3,...) for stretching bonds of molecule will be calculated by the following relation

$$N_i = \frac{\omega_e}{\omega_e \chi_e} - 2, i = 1, 2, 3, \ldots \quad (4)$$

Where ω_e and $\omega_e\chi_e$ are spectroscopic constants. The initial guess value for the parameter A_i is obtained by using the energy equation for the single-oscillator fundamental mode, which is given as,

$$E(v = 1) = -4A_i(N_i - 1). \quad (5)$$

Initial guess for A_{ij} may be taken as zero. The parameter λ_{ij} obtained from the relation

$$\lambda_{ij} = \frac{\left|E_i - E_j\right|}{aN} (a = 3, 6). \quad (6)$$

RESULTS

Table. 1: Vibrational spectra of Cu(TMP)

Symmetry Species	Vibrational mode	Vibrational frequencies (cm^{-1})
A_{1g}	(C_m-C)	1235.04348
B_{2g}	(C_m-C)	1247.03267
E_u	(C_m-C)	1256.90364
A_{1g}	(C_b-H)	1470.00431
B_{2g}	(C_b-H)	1476.05321
E_u	(C_b-H)	1470.87451

Table. 2: Algebraic parameters

Algebraic parameters	C_m - C	C_b - H
A	-2.19234 cm^{-1}	-5.90923 cm^{-1}
A_{ij}	-0.98232 cm^{-1}	-2.92012 cm^{-1}
λ_{ij}(a=3)	0.02421 cm^{-1}	0.80834 cm^{-1}
λ_{ij}(a=6)	0.20091 cm^{-1}	0.03421 cm^{-1}
N (Dimensionless)	140	44

CONCLUSION

In this paper we have calculated the vibrational frequencies of copper tetramesityl porphyrin (Cu(TMP)) for the stretching modes (C_m-C) and (C_b-H).

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