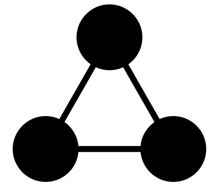
Physics 745 - Group Theory

Solution Set 16



Under each symmetry element we are considering, we need only consider which atoms go to themselves, and then for those atoms, take the trace of the corresponding matrix element. For E, of course, that trace is 9. Under C_3 and S_3, no atom maps to itself, so the trace is 0 in both cases. Under C_2', one atom maps to itself, and the rotation reverses two of the components while leaving the third unchanged, so it has trace -1. Under σ_h, all the atoms map to themselves, and z is reversed while the other two components remain unchanged, so the trace is 3. Under σ_v, one atom maps to itself, and it reverses only one coordinate, so its trace is 1.

D_{3h}	E	$2C_3$	$3C_2'$	σ_h	$2S_3$	$3\sigma_v$
A_1'	1	1	1	1	1	1
A_2'	1	1	-1	1	1	-1
A_1''	1	1	1	-1	-1	-1
A_2''	1	1	-1	-1	-1	1
E	2	-1	0	2	-1	0
E'	2	-1	0	-2	1	0
Γ	9	0	-1	3	0	1

It isn't that hard to complete the computation by the conventional rules. The number of copies of each representation is just:

$$A_1': \quad \tfrac{1}{12}\left(1\cdot 9+3\cdot 1\cdot(-1)+1\cdot 3+3\cdot 1\cdot 1\right)=1$$

$$A_2': \quad \tfrac{1}{12}\left(1\cdot 9+3\cdot(-1)\cdot(-1)+1\cdot 3+3\cdot(-1)\cdot 1\right)=1$$

$$A_1'': \quad \tfrac{1}{12}\left(1\cdot 9+3\cdot 1\cdot(-1)+(-1)\cdot 3+3\cdot(-1)\cdot 1\right)=0$$

$$A_2'': \quad \tfrac{1}{12}\left(1\cdot 9+3\cdot(-1)\cdot(-1)+(-1)\cdot 3+3\cdot 1\cdot 1\right)=1$$

$$E: \quad \tfrac{1}{12}\left(2\cdot 9+2\cdot 3\right)=2$$

$$E': \quad \tfrac{1}{12}\left(2\cdot 9+(-2)\cdot 3\right)=1$$

We therefore have

$$\Gamma = A_1' \oplus A_2' \oplus A_2'' \oplus 2E \oplus E'$$

As a check, we note that this has total dimension nine, as it should. According to Tinkham, the rotations and translations correspond to $A_2' \oplus A_2'' \oplus E \oplus E'$. If we "subtract" this from above, we are left with $\Gamma = A_1' \oplus E$, corresponding to the three true vibrational modes.

Incidentally, according to

http://arxiv.org/ftp/arxiv/papers/0811/0811.4320.pdf

this configuration of carbon atoms is stable, though not the most stable configuration for three atoms.