Solution Set 11

First we need the character table for O_h , which is easily determined from the character table for O and that for the inversion group J. They are in the table below.

J	E	J
Γ^+	1	1
Γ	1	-1

Next we need to work out the characters for the l =6 representation of the rotation group. We will assume that under parity, we are working with a system where the wave function goes like $(-1)^{l} = +1$, so that makes that part of the problem easy. The character of E is the

\mathcal{O}_{h}	E	8C ₃	$3C_4^2$	6C ₂	6C4	J	8S ₆	3σ	$6\sigma_d$	6S4
A_1^+	1	1	1	1	1	1	1	1	1	1
A_2^+	1	1	1	-1	-1	1	1	1	-1	-1
E^+	2	-1	2	0	0	2	-1	2	0	0
T_{1}^{+}	3	0	-1	-1	1	3	0	-1	-1	1
T_2^+	3	0	-1	1	-1	3	0	-1	1	-1
A_1	1	1	1	1	1	-1	-1	-1	-1	-1
A_2	1	1	1	-1	-1	-1	-1	-1	1	1
E	2	-1	2	0	0	-2	1	-2	0	0
T_1	3	0	-1	-1	1	-3	0	1	1	-1
T_2	3	0	-1	1	-1	-3	0	1	-1	1
Γ_6	13	1	1	1	-1	13	1	1	1	-1

dimensionality of the representation, which is 13. For the others, we use the formula

$$\chi(\alpha) = \frac{\sin\left\lfloor \left(l + \frac{1}{2}\right)\alpha\right\rfloor}{\sin\left\lfloor \frac{1}{2}\alpha\right\rfloor}$$

The results are included in the table, and then just copied for the improper rotations. Noting that the second half always matches the first, we need only look at the + representations, which means we can focus just on *O*, the first twenty-four elements. Using orthogonality, it's easy to see that the number of copies of A_1 and A_2 is (13*1+8+3+6-6)/24 = 1. The number of copies of T_1 is (13*3-3-6-6)/24 = 1, and of T_2 is (13*3-3+6+6)/24 = 2. Finally, there is (13*2-8+3*2)/24 = 1 copy of *E*. So in summary,

$$\Gamma_6 = A_1^+ \oplus A_2^+ \oplus E^+ \oplus T_1^+ \oplus 2T_2^+$$