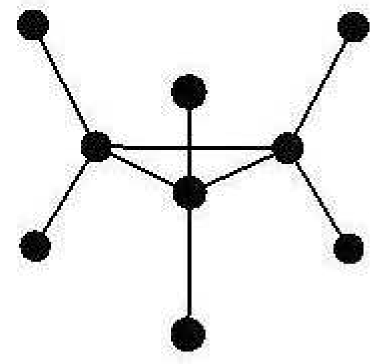
D_{3h} Symmetry - C_3H_6

The following IR and Raman spectroscopic data is available for cyclopropane, C_3H_6. Demonstrate that this data is consistent with a D_{3h} symmetry assignment for cyclopropane.



Frequency	3038	1479	1188	3025	1438	1029	866	3103	854	3082	1188	734
Activity	R	R	R	R, IR	R, IR	R, IR	R, IR	IR	IR	R	R	R
Type	▪	▪	▪	▪	▪	▪	▪	▪	▪	▪	▪	▪
Symmetry	▪	▪	▪	▪	▪	▪	▪	▪	▪	▪	▪	▪

$$\begin{array}{cccccc} E & C_3 & C_2 & \sigma_h & S_3 & \sigma_v \end{array}$$

$$C_{D3h} := \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & -1 \\ 2 & -1 & 0 & 2 & -1 & 0 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 & 1 \\ 2 & -1 & 0 & -2 & 1 & 0 \end{pmatrix}$$

A1': x² + y², z²
A2': Rz
E': (x,y), (x² - y², xy)
A1":
A2": z
E": (Rx, Ry), (xz, yz)

$$D3h := \begin{pmatrix} 1 \\ 2 \\ 3 \\ 1 \\ 2 \\ 3 \end{pmatrix} \qquad \Gamma_{uma} := \begin{pmatrix} 9 \\ 0 \\ 1 \\ 3 \\ 0 \\ 3 \end{pmatrix} \qquad \Gamma_{bonds} := \begin{pmatrix} 9 \\ 0 \\ 1 \\ 3 \\ 0 \\ 3 \end{pmatrix}$$

$$A_1 := \left(C_{D3h}{}^T\right)^{\langle 1 \rangle} \qquad A_2 := \left(C_{D3h}{}^T\right)^{\langle 2 \rangle} \qquad E := \left(C_{D3h}{}^T\right)^{\langle 3 \rangle} \qquad A_{11} := \left(C_{D3h}{}^T\right)^{\langle 4 \rangle}$$

$$A_{21} := \left(C_{D3h}{}^T\right)^{\langle 5 \rangle} \qquad E_1 := \left(C_{D3h}{}^T\right)^{\langle 6 \rangle} \qquad h := \sum D3h \qquad \Gamma_{tot} := \overrightarrow{\left[\Gamma_{uma} \cdot (A_{21} + E)\right]}$$

$$\Gamma_{tot}{}^T = (27 \;\; 0 \;\; -1 \;\; 3 \;\; 0 \;\; 3) \qquad \Gamma_{vib} := \Gamma_{tot} - A_2 - E - A_{21} - E_1 \qquad i := 1..6$$

$$\Gamma_{stretch} := \Gamma_{bonds} \qquad \Gamma_{bend} := \Gamma_{vib} - \Gamma_{stretch}$$

$$Vib_i := \frac{\sum \overrightarrow{\left[D3h \cdot \left(C_{D3h}{}^T\right)^{\langle i \rangle} \cdot \Gamma_{vib}\right]}}{h} \qquad Stretch_i := \frac{\sum \overrightarrow{\left[D3h \cdot \left(C_{D3h}{}^T\right)^{\langle i \rangle} \cdot \Gamma_{stretch}\right]}}{h} \qquad Bend_i := \frac{\sum \overrightarrow{\left[D3h \cdot \left(C_{D3h}{}^T\right)^{\langle i \rangle} \cdot \Gamma_{bend}\right]}}{h}$$

$$\text{Vib} = \begin{pmatrix} 3 \\ 1 \\ 4 \\ 1 \\ 2 \\ 3 \end{pmatrix} \quad \begin{array}{l} \text{A1}'\text{:}\ \ x^2 + y^2, z^2 \\ \text{A2}'\text{:}\ \ Rz \\ \text{E}'\text{:}\ \ (x,y), (x^2 - y^2, xy) \\ \text{A1}''\text{:} \\ \text{A2}''\text{:}\ \ z \\ \text{E}''\text{:}\ \ (Rx, Ry), (xz, yz) \end{array}$$

$$\text{Stretch} = \begin{pmatrix} 2 \\ 0 \\ 2 \\ 0 \\ 1 \\ 1 \end{pmatrix} \quad \begin{array}{l} \text{A1}'\text{:}\ \ x^2 + y^2, z^2 \\ \text{A2}'\text{:}\ \ Rz \\ \text{E}'\text{:}\ \ (x,y), (x^2 - y^2, xy) \\ \text{A1}''\text{:} \\ \text{A2}''\text{:}\ \ z \\ \text{E}''\text{:}\ \ (Rx, Ry), (xz, yz) \end{array}$$

$$\text{Bend} = \begin{pmatrix} 1 \\ 1 \\ 2 \\ 1 \\ 1 \\ 2 \end{pmatrix} \quad \begin{array}{l} \text{A1}'\text{:}\ \ x^2 + y^2, z^2 \\ \text{A2}'\text{:}\ \ Rz \\ \text{E}'\text{:}\ \ (x,y), (x^2 - y^2, xy) \\ \text{A1}''\text{:} \\ \text{A2}''\text{:}\ \ z \\ \text{E}''\text{:}\ \ (Rx, Ry), (xz, yz) \end{array}$$

Frequency	3038	1479	1188	3025	1438	1029	866	3103	854	3082	1188	734
Activity	R	R	R	R, IR	R, IR	R, IR	R, IR	IR	IR	R	R	R
Type	S	S	B	S	S	B	B	S	B	S	B	B
Symmetry	A1'	A1'	A1'	E'	E'	E'	E'	A2"	A2"	E"	E"	E"

There are 9 Raman active modes, 2 IR active modes, 8 IR/Raman active, and 2 modes that are neither Raman or IR active. This gives a total of 21 vibrational modes which is consistent with the total degrees of freedom (27=3x9) minus 6 for translation and rotation.