# 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.

$$C_{Td} := \begin{array}{c} \begin{matrix} E & C_3 & C_2 & S_4 & \sigma \end{matrix} \\ \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & -1 \\ 2 & -1 & 2 & 0 & 0 \\ 3 & 0 & -1 & 1 & -1 \\ 3 & 0 & -1 & -1 & 1 \end{pmatrix} \end{array} \quad \begin{array}{l} A_1\text{: } x^2 + y^2 + z^2 \\ A_2 \\ E\text{: } 2z^2 - x^2 - y^2,\ x^2 - y^2 \\ T_1\text{: } (R_x, R_y, R_z) \\ T_2\text{: } (x, y, z), (xy, xz, yz) \end{array}$$

$$Td := \begin{pmatrix} 1 \\ 8 \\ 3 \\ 6 \\ 6 \end{pmatrix} \qquad \Gamma_{uma} := \begin{pmatrix} 8 \\ 2 \\ 0 \\ 0 \\ 4 \end{pmatrix} \qquad \Gamma_{bonds} := \begin{pmatrix} 10 \\ 1 \\ 2 \\ 0 \\ 4 \end{pmatrix}$$

$$A_1 := \left(C_{Td}{}^T\right)^{\langle 1 \rangle} \qquad A_2 := \left(C_{Td}{}^T\right)^{\langle 2 \rangle} \qquad E := \left(C_{Td}{}^T\right)^{\langle 3 \rangle} \qquad T_1 := \left(C_{Td}{}^T\right)^{\langle 4 \rangle}$$

$$T_2 := \left(C_{Td}{}^T\right)^{\langle 5 \rangle} \qquad \Gamma_{tot} := \overrightarrow{\left(\Gamma_{uma} \cdot T_2\right)} \qquad h := \sum Td \qquad \Gamma_{tot}{}^T = \begin{pmatrix} 24 & 0 & 0 & 0 & 4 \end{pmatrix}$$

$$i := 1 .. 5$$

$$\Gamma_{vib} := \Gamma_{tot} - T_1 - T_2 \qquad Vib_i := \frac{\sum \overrightarrow{\left[Td \cdot \left(C_{Td}{}^T\right)^{\langle i \rangle} \cdot \Gamma_{vib}\right]}}{h} \qquad Vib = \begin{pmatrix} 2 \\ 0 \\ 2 \\ 1 \\ 3 \end{pmatrix} \quad \begin{array}{l} A_1\text{: } x^2 + y^2 + z^2 \\ A_2 \\ E\text{: } 2z^2 - x^2 - y^2,\ x^2 - y^2 \\ T_1\text{: } (R_x, R_y, R_z) \\ T_2\text{: } (x, y, z), (xy, xz, yz) \end{array}$$

$$\Gamma_{stretch} := \Gamma_{bonds} \qquad Stretch_i := \frac{\sum \overrightarrow{\left[Td \cdot \left(C_{Td}{}^T\right)^{\langle i \rangle} \cdot \Gamma_{stretch}\right]}}{h} \qquad Stretch = \begin{pmatrix} 2 \\ 0 \\ 1 \\ 0 \\ 2 \end{pmatrix} \quad \begin{array}{l} A_1\text{: } x^2 + y^2 + z^2 \\ A_2 \\ E\text{: } 2z^2 - x^2 - y^2,\ x^2 - y^2 \\ T_1\text{: } (R_x, R_y, R_z) \\ T_2\text{: } (x, y, z), (xy, xz, yz) \end{array}$$

$$\Gamma_{bend} := \Gamma_{vib} - \Gamma_{stretch} \qquad Bend_i := \frac{\sum \overrightarrow{\left[Td \cdot \left(C_{Td}{}^T\right)^{\langle i \rangle} \cdot \Gamma_{bend}\right]}}{h} \qquad Bend = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \\ 1 \end{pmatrix} \quad \begin{array}{l} A_1\text{: } x^2 + y^2 + z^2 \\ A_2 \\ E\text{: } 2z^2 - x^2 - y^2,\ x^2 - y^2 \\ T_1\text{: } (R_x, R_y, R_z) \\ T_2\text{: } (x, y, z), (xy, xz, yz) \end{array}$$

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.