

## Vibrational Frequencies of Oxygen Difluoride using Lie Algebraic Model

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### ABSTRACT

In one-dimensional Lie algebraic framework, we calculated the vibrational frequencies of oxygen difluoride (F<sub>2</sub>O) molecule in fundamental mode, higher overtones and their combinational bands.

**Keywords:** Vibrational frequencies, Lie algebraic model, Oxygen difluoride.

### INTRODUCTION

Analysis of vibrational spectra of small-size molecules is among the most challenging aspects of current studies in molecular physics. The emergence of novel experimental techniques to produce vibrational spectra of molecules in higher overtones, requires reliable theoretical models for their interpretation. In this paper we are concerned with the vibrational spectra of oxygen difluoride using Lie algebraic approach. In this model, vibrational Hamiltonian matrix describes the vibrational energies of the molecule. In 1991, one-dimensional Lie algebraic method applied for the study of vibrational frequencies of small size molecules by Iachello and co-researchers<sup>1,2</sup> and then this method was subsequently improved in vibrational spectra of medium-size molecules<sup>3-10</sup>.

### Lie algebraic method<sup>11,12</sup>

The general Hamiltonian for  $n$  vibrational modes of oxygen difluoride (F-O and F-O) is

$$H = E_0 + \sum_{i=1}^n p_i b_i + \sum_{i < j} p_{ij} b_{ij} + \sum_{i < j} q_{ij} f_{ij} \quad (1)$$

According to equation (1),  $b_i$  and  $b_{ij}$  are invariant operators for uncoupled and coupled bonds respectively and are known as

$$\langle b_i \rangle = -4(N_i^{F-O} v_i - v_i^2) \quad (2)$$

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

and the Majorana operator  $f_{ij}$  is used to express the local mode interactions in pairs and contains non-diagonal and diagonal matrix elements,

$$\begin{aligned} \langle N_i^{F-O}, v_i; N_j^{F-O}, v_j | f_{ij} | N_i^{F-O}, v_i; N_j^{F-O}, v_j \rangle &= (N_i^{F-O} v_j + N_j^{F-O} v_i - 2v_i v_j) \\ \langle N_i^{F-O}, v_i + 1; N_j^{F-O}, v_j - 1 | f_{ij} | N_i^{F-O}, v_i; N_j^{F-O}, v_j \rangle &= -[v_j(v_i + 1)(N_i^{F-O} - v_i)(N_j^{F-O} - v_j + 1)]^{1/2} \\ \langle N_i^{F-O}, v_i - 1; N_j^{F-O}, v_j + 1 | f_{ij} | N_i^{F-O}, v_i; N_j^{F-O}, v_j \rangle &= -[v_i(v_j + 1)(N_j^{F-O} - v_j)(N_i^{F-O} - v_i + 1)]^{1/2} \end{aligned} \quad (4)$$

Hamiltonian for two stretching vibrations of oxygen difluoride molecule with  $C_{2v}$  symmetry point group can be written as

$$H = E_0 + p_1 b_1 + p_2 b_2 + p_{12} b_{12} + q_{12} f_{12} \quad (5)$$

In equation (5),  $p_1$ ,  $p_2$ ,  $p_{12}$  and  $q_{12}$  are algebraic parameters ( $\text{cm}^{-1}$ ), estimated from the spectroscopic data. Two bonds (F-O) are equivalent in the oxygen difluoride; so, we consider as  $p_1 = p_2 = p$ ,  $N_1^{F-O} = N_2^{F-O} = N^{F-O}$  in equations (2), (3) and (4).

The Hamiltonian matrix for the first two local oscillators is

$$H = \begin{bmatrix} -4p(N^{F-O}-1) - 4p_{12}(2N^{F-O}-1) + q_{12}N^{F-O} & -q_{12}N^{F-O} \\ -q_{12}N^{F-O} & -4p(N^{F-O}-1) - 4p_{12}(2N^{F-O}-1) + q_{12}N^{F-O} \end{bmatrix}$$

## RESULTS AND DISCUSSION

The energy equation (6) is used to find the initial value of the parameter  $p$ ,

$$E(v=1) = -4p(N^{F-O}-1) \quad (6)$$

and the value for  $q_{12}$  determined from the relation,

$$q_{12} = \frac{|E_1 - E_2|}{2 N^{F-O}} \quad (7)$$

Where,  $E_1$ ,  $E_2$  are the oxygen difluoride, symmetric and antisymmetric vibrational frequencies, respectively. The oxygen difluoride vibrational frequencies were calculated using the Lie algebraic approach and the obtained results reported in (2) and Table (3).

The dimensionless Vibron number  $N_i$  for stretching and bending bonds of oxygen difluoride is determined using the following relation,

$$N_i^{F-O} = \frac{\omega_e}{\omega_e \chi_e} - 1, i=1, 2.$$

Where,  $\omega_e (=1053.0138)$ ,  $\omega_e \chi_e (=9.9194)$  are the vibrational harmonic and anharmonic (spectroscopic) constants, respectively for the bond F-O<sup>13</sup>.

**Table 1: Algebraic parameters**

|                        |         |
|------------------------|---------|
| $N^{F-O}$ (stretching) | 106     |
| $N^{O-F-O}$ (bending)  | 62      |
| $p$ (stretching)       | -2.094  |
| $p$ (bending)          | -1.8893 |
| $p_{12}$ (stretching)  | 0.0574  |
| $p_{12}$ (bending)     | 0.4685  |
| $q_{12}$ (stretching)  | 0.4575  |
| $q_{12}$ (bending)     | 3.7177  |

**Table 2: Fundamental vibrational frequencies (in  $\text{cm}^{-1}$ )**

| Vibrational Mode                | Symmetry | Observed <sup>14</sup> | Calculated |
|---------------------------------|----------|------------------------|------------|
| $\nu_1$ (symmetric stretch)     | $A_1$    | 928                    | 928.0244   |
| $\nu_2$ (bend)                  | $A_1$    | 461                    | 459.8062   |
| $\nu_3$ (antisymmetric stretch) | $B_1$    | 831                    | 831.0344   |

**Table 3: Higher overtone vibrational frequencies (in  $\text{cm}^{-1}$ )**

| Overtone | Symmetric stretch ( $A_1$ ) | Bend ( $A_1$ )     | Antisymmetric stretch ( $B_1$ ) |
|----------|-----------------------------|--------------------|---------------------------------|
| 1        | $2\nu_1(1847.133)$          | $2\nu_2(906.247)$  | $2\nu_3(1632.923)$              |
| 2        | $3\nu_1(2743.971)$          | $3\nu_2(1357.693)$ | $3\nu_3(2427.607)$              |
| 3        | $4\nu_1(3694.012)$          | $4\nu_2(1794.012)$ | $4\nu_3(3287.437)$              |
| 4        | $5\nu_1(4571.063)$          | $5\nu_2(2269.624)$ | $5\nu_3(4071.773)$              |
| 5        | $6\nu_1(5513.453)$          | $6\nu_2(2683.483)$ | $6\nu_3(4870.003)$              |
| 6        | $7\nu_1(6384.138)$          | $7\nu_2(3172.896)$ | $7\nu_3(5783.896)$              |
| 7        | $8\nu_1(7353.148)$          | $8\nu_2(3523.312)$ | $8\nu_3(6561.324)$              |
| 8        | $9\nu_1(8208.200)$          | $9\nu_2(4004.915)$ | $9\nu_3(7318.005)$              |

**Table 4: Combinational bands (in  $\text{cm}^{-1}$ )**

| Combinational band | Calculated | Combinational band | Calculated |
|--------------------|------------|--------------------|------------|
| $\nu_1 + \nu_2$    | 1389.933   | $2\nu_1 + \nu_2$   | 2309.042   |
| $\nu_1 + \nu_3$    | 1759.518   | $\nu_2 + 2\nu_2$   | 1369.801   |
| $\nu_2 + \nu_3$    | 1292.943   | $\nu_2 + 2\nu_3$   | 2094.832   |
| $\nu_1 + 2\nu_1$   | 2775.616   | $2\nu_1 + \nu_3$   | 2678.626   |
| $\nu_1 + 2\nu_2$   | 1836.374   | $\nu_3 + 2\nu_2$   | 1739.384   |
| $\nu_1 + 2\nu_3$   | 2561.406   | $\nu_3 + 2\nu_3$   | 2464.416   |

## CONCLUSION

In the Table (2), the estimated fundamental vibrational frequencies were compared with the observed data. In Table (3) and (4), vibrational frequencies upto the ninth harmonic and combinational bands upto third harmonic reported accordingly by the Lie algebraic method.

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## Conflict of interest

The author declare that we have no conflict of interest.

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