

# Unit 7 - 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.

## 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

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.

Lecture 21

Lecture 22

Lecture 23

Lecture 24

Lecture 25

Quiz : Assignment 5

Feedback form 5

Solutions of Assignment 5

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 5

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

Due on 2020-03-04, 23:59 IST.

1) The order of the group equals to \_\_\_\_\_

1 point

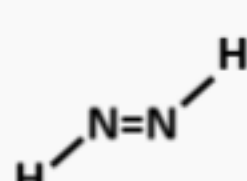
- dimension of the irreducible representation  
 sum of the squares of the characters in an irreducible representation  
 number of classes  
 none of the above

No, the answer is incorrect. Score: 0

Accepted Answers: sum of the squares of the characters in an irreducible representation

2) Consider trans-N<sub>2</sub>H<sub>2</sub> molecule in its planar form. What will be the reducible representation taking 3N Cartesian coordinates as basis set (take xz as the molecular plane)?

1 point



- |    |                |   |                |
|----|----------------|---|----------------|
| E  | C <sub>2</sub> | i | σ <sub>h</sub> |
| 12 | 0              | 0 | 4              |
- |    |                |   |                |
|----|----------------|---|----------------|
| E  | C <sub>2</sub> | i | σ <sub>h</sub> |
| 12 | -2             | 1 | 4              |
- |    |                |   |                |
|----|----------------|---|----------------|
| E  | C <sub>2</sub> | i | σ <sub>h</sub> |
| 12 | 1              | 2 | 4              |
- |    |                |    |                |
|----|----------------|----|----------------|
| E  | C <sub>2</sub> | i  | σ <sub>h</sub> |
| 12 | 0              | -2 | 4              |

No, the answer is incorrect. Score: 0

Accepted Answers:

E	C <sub>2</sub>	i	σ <sub>h</sub>
12	0	0	4

3) Consider the point group C<sub>3v</sub>. how many irreducible representations it will have?

1 point

- 3  
 2  
 4  
 1

No, the answer is incorrect. Score: 0

Accepted Answers: 3

4) A point group 'W' has 24 symmetry operations and 12 classes given that it has only one-dimensional and two-dimensional irreducible representations. The number of one-dimensional and two-dimensional irreducible representations respectively are

1 point

- 12,3  
 8,4  
 16,2  
 6,5

No, the answer is incorrect. Score: 0

Accepted Answers: 8,4

5) A point group 'Q' has 48 symmetry operations and 10 classes given that it has one-dimensional, two-dimensional and three-dimensional irreducible representations. If it has 4 three-dimensional irreducible representations then number of one-dimensional and two-dimensional irreducible representations respectively are

1 point

- 4,2  
 6,5  
 2,8  
 6,2

No, the answer is incorrect. Score: 0

Accepted Answers: 4,2

6) Identify the Mulliken notation for the following irreducible representation, G ?

1 point

	E	2C <sub>3</sub>	3C' <sub>2</sub>	i	2S <sub>6</sub>	3σ <sub>d</sub>
Γ	+1	+1	-1	-1	-1	+1

- A<sub>1</sub>  
 A<sub>1u</sub>  
 A<sub>2</sub>  
 A<sub>2u</sub>

No, the answer is incorrect. Score: 0

Accepted Answers: A<sub>2u</sub>

7) Consider the above character table and answer the following questions.

1 point

	E	2C <sub>4</sub> (z)	C <sub>2</sub>	2σ <sub>v</sub>	2σ <sub>d</sub>	linear functions, rotations	quadratic functions
Γ <sub>1</sub>	+1	+1	+1	-1	-1	'\$'	-
Γ <sub>2</sub>	+1	-1	+1	-1	+1	-	xy
Γ <sub>3</sub>	+1	+1	+1	+1	+1	z	x <sup>2</sup> +y <sup>2</sup> , '#'
Γ <sub>4</sub>	+1	-1	+1	+1	-1	-	x <sup>2</sup> -y <sup>2</sup>
Γ <sub>5</sub>	+2	0	-2	0	0	(x, y) (R <sub>x</sub> , R <sub>y</sub> )	(xz, yz)

Replace 'G<sub>2</sub>' with correct Mulliken symbol.

- B<sub>1</sub>  
 A<sub>2</sub>  
 B<sub>2</sub>  
 A<sub>1</sub>

No, the answer is incorrect. Score: 0

Accepted Answers: B<sub>2</sub>

8) Replace '\$' with the correct term.

1 point

- x  
 y  
 R<sub>z</sub>  
 z<sup>2</sup>

No, the answer is incorrect. Score: 0

Accepted Answers: R<sub>z</sub>

9) Replace '#' with correct quadratic function.

1 point

- x  
 y  
 z<sup>2</sup>  
 R<sub>x</sub>

No, the answer is incorrect. Score: 0

Accepted Answers: z<sup>2</sup>

10) The following are the characters of irreducible representation A<sup>\*</sup><sub>2u</sub>. What is the character of 'i' ?

1 point

	E	C <sub>n</sub>	nC <sub>2</sub>	i	σ
Γ	1	1	-1	*	-1

- 2  
 0  
 1  
 -1

No, the answer is incorrect. Score: 0

Accepted Answers: -1