Solutions for problem set 11

Problem 1. Crystal field splitting *Here is the example of the proper group table (i.e., no inversions) for a equilateral triangular pyramid (i.e, the basis is an equilateral triangle, but the height is arbitrary, such that the result is not tetrahedral) – which is actually the same as the group for even permutations of 3 elements.*

	E	C_3	C_3^2
$\Gamma^{(1)}$	*1*	*1*	*1*
$\Gamma^{(2)}$	*1*	$e^{i\frac{2\pi}{3}}$	$e^{i\frac{4\pi}{3}}$
$\Gamma^{(3)}$	*1*	$e^{i\frac{4\pi}{3}}$	$e^{i\frac{2\pi}{3}}$

a) Make a group table for SO(3) and for the proper tetrahedral group T.

b) Use the orthogonality relation of the characters to find into which irreducible representations (i) the $D^{(\ell)}$ for $\ell = 0, 1, 2, 3$ split if the symmetry is lowered to T, and (i) into which irreducible representation the elements of T split if the symmetry is lowered to that of an equilateral triangular pyramid. Hint: Start with $D^{(\ell)} = \sum_i a_i \Gamma^{(i)}$.

c) Why is part (b) important for diamond color centers?

Solution

Problem 2. Selection rules *Give a group theory argument along the lines of (see class)*

$$\left\langle \phi^{(\nu)} \middle| V \middle| \phi^{(\mu)} \right\rangle = 0 \quad \text{iff} \quad \mathrm{a}_{\mathrm{V},\nu\mu} = 0$$

to explain which transitions between $ns_{1/2}$ and $(n+1)p_{3/2}$ of hydrogen are allowed electric and magnetic dipole transitions, and how this changes if you put the H atom into a diamond lattice without and with a strong electric field. Hint: For the first part, use the fact that $V_{\mathrm{el}} = -e\vec{r} \cdot \vec{E}$ and $V_{\mathrm{mgn}} = -\mu\vec{j} \cdot \vec{B}$, where $\vec{j}$ is any angular momentum vector.

Solution