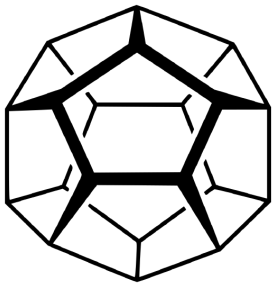
6.2: Dodecahedrane

When Paquette's group synthesized dodecahedrane, $C_{20}H_{20}$, they measured its infrared and Raman spectra (JACS 1983, 105, 5446-5450).



Dodecahedrane: (Public Domain; Yikrazuul).

They found three IR active bands at 2945, 1298, and 728 cm^{-1} and eight Raman frequencies at 2924, 2938, 1324, 1164, 1092, 840, 676, and 480 cm^{-1}. Use group theory to show that these data are consistent with the fact that dodecahedrane has icosahedral symmetry.

$$\begin{array}{cc} E & C_5 \quad C_5^2 \quad C_3 \quad C_2 \quad i \quad S_{10} \quad S_{10}^3 \quad S_6 \quad \sigma \\ \mathrm{CIh} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 3 & \frac{1+\sqrt{5}}{2} & \frac{1-\sqrt{5}}{2} & 0 & -1 & 3 & \frac{1-\sqrt{5}}{2} & \frac{1+\sqrt{5}}{2} & 0 & -1 \\ 3 & \frac{1-\sqrt{5}}{2} & \frac{1+\sqrt{5}}{2} & 0 & -1 & 3 & \frac{1+\sqrt{5}}{2} & \frac{1-\sqrt{5}}{2} & 0 & -1 \\ 4 & -1 & -1 & 1 & 0 & 4 & -1 & -1 & 1 & 0 \\ 5 & 0 & 0 & -1 & 1 & 5 & 0 & 0 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 \\ 3 & \frac{1+\sqrt{5}}{2} & \frac{1-\sqrt{5}}{2} & 0 & -1 & -3 & \frac{1-\sqrt{5}}{2} & \frac{1+\sqrt{5}}{2} & 0 & 1 \\ 3 & \frac{1-\sqrt{5}}{2} & \frac{1+\sqrt{5}}{2} & 0 & -1 & -3 & -\frac{1-\sqrt{5}}{2} & -\frac{1+\sqrt{5}}{2} & 0 & 1 \\ 4 & -1 & -1 & 1 & - & -4 & 1 & 1 & -1 & 0 \\ 5 & 0 & 0 & -1 & 1 & -5 & 0 & 0 & 1 & -1 \end{bmatrix} & \begin{array}{l} Ag : x^2+y^2+z^2 \\ \mathrm{T1g: Rx, Ry, Rz} \\ \mathrm{T2g} \\ \mathrm{Gg} \\ \mathrm{Hg:}\ 2z^2-x^2-y^2,\ x^2-y^2, xy, yz, xz \\ \mathrm{Au} \\ \mathrm{T1u: x, y, z} \\ \mathrm{T2u} \\ \mathrm{Gu} \\ \mathrm{Hu} \end{array} \end{array}$$

$$\mathrm{Ih} = (1 \quad 12 \quad 12 \quad 20 \quad 15 \quad 1 \quad 12 \quad 12 \quad 20 \quad 15) \quad \mathrm{Ih} = \mathrm{Ih}^T \quad \Gamma\mathrm{uma} = (40 \quad 0 \quad 0 \quad 4 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 8) \quad \Gamma\mathrm{uma} = \Gamma\mathrm{uma}^T$$

$$\mathrm{Ag} = (\mathrm{CIh}^T)^{<1>} \quad \mathrm{T1g} = (\mathrm{CIh}^T)^{<2>} \quad \mathrm{T2g} = (\mathrm{CIh}^T)^{<3>} \quad \mathrm{Gg} = (\mathrm{CIh}^T)^{<4>} \quad \mathrm{Hg} = (\mathrm{CIh}^T)^{<5>}$$
$$\mathrm{Au} = (\mathrm{CIh}^T)^{<6>} \quad \mathrm{T1u} = (\mathrm{CIh}^T)^{<7>} \quad \mathrm{T2u} = (\mathrm{CIh}^T)^{<8>} \quad \mathrm{Gu} = (\mathrm{CIh}^T)^{<9>} \quad \mathrm{Hu} = (\mathrm{CIh}^T)^{<10>}$$

$$h = \sum Ih \quad h = 120 \quad \Gamma_{tot} = \overrightarrow{(\Gamma T1u)} \quad \Gamma_{vib} = \Gamma_{tot} - T1g - T1u \quad \Gamma_{bend} = \Gamma_{vib} - \Gamma_{stretch} \quad i = 1..10$$

$$\mathrm{Vib}_i = \frac{\overrightarrow{[\mathrm{Ih}(\mathrm{CIh}^T)^{<i>}\,\Gamma\mathrm{vib}]}}{h} \quad \mathrm{Stretch}_i = \frac{\overrightarrow{[\mathrm{Ih}(\mathrm{CIh}^T)^{<i>}\,\Gamma\mathrm{stretch}]}}{h} \quad \mathrm{Bend}_i = \frac{\overrightarrow{[\mathrm{Ih}(\mathrm{CIh}^T)^{<i>}\,\Gamma\mathrm{bend}]}}{h}$$

$$\mathrm{Vib} = \begin{bmatrix} 2 \\ 1 \\ 2 \\ 4 \\ 6 \\ 0 \\ 3 \\ 4 \\ 4 \\ 4 \end{bmatrix} \begin{array}{l} Ag : x^2+y^2+z^2 \\ \mathrm{T1g: Rx, Ry, Rz} \\ \mathrm{T2g} \\ \mathrm{Gg} \\ \mathrm{Hg:}\ 2z^2-x^2-y^2,\ x^2-y^2, xy, yz, xz \\ \mathrm{Au} \\ \mathrm{T1u: x, y, z} \\ \mathrm{T2u} \\ \mathrm{Gu} \\ \mathrm{Hu} \end{array} \qquad \mathrm{Stretch} = \begin{bmatrix} 2 \\ 0 \\ 0 \\ 2 \\ 3 \\ 0 \\ 2 \\ 2 \\ 2 \\ 1 \end{bmatrix} \begin{array}{l} Ag : x^2+y^2+z^2 \\ \mathrm{T1g: Rx, Ry, Rz} \\ \mathrm{T2g} \\ \mathrm{Gg} \\ \mathrm{Hg:}\ 2z^2-x^2-y^2,\ x^2-y^2, xy, yz, xz \\ \mathrm{Au} \\ \mathrm{T1u: x, y, z} \\ \mathrm{T2u} \\ \mathrm{Gu} \\ \mathrm{Hu} \end{array}$$

$$\text{Bend} = \begin{bmatrix} 0 & Ag: x^2+y^2+z^2 \\ 1 & \text{T1g: Rx, Ry, Rz} \\ 2 & \text{T2g} \\ 2 & \text{Gg} \\ 3 & \text{Hg: } 2z^2-x^2-y^2,\ x^2-y^2, xy, yz, xz \\ 0 & \text{Au} \\ 1 & \text{T1u: x, y, z} \\ 2 & \text{T2u} \\ 2 & \text{Gu} \\ 3 & \text{Hu} \end{bmatrix}$$

According to the usual selection rules only the three T_{1u} vibrations are IR active. The A_g and H_g vibrations are Raman active giving a total of eigth frequencies in the Raman spectra. This analysis is in agreement with the experimental spectroscopic results quoted by Paquette. Note also that, as is usual for molecules with a center of inversion, there are no coincidences between the IR and Raman active modes.

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