

Exercise 7.1

Given the characters χ of a reducible representation Γ of the indicated point group \mathcal{G} for the various classes of \mathcal{G} in the order in which these classes appear in the character table, find the number of times irreducible representation occurs in Γ .

- (a) \mathcal{C}_{2v} $\chi = 4, -2, 0, -2$,
 (b) \mathcal{C}_{3h} $\chi = 4, 1, 1, 2, -1, -1$,
 (c) \mathcal{D}_{4d} $\chi = 6, 0, -2, 0, -2, 0, 0$,
 (d) \mathcal{O}_h $\chi = 15, 0, -1, 1, 1, -3, 0, 5, -1, 3$.

Solution 7.1

- (a) 1

\mathcal{C}_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

- (b) 2

\mathcal{C}_{3h}	E	C_3	C_3^2	σ_h	S_3	S_3^5
A'	1	1	1	1	1	1
E'	1	ε	ε^*	1	ε	ε^*
	1	ε^*	ε	1	ε^*	ε
A''	1	1	1	-1	-1	-1
E''	1	ε	ε^*	-1	$-\varepsilon$	$-\varepsilon^*$
	1	ε^*	ε	-1	$-\varepsilon^*$	$-\varepsilon$

- (c) 3

\mathcal{D}_{4d}	E	$2S_8$	$2C_4$	$2S_8^3$	C_2	$4C_2'$	$4\sigma_d$
A_1	1	1	1	1	1	1	1
A_2	1	1	1	1	1	-1	-1
B_1	1	-1	1	-1	1	1	-1
B_2	1	-1	1	-1	1	-1	1
E_1	2	$\sqrt{2}$	0	$-\sqrt{2}$	-2	0	0
E_2	2	0	-2	0	2	0	0
E_3	2	$-\sqrt{2}$	0	$\sqrt{2}$	-2	0	0

- (d) 4

\mathcal{O}_h	E	$8C_3$	$3C_2$	$6C_4$	$6C_2'$	i	$8S_6$	$3\sigma_h$	$6S_4$	$6\sigma_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1
E_g	2	-1	2	0	0	2	-1	2	0	0
T_{1g}	3	0	-1	1	-1	3	0	-1	1	-1
T_{2g}	3	0	-1	-1	1	3	0	-1	-1	1
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1
E_g	2	-1	2	0	0	-2	1	-2	0	0
T_{1u}	3	0	-1	1	-1	-3	0	1	-1	1
T_{2u}	3	0	-1	-1	1	-3	0	1	1	-1

Exercise 7.2

Consider the four functions of Problem 5.2 which form a basis for a reducible representation Γ of \mathcal{D}_4 . Using projection operators find the orthonormal basis functions which reduce Γ . Assume $(f_i, f_j) = \delta_{ij}$.

Solution 7.2

Table 7.1: The character table for the \mathcal{D}_4 point group.

\mathcal{D}_4	E	$2C_4$	C_2	$2C_2'$	$2C_2''$
A_1	1	1	1	1	1
A_1	1	1	1	-1	-1
B_1	1	-1	1	1	-1
B_2	1	-1	1	-1	1
E	2	0	-2	0	0

Exercise 7.3

Show that the characters of \mathcal{C}_{4v} obey the orthogonality rules of eqns (7.3-5) and (A.7-3.10).

Solution 7.3**Exercise 7.4**

How many times does each irreducible representation of the \mathcal{C}_{2v} point group occur in the nine-dimensional representation found in Problem 5.3?

Solution 7.4**Exercise 7.5**

Consider the group whose group table is

	E	A	B	C
E	E	A	B	C
A	A	C	E	B
B	B	E	C	E
C	C	B	A	A

write out the matrices and characters for the regular representation of this group.

Solution 7.5**Exercise 7.6**

Determine the irreducible representation to which the following real orbitals belong for the indicated point group:

1. p_1, p_2, p_3 in \mathcal{D}_4 and \mathcal{D}_{2h} ,
2. d_1, d_2, d_3, d_4, d_5 in \mathcal{O}_h ,
3. d_1, d_2, d_3, d_4, d_5 in \mathcal{D}_{3h} ,
4. d_1, d_2, d_3, d_4, d_5 in \mathcal{T}_d .

Solution 7.6