6.5.1: Buckminsterfulerene

C_{60} Has Icosahedral Symmetry

Buckminsterfulerene has four IR active vibrational modes (528, 577, 1180, 1430 cm^{-1}) and ten Raman active modes (273, 436, 496, 710, 773, 110, 1250, 1435, 1470, 1570 cm^{-1}). Demonstrate that the assumption of icosahedral symmetry for C_{60} is consistent with this data.

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

$$\mathrm{Ih:} \begin{pmatrix} 1 & 12 & 12 & 20 & 15 & 1 & 12 & 12 & 20 & 15 \end{pmatrix} \quad \mathrm{Ih} = \mathrm{Ih}^T \quad \Gamma_{uma} = \begin{pmatrix} 60 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 \end{pmatrix} \quad \Gamma_{uma} = \Gamma_{uma}^T$$

$$\Gamma_{bonds} = \begin{pmatrix} 90 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 8 \end{pmatrix} \quad \Gamma_{bonds} = \Gamma_{bonds}^T \quad \Gamma_{stretch} = \Gamma_{bonds}$$

$$\mathrm{Ag} = (\mathrm{CIh}^T)^{<1>} \quad \mathrm{T}_{1g} = (\mathrm{CIh}^T)^{<2>} \quad \mathrm{T}_{2g} = (\mathrm{CIh}^T)^{<3>} \quad \mathrm{G}_g = (\mathrm{CIh}^T)^{<4>} \quad \mathrm{H}_g = (\mathrm{CIh}^T)^{<5>}$$

$$\mathrm{A}_u = (\mathrm{CIh}^T)^{<6>} \quad \mathrm{T}_{1u} = (\mathrm{CIh}^T)^{<7>} \quad \mathrm{A}_u = (\mathrm{CIh}^T)^{<8>} \quad \mathrm{G}_u = (\mathrm{CIh}^T)^{<9>} \quad \mathrm{H}_u = (\mathrm{CIh}^T)^{<10>}$$

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

$$\mathrm{Vib}_i = \frac{\sum \overrightarrow{[\mathrm{Ih}(\mathrm{CIh}^T)^{<i>}\Gamma_{vib}]}}{h} \qquad \mathrm{Vib} = \begin{bmatrix} 2 \\ 3 \\ 4 \\ 6 \\ 8 \\ 1 \\ 4 \\ 5 \\ 6 \\ 7 \end{bmatrix} \quad \begin{array}{l} Ag: x^2+y^2+z^2 \\ \mathrm{Eg:}\ 2z^2-x^2-y^2, x^2-y^2 \\ \mathrm{T1g:\ Rx, Ry, Rz} \\ \mathrm{T2g} \\ \mathrm{Gg} \\ \mathrm{Hg:}\ 2z^2-x^2-y^2,\ x^2-y^2,\ xy,\ yz,\ xz \\ \mathrm{Au} \\ \mathrm{T1u:\ x, y, z} \\ \mathrm{T2u} \\ \mathrm{Gu} \\ \mathrm{Hu} \end{array}$$

The 4 T_{1u} modes are IR active and the 2 A_g and 8 H_g modes are Raman active. Also there are no coincidences. Thus the assumption of icosahedral symmetry is consistent with the spectroscopic data.