

Symmetry Analysis for Tetrahedrane

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

$C_{Td} := \begin{pmatrix} E & C_3 & C_2 & S_4 & \sigma \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & -1 \\ 2 & -1 & 2 & 0 & 0 \\ 3 & 0 & -1 & 1 & -1 \\ 3 & 0 & -1 & -1 & 1 \end{pmatrix}$	$A_1: x^2 + y^2 + z^2$ A_2 $E: 2z^2 - x^2 - y^2, x^2 - y^2$ $T_1: (R_x, R_y, R_z)$ $T_2: (x, y, z), (xy, xz, yz)$	$Td := \begin{pmatrix} 1 \\ 8 \\ 3 \\ 6 \\ 6 \end{pmatrix}$	$\Gamma_{uma} := \begin{pmatrix} 8 \\ 2 \\ 0 \\ 0 \\ 4 \end{pmatrix}$	$\Gamma_{bonds} := \begin{pmatrix} 10 \\ 1 \\ 2 \\ 0 \\ 4 \end{pmatrix}$
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$A_1 := (C_{Td} T)^{\langle 1 \rangle}$	$A_2 := (C_{Td} T)^{\langle 2 \rangle}$	$E := (C_{Td} T)^{\langle 3 \rangle}$	$T_1 := (C_{Td} T)^{\langle 4 \rangle}$
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$T_2 := (C_{Td} T)^{\langle 5 \rangle}$	$\Gamma_{tot} := \overrightarrow{(\Gamma_{uma} \cdot T_2)}$	$h := \sum Td$	$\Gamma_{tot}^T = (24 \ 0 \ 0 \ 0 \ 4)$
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$i := 1..5$

$\Gamma_{vib} := \Gamma_{tot} - T_1 - T_2$	$Vib_i := \frac{\sum [Td \cdot (C_{Td} T)^{\langle i \rangle} \cdot \Gamma_{vib}]}{h}$	$Vib = \begin{pmatrix} 2 \\ 0 \\ 2 \\ 1 \\ 3 \end{pmatrix}$	$A_1: x^2 + y^2 + z^2$ A_2 $E: 2z^2 - x^2 - y^2, x^2 - y^2$ $T_1: (R_x, R_y, R_z)$ $T_2: (x, y, z), (xy, xz, yz)$
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$\Gamma_{stretch} := \Gamma_{bonds}$	$Stretch_i := \frac{\sum [Td \cdot (C_{Td} T)^{\langle i \rangle} \cdot \Gamma_{stretch}]}{h}$	$Stretch = \begin{pmatrix} 2 \\ 0 \\ 1 \\ 0 \\ 2 \end{pmatrix}$	$A_1: x^2 + y^2 + z^2$ A_2 $E: 2z^2 - x^2 - y^2, x^2 - y^2$ $T_1: (R_x, R_y, R_z)$ $T_2: (x, y, z), (xy, xz, yz)$
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$\Gamma_{bend} := \Gamma_{vib} - \Gamma_{stretch}$	$Bend_i := \frac{\sum [Td \cdot (C_{Td} T)^{\langle i \rangle} \cdot \Gamma_{bend}]}{h}$	$Bend = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \\ 1 \end{pmatrix}$	$A_1: x^2 + y^2 + z^2$ A_2 $E: 2z^2 - x^2 - y^2, x^2 - y^2$ $T_1: (R_x, R_y, R_z)$ $T_2: (x, y, z), (xy, xz, yz)$
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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.