

Unit 6 - Week 4- Matrix Representation of Point Group, Introduction to Reducible and Irreducible Representation, Description of Character Table , Great Orthogonality Theorem and its consequences

Course outline

How does an NPTEL online course work?

Week-1: Introduction to Symmetry elements, Symmetry operations and Group Theory

Week 2- Generation of Symmetry Operations from Symmetry Elements; Point Group analysis; Relation between molecular symmetry and physical properties(polarity and chirality).

Week 3 - Introduction to Group Multiplication Tables; Stereographic Projections and Matrix Representations of Symmetry Operations

Week 4- Matrix Representation of Point Group, Introduction to Reducible and Irreducible Representation, Description of Character Table , Great Orthogonality Theorem and its consequences

Lecture 16

Lecture 17

Lecture 18

Lecture 19

Lecture 20

Quiz : Assignment 4

Feedback form 4

Solutions of Assignment 4

Week 5 - Constructing Character table using the consequences of GOT, Relation between group theory and quantum mechanics, Introduction to Symmetry Adapted Linear Combinations: Projection operator.

Week 6 - Projection operator, concept of Symmetry Adapted Linear Combination(SALC), concept of Linear Combination of Atomic Orbitals(LCAO),LCAO-MO, Hückle Approximations and Introduction to Normal Mode of Vibration.

Week 7 - Molecular Vibrations: Normal modes and their symmetry aspects, Selection rules of fundamental vibrational transitions.

Text Transcripts

Week - 8 - Electronic Transitions

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Assignment 4

The due date for submitting this assignment has passed. As per our records you have not submitted this assignment.

Due on 2020-02-26, 23:59 IST.

1) What is the trace of the matrix for $C_3(z)$ (clockwise rotation) operation if x, y and z coordinates are used as the bases? 1 point

- 1
 -1
 0
 2

No, the answer is incorrect. Score: 0

Accepted Answers: 0

2) What is the trace of the matrix for $S_4(z)$ (clockwise rotation) operation if x, y and z coordinates are used as the bases? 1 point

- 1
 2
 0
 -1

No, the answer is incorrect. Score: 0

Accepted Answers: -1

3) A complete set of elements that are conjugate to one and another is called..... 1 point

- order
 class
 representation
 none of the above

No, the answer is incorrect. Score: 0

Accepted Answers: class

4) Consider the following table and replace Γ by the correct Mulliken's notation (take xz as the molecular plane)? 1 point

C_{2v}	E	$C_2(z)$	$\sigma_v(xz)$	$\sigma_v(yz)$
Γ	+1	-1	+1	-1

- A_1
 B_1
 A_2
 B_2

No, the answer is incorrect. Score: 0

Accepted Answers: B_1

5) Consider the following table and replace Γ by correct Mulliken's notation (take z as the principle axis)? 1 point

D_3	E	$3C_3(z)$	$3C'_2$
Γ	+1	+1	-1

- A_2
 B_2
 A_1
 B_1

No, the answer is incorrect. Score: 0

Accepted Answers: A_2

6) Consider $POCl_3$ molecule. what will be the reducible representation of its point group if 3N Cartesian coordinates are used as basis set? 1 point

- | | | |
|----|--------|-------------|
| E | $2C_3$ | $3\sigma_v$ |
| 15 | 0 | 3 |
- | | | |
|----|--------|-------------|
| E | $2C_3$ | $3\sigma_v$ |
| 15 | -1 | 2 |
- | | | |
|----|--------|-------------|
| E | $2C_3$ | $3\sigma_v$ |
| 12 | 0 | 3 |
- | | | |
|----|--------|-------------|
| E | $2C_3$ | $3\sigma_v$ |
| 15 | 0 | -3 |

No, the answer is incorrect. Score: 0

Accepted Answers:

E	$2C_3$	$3\sigma_v$
15	0	3

7) A point group has four 1-D and two 2-D irreducible representations. What is the order of the point group? 1 point

- 6
 8
 12
 10

No, the answer is incorrect. Score: 0

Accepted Answers: 12

8) Consider a molecule which belongs to C_{3v} point group. The reducible representation (Γ) is given below taking 3N Cartesian coordinates as basis set. 1 point

C_{3v}	E	$2C_3$	$3\sigma_v$
Γ	a	b	c

The reducible representation can be expressed as $\Gamma_{\text{reducible}} = pA_1 + qA_2 + rE$. Find out the value of q. Character table of C_{3v} point group is given below

C_{3v}	E	$2C_3(z)$	$3\sigma_v$
A_1	+1	+1	+1
A_2	+1	+1	-1
E	+2	-1	0

- $[a+b+3c]/6$
 $[a+3b+3c]/6$
 $[a+2b+3c]/6$
 $[a+2b-3c]/6$

No, the answer is incorrect. Score: 0

Accepted Answers: $[a+2b-3c]/6$

9) Matrices which describe the transformation of a set of orthogonal coordinates by proper and improper rotations are called _____ matrices. 1 point

- orthogonal
 conjugate
 inverse
 diagonal

No, the answer is incorrect. Score: 0

Accepted Answers: orthogonal

10) What is $c[S_2(z)]$ if x, y and z coordinates are used as the bases? 1 point

- 3
 2
 1
 None of the above

No, the answer is incorrect. Score: 0

Accepted Answers: None of the above