6.10: Tetrahedrane

Symmetry Analysis for Tetrahedrane

Tetrahedrane, C_4H_4, belongs to the Td point group. Use group theory to predict the number of IR and Raman acitive vibrational modes it has. To date tetrahedrane has not been synthesized.

$$C_{Td} = \begin{array}{c} \begin{array}{ccccc} E & C_3 & C_2 & S_4 & \sigma \end{array} \\ \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & -1 \\ 2 & -1 & 2 & 0 & 0 \\ 3 & 0 & -1 & 1 & -1 \\ 3 & 0 & -1 & -1 & 1 \end{pmatrix} \end{array} \quad \begin{array}{l} {}_1 : x^2+y^2+z^2 \\ A_2 \\ E: 2z^2-x^2-y^2,\ x^2-y^2 \\ T_1: (R_x,\ R_y,\ R_z) \\ T_2: (x,\ y,\ z),\ (xy,\ xz,\ yz) \end{array} \quad Td = \begin{pmatrix} 1 \\ 8 \\ 3 \\ 6 \\ 6 \end{pmatrix} \quad \Gamma_{uma} = \begin{pmatrix} 8 \\ 2 \\ 0 \\ 0 \\ 4 \end{pmatrix} \quad \Gamma_{bonds} = \begin{pmatrix} 10 \\ 1 \\ 2 \\ 0 \\ 4 \end{pmatrix}$$

$$A_1 = (C_{Td}^T)^{<1>} \quad A_2 = (C_{Td}^T)^{<2>} \quad E = (C_{Td}^T)^{<3>} \quad T_1 = (C_{Td}^T)^{<4>}$$

$$T_2 = (C_{Td}^T)^{<5>} \quad \Gamma_{tot} = \overrightarrow{(\Gamma_{uma} T_2)} \quad h = \sum Td \quad \Gamma_{tot}^T = \begin{pmatrix} 20 & 0 & 0 & 0 & 4 \end{pmatrix}$$

$$i = 1..5$$

$$\Gamma_{vib} = \Gamma_{tot} - T_1 - T_2 \qquad \mathrm{Vib}_i = \frac{\sum \overrightarrow{[Td(C_{Td}^T)^{<i>}\Gamma_{vib}]}}{h} \qquad \mathrm{Vib} = \begin{pmatrix} 2 \\ 0 \\ 2 \\ 1 \\ 3 \end{pmatrix} \quad \begin{array}{l} {}_1 : x^2+y^2+z^2 \\ A_2 \\ E: 2z^2-x^2-y^2,\ x^2-y^2 \\ T_1: (R_x,\ R_y,\ R_z) \\ T_2: (x,\ y,\ z),\ (xy,\ xz,\ yz) \end{array}$$

$$\Gamma_{stretch} = \Gamma_{bonds} \qquad \mathrm{Stretch}_i = \frac{\sum \overrightarrow{[Td(C_{Td}^T)^{<i>}\Gamma_{stretch}]}}{h} \qquad \mathrm{Stretch} = \begin{pmatrix} 2 \\ 0 \\ 1 \\ 0 \\ 2 \end{pmatrix} \quad \begin{array}{l} {}_1 : x^2+y^2+z^2 \\ A_2 \\ E: 2z^2-x^2-y^2,\ x^2-y^2 \\ T_1: (R_x,\ R_y,\ R_z) \\ T_2: (x,\ y,\ z),\ (xy,\ xz,\ yz) \end{array}$$

$$\Gamma_{bend} = \Gamma_{vib} - \Gamma_{stretch} \qquad \mathrm{Bend}_i = \frac{\sum \overrightarrow{[Td(C_{Td}^T)^{<i>}\Gamma_{bend}]}}{h} \qquad \mathrm{Bend} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \\ 1 \end{pmatrix} \quad \begin{array}{l} {}_1 : x^2+y^2+z^2 \\ A_2 \\ E: 2z^2-x^2-y^2,\ x^2-y^2 \\ T_1: (R_x,\ R_y,\ R_z) \\ T_2: (x,\ y,\ z),\ (xy,\ xz,\ yz) \end{array}$$

According to the selection rules, tetrahedrane should have three IR active modes ($3T_2$) and seven Raman active modes ($2A_1$ + 2E + $3T_2$). Two of the IR modes are stretches, while five of the Raman modes are stretches.