

6.11: PH3

C_{3v} Symmetry - PH_3

PH_3 (pyramidal) has IR and Raman active vibrations at 2421, 2327, 1121, and 991 cm^{-1} . Make assignments in terms of stretches and bends.

$$\begin{array}{l}
 \begin{array}{c} E \quad C_3 \quad \sigma_v \\
 C_{3v} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 2 & -1 & 0 \end{pmatrix} \begin{array}{l} 1 : z, x^2 + y^2, z^2 \\ A_2 : R_z \\ E : (x, y), (R_x, R_y), (x^2 + y^2, xy)(xz, yz) \end{array}
 \end{array}
 \end{array}
 \quad
 \begin{array}{l}
 C_{3v} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \quad \Gamma_{uma} = \begin{pmatrix} 4 \\ 1 \\ 2 \end{pmatrix} \quad \Gamma_{bonds} = \begin{pmatrix} 3 \\ 0 \\ 1 \end{pmatrix}
 \end{array}$$

$$\begin{array}{l}
 A_1 = (C_{C_{3v}}^T)^{<1>} \quad A_2 = (C_{C_{3v}}^T)^{<2>} \quad E = (C_{C_{3v}}^T)^{<3>} \quad h = \sum C_{3v} \\
 \Gamma_{tot} = \overline{[\Gamma_{uma}(A_1 + E)]} \quad \Gamma_{tot}^T = \begin{pmatrix} 12 & 0 & 2 \end{pmatrix} \quad \Gamma_{vib} = \Gamma_{tot} - A_1 - A_2 - 2E
 \end{array}$$

$$\begin{array}{l}
 i = 1..3 \quad \text{Vib}_i = \frac{\sum [C_{3v}(C_{C_{3v}}^T)^{<i>} \Gamma_{vib}]}{h} \quad \text{Vib} = \begin{pmatrix} 2 \\ 0 \\ 2 \end{pmatrix} \begin{array}{l} 1 : z, x^2 + y^2, z^2 \\ A_2 : R_z \\ E : (x, y), (R_x, R_y), (x^2 + y^2, xy)(xz, yz) \end{array}
 \end{array}$$

$$\begin{array}{l}
 \Gamma_{stretch} = \Gamma_{bonds} \quad \text{Stretch}_i = \frac{\sum [C_{3v}(C_{C_{3v}}^T)^{<i>} \Gamma_{stretch}]}{h} \quad \text{Stretch} = \begin{pmatrix} 2 \\ 0 \\ 2 \end{pmatrix} \begin{array}{l} 1 : z, x^2 + y^2, z^2 \\ A_2 : R_z \\ E : (x, y), (R_x, R_y), (x^2 + y^2, xy)(xz, yz) \end{array}
 \end{array}$$

$$\begin{array}{l}
 \Gamma_{bend} = \Gamma_{vib} - \Gamma_{stretch} \quad \text{Bend}_i = \frac{\sum [C_{3v}(C_{C_{3v}}^T)^{<i>} \Gamma_{bend}]}{h} \quad \text{Bend} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \begin{array}{l} 1 : z, x^2 + y^2, z^2 \\ A_2 : R_z \\ E : (x, y), (R_x, R_y), (x^2 + y^2, xy)(xz, yz) \end{array}
 \end{array}$$

Group theory predicts two singly degenerate (A_1) vibrational modes and two doubly degenerate (E) vibrational modes. This is consistent with the appearance of four fundamentals in the experimental IR and Raman spectra. It further predicts that there are two stretches and two bends. This is also consistent with the experimental data.

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