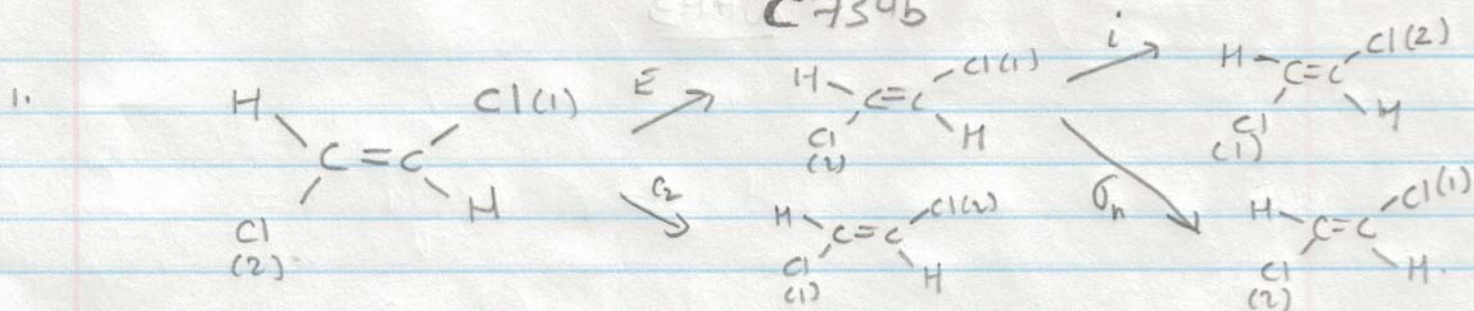


Solutions Problem Set 3 2008-04

CH₂Cl₂ C₂H₂Cl₂



a) $\langle Cl(1) \ Cl(2) | \Gamma(E) = \langle Cl(1) \ Cl(2) |$
 $\therefore \Gamma(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \chi = 2$

$\langle Cl(1) \ Cl(2) | \Gamma(C_2) = \langle Cl(2) \ Cl(1) |$
 $\therefore \Gamma(C_2) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \chi = 0$

$\langle Cl(1) \ Cl(2) | \Gamma(\sigma_v) = \langle Cl(2) \ Cl(1) |$
 $\therefore \Gamma(\sigma_v) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \chi = 0$

$\langle Cl(1) \ Cl(2) | \Gamma(\sigma_h) = \langle Cl(1) \ Cl(2) |$
 $\therefore \Gamma(\sigma_h) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \chi = 2$

if irreducible $\sum_{\Gamma} |\chi(\Gamma)|^2 = h = 4$

but $\sum_{\Gamma} |\chi(\Gamma)|^2 = 4 + 0 + 0 + 4 = 8 > 4 \therefore$ reducible.

b) given $\{1, 1, 1, 1\} \Rightarrow \chi(E)=1, \chi(C_2)=1, \chi(\sigma_v)=1$
 $\therefore [A_g]$

$\{1, -1, -1, 1\} \Rightarrow \chi(E)=1, \chi(C_2)=-1, \chi(\sigma_v)=1 \therefore [B_u]$

$$c) \quad \langle z | \Gamma(E) = +\langle z | \quad \therefore \Gamma(E) = (1) \quad \chi = 1$$

$$\langle z | \Gamma(G_2) = +\langle z | \quad \therefore \Gamma(G_2) = (1) \quad \chi = 1$$

$$\langle z | \Gamma(i) = -\langle z | \quad \therefore \Gamma(i) = (-1) \quad \chi = -1$$

$$\langle z | \Gamma(\sigma_h) = -\langle z | \quad \therefore \Gamma(\sigma_h) = (-1) \quad \chi = -1$$

$$\{1 \quad 1 \quad -1 \quad -1\} \quad \chi(E) = 1, \quad \chi(G_2) = 1 \quad \chi(i) = -1$$

$\therefore \boxed{A_u}$

d) Here we can use orthogonality of IRs

$$\sum_T |\chi_4(T)|^2 = 4$$

$$\text{and } \sum_{IR} l_{IR}^2 = 4 \quad \therefore (1)^2 + (1)^2 + (1)^2 + l_4^2 = 4$$

$$\therefore l_4^2 = 4 - 3 = 1 = 1$$

$$\boxed{l_4 = 1}$$

$$\therefore \chi_4(E) = 1$$

$$\therefore (1)^2 + \chi_4(G_2)^2 + \chi_4(i)^2 + \chi_4(\sigma_h)^2 = 4$$

$$\text{or } \chi_4(G_2)^2 + \chi_4(i)^2 + \chi_4(\sigma_h)^2 = 3 \quad (1)$$

$$\chi_1(E)\chi_4(E) + \chi_4(G_2)(1) + \chi_4(i)(1) + \chi_4(\sigma_h)(1) = 0$$

$$\text{or } \chi_4(G_2) + \chi_4(i) + \chi_4(\sigma_h) = -1 \quad (2)$$

$$\text{Similarly: } \chi_2(E)\chi_4(E) + \chi_4(G_2)(-1) + \chi_4(i)(-1) + \chi_4(\sigma_h)(1) = 0$$

$$\text{or } -\chi_4(G_2) - \chi_4(i) + \chi_4(\sigma_h) = -1 \quad (3)$$

$$\text{add (2) + (3)} \quad 2\chi_4(\sigma_h) = -2 \quad \therefore \chi_4(\sigma_h) = -1$$

$$\text{subtract (2) - (3)} \quad 2\chi_4(G_2) + 2\chi_4(i) = 0$$

$$\therefore \chi_4(i) = -\chi_4(G_2)$$

$$\text{Into (1)} \Rightarrow 2\chi_4(i) + (-1)^2 = 3 \quad \chi_4(i) + \chi_4(\sigma_h) = 0$$

$$\text{or } (2) + (3) \quad \chi_4(i) = -1 \quad \chi_4(G_2) + (-1) + \chi_4(\sigma_h) = 0$$

$$\therefore \chi_4(G_2) = -1 \quad \chi_4(i) = -1 \Rightarrow \boxed{B_g} \quad \chi_4(G_2) = -1 = -\chi_4(G_2) + \chi_4(G_2) + \chi_4(\sigma_h)$$

Hilroy

(2)

Character Table:

C_{2h}	E	C_2	i	σ_h
A_g	1	1	1	1
B_g	1	-1	1	-1
A_u	1	1	-1	-1
B_u	1	-1	-1	-1

② $\langle x, y, z | \Gamma_m(E) = \langle x, y, z |$
 $\therefore \Gamma_m(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \chi = 3$

$\langle x, y, z | \Gamma_m(C_2) = \langle -x, -y, z |$
 $\therefore \Gamma_m(C_2) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \chi = -1$

$\langle x, y, z | \Gamma_m(i) = \langle -x, -y, -z |$
 $\therefore \Gamma_m(i) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \chi = -3$

$\langle x, y, z | \Gamma_m(\sigma_h) = \langle x, y, -z |$
 $\therefore \Gamma_m(\sigma_h) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \chi = +1$

character set = $\{3, -1, -3, 1\}$ (clearly reducible!)

b) use $a_j = \frac{1}{h} \sum_R \chi_m(R) \chi_j(R) \quad h=4$

$a_{A_g} = \frac{1}{4} [(3)(1) + (-1)(1) + (-3)(1) + (1)(1)] = 0$

$$a_{B_g} = \frac{1}{4} [(3)(1) + (-1)(-1) + (-3)(1) + (1)(-1)] = 0$$

$$a_{A_u} = \frac{1}{4} [(3)(1) + (-1)(1) + (-3)(-1) + (1)(-1)] = 1$$

$$a_{B_u} = \frac{1}{4} [(3)(1) + (-1)(-1) + (-3)(-1) + (1)(1)] = 2$$

$$\therefore \Gamma_m = A_u \oplus 2B_u$$

c) Group Multiplication Table

C_{2h}	E	C_2	i	σ_h
E	EE	C_2E	iE	σ_hE
C_2	EC_2	C_2C_2	iC_2	σ_hC_2
i	Ei	C_2i	ii	σ_hi
σ_h	$E\sigma_h$	$C_2\sigma_h$	$i\sigma_h$	$\sigma_h\sigma_h$

$$EE = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = E$$

$$EC_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} C_2$$

$$= C_2E$$

$$Ei = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} i$$

$$= iE$$

$$E\sigma_h = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \sigma_h$$

$$= \sigma_h E$$

(4)

$$C_2 C_2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = E$$

$$i i = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = E$$

$$\sigma_h \sigma_h = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = E$$

$$C_2 i = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \sigma_h$$
$$= i C_2$$

$$C_2 \sigma_h = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = i$$
$$= \sigma_h C_2$$

$$i \sigma_h = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = C_2$$
$$= \sigma_h i$$

Note all matrices are diagonal \Rightarrow group is Abelian.

Table is

	E	C_2	σ_n	σ_n
E	E	C_2	σ_n	σ_n
C_2	C_2	E	E	σ_n
σ_n	σ_n	σ_n	E	C_2

obeys rearrangement theorem.