Important Questions on Group Theory

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1.Which of the following is not the symmetry element that is not present in CH_4?

A. S_4

B. C_2

C. σ_d

D. C_4

2. What is the point group of H_2O_2 ?

A. C_{2V}

B. C_3

C. C_{3h}

D. C_2

3. Identify the Mulliken notation of the following irreducible representation.

E	C_2	σ_v (xz)	σ_v(yz)
1	1	−1	−1

A. A_1

B. A_2

C. B_2'

D. A_1''

4. No. of C_2 axis in $SiCl_4$ are .....

A. 2

B. 0

C. 3

D. 6

5. Point group of trans N_2F_2 is:

A. C_{2h}

B. C_{2v}

C. D_{2h}

D. None of above

6. The character of S_6 is:

A. 0

B. 2

C. 1

D. −1

7. The pair of non-polar point group is:

A. C_{2h}, C_i

B. C_3, D_{4d}

C. C_1, C_{3v}

D. S_4, D_4

8.What will be the final operation of $C_2(x).C_2(y).C_2(z).\ \sigma_{xz}$?

A. $C_2(z)$ B. σ_{xz}

C. $C_4(z)$ D. I

9. For H_2O, the electronic transition from ground state to B_2 symmetry is:

C_{2v}	E	C_2	σ_v	$\sigma_{v'}$	
A_1	1	1	1	1	Z, x^2, $x^2 - y^2$
A_2	1	1	−1	−1	Xy
B_1	1	−1	1	−1	Xz, x
B_2	1	−1	−1	1	Y, yz

A. Not allowed

B. Allowed with x polarisation

C. Allowed with y polarisation

D. Allowed with z polarisation

10. Phosphorus pentachloride, PCl_5 is a trigonal bipyramidal molecule. To what point group does it belong?

A. D_{3v}

B. D_{3h}

C. C_{3h}

D. D_{5h}

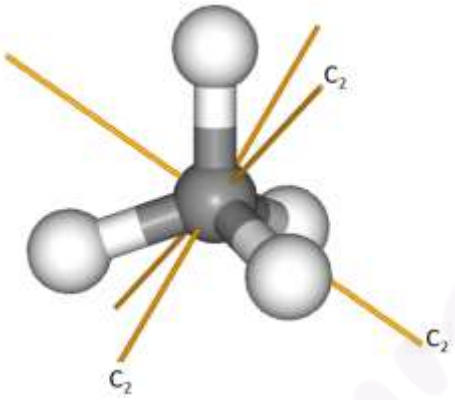
Answer Key:

1. D	6. A
2. D	7. C
3. B	8. B
4. C	9. C
5. A	10. B

Solutions:

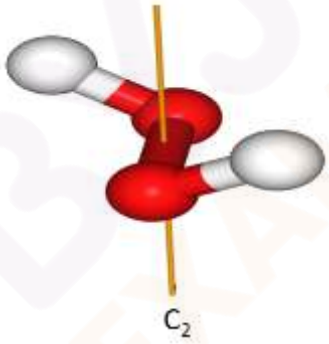
Solution 1: The point group of CH_4 is tetrahedral.

The symmetry elements present in this are: E, $4C_3$, $3C_2$, $6\sigma_d$, $3S_4$.



According to the above representation, C_4 is not present in methane.

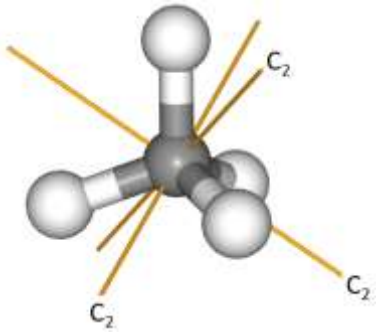
Solution 2: In this question, the form in which H_2O_2 exists is not given. In general, we take its gauche or open book form.



It has only C_2 axis and E symmetry operation. According to this, its point group is C_2.

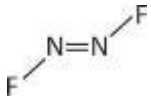
Solution 3: For Mulliken notation, we need to see the character below the symmetry operation of a given point group. In the given table, it is symmetric w.r.t E, so, A. Since the subsidiary axis is absent, we will check the molecular plane (xz), it is antisymmetric to that, so, it will be A_2. Further there is no horizontal plane present due to which 'or '' will not be applied.

Solution 4: $SiCl_4$ is a tetrahedral molecule, just like CH_4.



As shown in the above figure, there are 3 C_2 axes present in this which is passing through all the pair of opposite faces of $SiCl_4$.

Solution 5: The structure of trans – N_2F_2 is given below as:



It has one C_2 axis perpendicular to the plane of paper. This is the only axis present in the molecule. There is no other C_2 axis present in the molecule. Also, it has a molecular plane which is also its horizontal plane. Based on symmetry operation, the molecule has a C_{2h} point group.

Solution 6: S_n: cos θ –sin θ 0

Sin θ cos θ 0

0 0 –1

The character of any matrix is the sum of its diagonal elements.

Character of $S_n(z)$ = 2cos θ – 1

For S_6, $\theta = \frac{360}{6} = 60°$

$\cos 60^\circ = \frac{1}{2}$, $\sin 60^\circ = \frac{\sqrt{3}}{2}$

Character of $S_6(z)$ = $2\cos 60^\circ - 1 = 0$

Solution 7: Polar molecules are those which do not have a plane of symmetry in the molecule. C_i has a centre of inversion so, molecule is nonpolar .C_{2h} molecule has a perpendicular plane of symmetry so it is also nonpolar. In general, all the molecules which have a C_n point group except C_i, C_{nh} are polar.

Solution 8: For the application of product of operations on Cartesian coordinates, we start applying from right side operations one by one.

σ_{xz} (x, y, z) = (x, –y, z)

$C_2(z)$. (x, –y, z) = (–x, y, z)

$C_2(y)$. (–x, y, z) = (x, y, –z)

$C_2(x)$. (x, y, –z) = (x, –y, z)

The final result of the product of symmetry operation on (x, y, z) will be (x, –y, z) which can be directly obtained by σ_{xz} .

Solution 9: Ground state is the most symmetric state so A_1 is the ground state.

E	C_2	σ_v	$\sigma_{v'}$
1	–1	–1	1

Direct product: $A_1 \times B_2$

This direct product resembles the B_2, so, this transition is Y polarised.

Solution 10: PCl_5 has trigonal bipyramidal molecular geometry and it contains a C_3 main rotation axis and 3 perpendicular C_2 axes. There are 3 σ_v planes and a σ_h plane. Hence PCl_5 belongs to the D_{3h} point group.

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