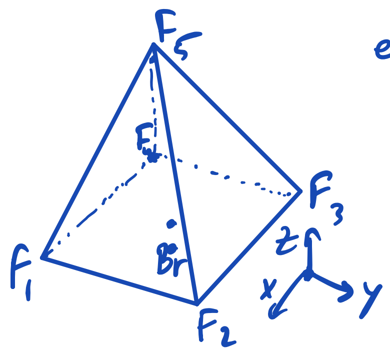
Answer model exam Symmetry in Physics of April 2, 2024

1 a)



effectively the molecule forms a pyramid, even though Br is below the base

Symmetries: 4 rotations around the F_5 - Br axis
$0°, 90°, 180°, 270°$
e, c, c^2, c^3

& 4 reflections: in the x-z & y-z plane
$\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad = b \quad\quad = bc^2$

and in the F_1-F_3-F_5 plane $= bc$
" $\quad$ F_2-F_4-F_5 plane $= bc^3$

forming gp called C_{4v} ($\cong D_4$)

Conjugacy classes: $(e) = \{e\}$
$(c) = \{c, c^3\}$ same angle & related by reflection
$(c^2) = \{c^2\}$
$(b) = \{b, bc^2\}$ related by $90°$ rotation
$(bc) = \{bc, bc^3\}$ "
related by $45°$, not in the gp

1 b)

	(e)	(c)	(c^2)	(b)	(bc)
$\chi^{(1)}$	1	1	1	1	1
$\chi^{(2)}$	1	1	1	-1	-1
$\chi^{(3)}$	1	-1	1	1	-1
$\chi^{(4)}$	1	-1	1	-1	1
$\chi^{(5)}$	2	a	b	c	d

$\Sigma n_\mu^2 = 8$ gives the 2 in the (e) column

fix by $\perp$: $a = c = d = 0$ & $b = -2$

$\leftrightarrow$ 1D irreps $\chi(c)^4 = 1$

$\chi(b)^2 = 1 = \chi(bc)^2$

$\underbrace{\chi(b)}_{\pm 1}\,\chi(c) = \underbrace{\chi(bc)}_{\pm 1}$

$\Rightarrow \chi(c) = \pm 1$

4 options

1 c) $\chi^v(\theta) = 1 + 2\cos\theta$ for rotations

$\chi^v(b)$: $D^v(b) = \begin{pmatrix} 1 & & \\ & -1 & \\ & & 1 \end{pmatrix} \to \chi^v(b) = 1$

$$D^V(bc) = D^V(b)\,D^V(c) \Rightarrow \chi^V(bc) = 1$$

$$\chi^V = (3, 1, -1, 1, 1) \qquad \begin{pmatrix} 1 & & \\ & -1 & \\ & & 1 \end{pmatrix}\begin{pmatrix} c\theta & & \\ & c\theta & \\ & & 1 \end{pmatrix}$$

$$\langle \chi^{(1)}, \chi^V \rangle = \frac{1}{8}(3 + 1\cdot 2 - 1 + 2\cdot 1 + 2\cdot 1) = 1$$

yes, BrF_5 allows for an EDM.

2a) $\sigma_{ij} = \varepsilon_0 E_i E_j - \frac{1}{2}\varepsilon_0 \vec{E}^2 \delta_{ij}$ is symmetric but not traceless.

isolate trace: $\delta_{ij}\sigma_{ij} = \varepsilon_0 \vec{E}^2 - \frac{3}{2}\varepsilon_0 \vec{E}^2 = -\frac{1}{2}\varepsilon_0 \vec{E}^2$

$$\sigma_{ij} = \underbrace{\left[\sigma_{ij} - \frac{\delta_{ij}\sigma_{kk}}{3}\right]}_{\text{symm traceless part}} + \underbrace{\delta_{ij}\frac{\sigma_{kk}}{3}}_{\text{invariant}} = \left[\varepsilon_0 E_i E_j - \frac{1}{3}\varepsilon_0 \vec{E}^2 \delta_{ij}\right] - \frac{1}{6}\varepsilon_0 \vec{E}^2 \delta_{ij}$$

5 indep comp so $D^{(2)}$ irrep of $SO(3)$

trivial rep $D^{(0)}$ of $SO(3)$

2b) rank 2 tensors transform like: $\sigma' = D^V \sigma (D^V)^{-1}$

invariant tensors have $\sigma' = \sigma \Rightarrow \sigma D^V = D^V \sigma$

or $[D^V, \sigma] = 0$

since D^V is an irrep, by Schur's lemma: $\sigma \propto \mathbb{1}$

2c) reflection in origin P: $\vec{E} \xrightarrow{P} -\vec{E}$ or $E_i \xrightarrow{P} -E_i$

Hence $\sigma_{ij} \xrightarrow{P} \sigma_{ij}$ invariant

Similarly for $\vec{E} \to \vec{B}$ case: $\vec{B} \xrightarrow{P} \vec{B}$ hence σ_{ij} invar.

3a) $L_z|2,m\rangle$: $\hbar\begin{pmatrix} 2 & & & & \\ & 1 & & & \\ & & 0 & & \\ & & & -1 & \\ & & & & -2 \end{pmatrix}$

3b) $D^{(2)}(R_z) = \langle 2\, m \,|\, U(R_z) \,|\, 2\, m' \rangle$

$$= \langle 2\, m \,|\, \exp\left(-\frac{i}{\hbar}\theta L_z\right) \,|\, 2\, m' \rangle$$

$$= \underbrace{\langle 2m | 2m' \rangle}_{\delta_{mm'}} e^{-i\theta m'} = \begin{pmatrix} e^{-2i\theta} & & & & 0 \\ & e^{i\theta} & & & \\ & & 1 & & \\ & & & e^{i\theta} & \\ 0 & & & & e^{i2\theta} \end{pmatrix}$$

3c) $D^{(2)}(R_z)$ is obviously fully reducible

on diagonal are the 1D complex irreps:

$e^{\pm i2\theta}$, $e^{\pm i\theta}$, 1

D.Boer, 28-3-2024