C_{60} Has Icosahedral Symmetry

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

CIh :=

E	C_5	C_5^2	C_3	C_2	i	S_{10}	S_{10}^3	S_6	σ	
1	1	1	1	1	1	1	1	1	1	Ag: $x^2 + y^2 + z^2$
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	T1g: Rx, Ry, Rz
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	T2g
4	-1	-1	1	0	4	-1	-1	1	0	Gg
5	0	0	-1	1	5	0	0	-1	1	Hg: $2z^2 - x^2 - y^2$, $x^2 - y^2$, xy, yz, xz
1	1	1	1	1	-1	-1	-1	-1	-1	Au
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	T1u: x, y, z
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	T2u
4	-1	-1	1	0	-4	1	1	-1	0	Gu
5	0	0	-1	1	-5	0	0	1	-1	Hu

$Ih := (1\ \ 12\ \ 12\ \ 20\ \ 15\ \ 1\ \ 12\ \ 12\ \ 20\ \ 15)$ $\quad Ih := Ih^T$ $\quad \Gamma uma := (60\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 4)$ $\quad \Gamma uma := \Gamma uma^T$

$\Gamma bonds := (90\ \ 0\ \ 0\ \ 0\ \ 2\ \ 0\ \ 0\ \ 0\ \ 0\ \ 8)$ $\quad \Gamma bonds := \Gamma bonds^T$ $\quad \Gamma stretch := \Gamma bonds$

$Ag := (CIh^T)^{\langle 1\rangle}$ $\quad T1g := (CIh^T)^{\langle 2\rangle}$ $\quad T2g := (CIh^T)^{\langle 3\rangle}$ $\quad Gg := (CIh^T)^{\langle 4\rangle}$ $\quad Hg := (CIh^T)^{\langle 5\rangle}$

$Au := (CIh^T)^{\langle 6\rangle}$ $\quad T1u := (CIh^T)^{\langle 7\rangle}$ $\quad T2u := (CIh^T)^{\langle 8\rangle}$ $\quad Gu := (CIh^T)^{\langle 9\rangle}$ $\quad Hu := (CIh^T)^{\langle 10\rangle}$

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

$$Vib_i := \frac{\sum \overrightarrow{\left[Ih \cdot (CIh^T)^{\langle i\rangle} \cdot \Gamma vib\right]}}{h}$$

Vib =

Vib	
2	Ag: $x^2 + y^2 + z^2$
3	T1g: Rx, Ry, Rz
4	T2g
6	Gg
8	Hg: $2z^2 - x^2 - y^2$, $x^2 - y^2$, xy, yz, xz
1	Au
4	T1u: x, y, z
5	T2u
6	Gu
7	Hu

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.