Exercise 7.1

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

(a) $\mathscr{C}_{2\mathrm{v}}$ $\chi = 4, -2, 0, -2,$

(b) $\mathscr{C}_{3\mathrm{h}}$ $\chi = 4, 1, 1, 2, -1, -1,$

(c) $\mathscr{D}_{4\mathrm{d}}$ $\chi = 6, 0, -2, 0, -2, 0, 0,$

(d) $\mathscr{O}_{\mathrm{h}}$ $\chi = 15, 0, -1, 1, 1, -3, 0, 5, -1, 3.$

Solution 7.1

(a) 1

Table 7.1: The character table for the $\mathscr{C}_{2\mathrm{v}}$ point group.

$\mathscr{C}_{2\mathrm{v}}$	E	C_2	$\sigma_\mathrm{v}(xz)$	$\sigma_\mathrm{v}(yz)$
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

Table 7.2: The character table for the $\mathscr{C}_{3\mathrm{h}}$ point group.

$\mathscr{C}_{3\mathrm{h}}$	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

Table 7.3: The character table for the $\mathscr{D}_{4\mathrm{d}}$ point group.

$\mathscr{D}_{4\mathrm{d}}$	E	$2S_8$	$2C_4$	$2S_8^3$	C_2	$4C_2'$	$4\sigma_\mathrm{d}$
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

Table 7.4: The character table for the $\mathscr{O}_{\mathrm{h}}$ point group.

$\mathscr{O}_\mathrm{h}$	E	$8C_3$	$3C_2$	$6C_4$	$6C_2'$	i	$8S_6$	$3\sigma_\mathrm{h}$	$6S_4$	$6\sigma_\mathrm{d}$
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 $\mathscr{D}_4$. Using projection operators find the orthonormal basis functions which reduce Γ. Assume $(f_i, f_j) = \delta_{ij}$.

Solution 7.2

Table 7.5: The character table for the $\mathscr{D}_4$ point group.

$\mathscr{D}_4$	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 $\mathscr{C}_{4\mathrm{v}}$ 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 $\mathscr{C}_{2\mathrm{v}}$ point group occur in the nine-dimentional 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 $\mathscr{D}_4$ and $\mathscr{D}_{2\mathrm{h}}$,
2. d_1, d_2, d_3, d_4, d_5 in $\mathscr{O}_\mathrm{h}$,
3. d_1, d_2, d_3, d_4, d_5 in $\mathscr{D}_{3\mathrm{h}}$,
4. d_1, d_2, d_3, d_4, d_5 in $\mathscr{T}_\mathrm{d}$.

Solution 7.6