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EXAMPLES OF SOME MOLECULES AND Their point groups

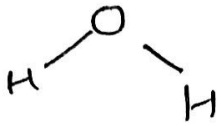
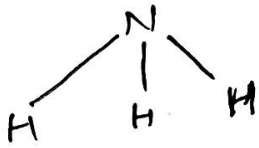
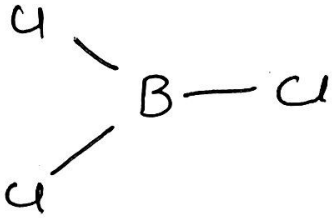
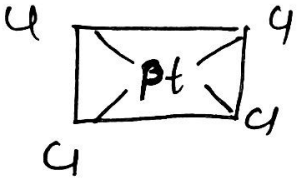
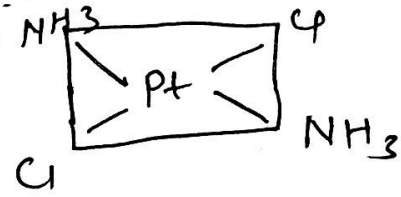
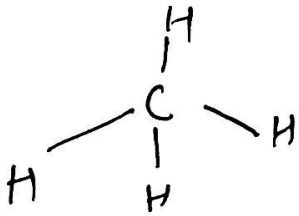
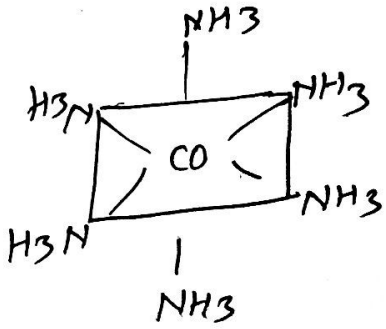
molecule	Structure	Symmetry elements
(1) H_2O		$E, C_2(z), \sigma_{xz}, \sigma_{yz}$
(2) NH_3		$E, C_3^1, C_3^2, \sigma_a, \sigma_b, \sigma_c$
(3) BCl_3		$E, C_3^2\ 3C_2\ 3\sigma_v, \sigma_h, S_3^1, S_3^5 = 12$
(4) $[PtCl_4]^{--}$		$E, C_4^1, C_4^2, C_4^3, 2C_2'\ 2C_2'', 4\sigma_v, \sigma_h, S_4^1, S_4^3, i = 14$
(5) $[Pt(NH_3)_2Cl_2]$ (Trans dichloro diamine Pt (II))		$E, C_2, 2C_2, 2\sigma_v, \sigma_h, i = 8$
(6) CH_4		$E, 8C_3, 3C_2, 6S_4, 6\sigma_d = 24$
(7) H_2	H—H	$E, C_\infty, \infty C_2, \infty\sigma_v', \sigma_h'$
(8) HCl	H—Cl	$E, C_\infty, \infty\sigma_v$
(9) $[Co(NH_3)_6]^{3+}$		$E, 6C_4, 3C_2, 8C_3, 6C_2', 6S_4, 8S_6, 6\sigma_v, 3\sigma_h, i = 48$

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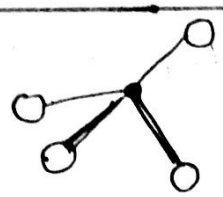
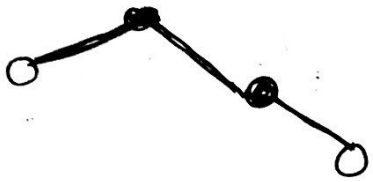
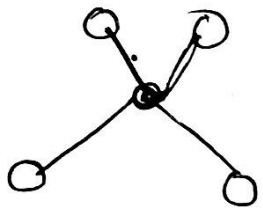
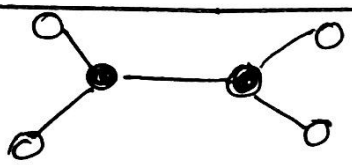
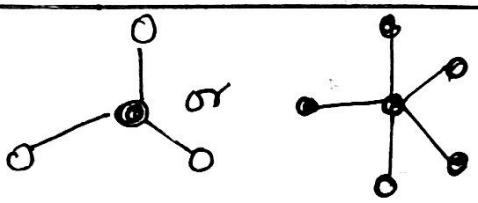
Table for point group and its symmetry elements

	Point group	symmetry elements	Structure	example.
	C_1	E		SiBrClFI
	C_2	E, C_2		H_2O_2
3.	C_s	E, σ		NHF_2
4.	C_{2v}	E, C_2, σ_v, σ_v'		H_2O, SO_2Cl_2
5.	C_{3v}	E, $2C_3$, $3\sigma_v$		NH_3, PCl_3, $POCl_2$
6.	$C_{\infty v}$	E, C_2, $2C_\phi$ ---- $\infty\sigma_v$		CO, HCl, OCS
7.	D_{2h}	E, $C_2(x,y,z)$, $\sigma(xy, yz, zx)$, i		N_2O_4, B_2H_6
8.	D_{3h}	E, C_3, $3C_2$, $3\sigma_v$, σ_h, S_3		BF_3, PCl_5
9.	D_{4h}	E, C_4, C_2, $2C_2''$		

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ASSIGNMENT

Group Theory

Try to Answer these Questions

1. a) Write symmetry elements and point group of following molecules.
   i) PCl_3 ii) NH_3 iii) BCl_3
   b) Differentiate between symmetry operations and symmetry elements.

2. a) Derive completely the Character table for C_{2v} point group.
   b) What is meant by Matrix representation of a point group? Describe representations for various symmetry elements.

3. a) Write complete ~~set~~ set of symmetry elements of BF_3 and NH_3. Assign point group of each molecule.
   b) Derive the complete matrices for all representations of point group C_{3v}.

4) Write properties of irreducible representations. Use them to construct character table for C_{2v} point group.

4. a) Write down the point groups to which the molecule AB_5 could belong. Draw the structure belonging to two point groups. Write down symmetry operations generated by each point group.

Explain application of group theory to find various normal modes of vibration of H_2O molecule.

(a) What is the point group of $POCl_3$? What will be the point group if one of the chlorine atom is replaced by Br.

6 a) Give examples of molecules with point group C_∞ and $D_{\infty h}$ clearly showing various elements of symmetry ~~ebt~~ in suitable diagrams.

b) Define order of a group.