

Unit 8 - 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.

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.

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.

Lecture 26

Lecture 27

Lecture 28

Lecture 29

Lecture 30

Feedback form 6

Quiz : Assignment 6

Solutions of Assignment 6

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 6

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

Due on 2020-03-11, 23:59 IST.

1) Consider ethylene molecule (point group = D_{2h}). The reducible representation formed using C – H σ -bonds as basis functions, can be reduced to $A_g + 1$ point $B_{1g} + B_{2u} + B_{3u}$. What will be the SALC corresponding to B_{3u} representation (only functional form)?

- $\sigma_1 - \sigma_2 + \sigma_3 - \sigma_4$
 $\sigma_1 - \sigma_2 - \sigma_3 + \sigma_4$
 $\sigma_1 - \sigma_2 + \sigma_3 + \sigma_4$
 $\sigma_1 + \sigma_2 - \sigma_3 - \sigma_4$

No, the answer is incorrect.
Score: 0

Accepted Answers:
 $\sigma_1 + \sigma_2 - \sigma_3 - \sigma_4$

2) Consider $PtCl_4^{2-}$ molecule (point group = D_{4h}).The irreducible representation using Pt-Cl σ -bonds as basis function, can be reduced to $A_{1g} + B_{1g} + E_u$. 1 point What will be the SALC corresponding to A_{1g} representation (only functional form)?

- $\sigma_1 - \sigma_2 + \sigma_3 - \sigma_4$
 $\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4$
 $\sigma_1 + \sigma_2 - \sigma_3 + \sigma_4$
 $\sigma_1 - \sigma_2 + \sigma_3 + \sigma_4$

No, the answer is incorrect.
Score: 0

Accepted Answers:
 $\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4$

3) Total number of the vibrational degrees of freedom for IF_5 molecule is

- 10
 12
 14
 16

No, the answer is incorrect.
Score: 0

Accepted Answers:
12

4) The number of vibrational degrees of freedom that the molecule XeO_4 can have is

- 8
 10
 9
 6

No, the answer is incorrect.
Score: 0

Accepted Answers:
9

5) The number of vibrational degrees of freedom that the molecule hydrogen chloride (HCl) can have is

- 1
 3
 5
 2

No, the answer is incorrect.
Score: 0

Accepted Answers:
1

6) Consider BF_3 molecule (point group = D_{3h}). The reducible representation formed using B – F σ -bonds as basis functions, can be reduced to $A'_1 + A'_2 + 3E'$ + $A''_2 + E''$. What will be the SALC corresponding to A'_1 representation (only functional form)?

- $\sigma_1 - \sigma_2 + 3\sigma_3$
 $\sigma_1 - 2\sigma_2 - \sigma_3$
 $\sigma_1 + \sigma_2 - \sigma_3$
 $\sigma_1 + \sigma_2 + \sigma_3$

No, the answer is incorrect.
Score: 0

Accepted Answers:
 $\sigma_1 + \sigma_2 + \sigma_3$

7) Under Hückel approximation, what does H_{ij} become when $i = j$?

- a
 b
 g
 E

No, the answer is incorrect.
Score: 0

Accepted Answers:
a

8) Under Hückel approximation, what does H_{ij} become when i and j are adjacent?

- a
 b
 g
 E

No, the answer is incorrect.
Score: 0

Accepted Answers:
b

9) The number of vibrational degrees of freedom that a gold atom can have is

- 73
 74
 1
 0

No, the answer is incorrect.
Score: 0

Accepted Answers:
0

10) Consider $PtCl_4^{2-}$ molecule (point group = D_{4h}). A representation made by considering the Pt-Cl σ bonds as basis functions, can be reduced to $A_{1g} + B_{1g} + E_u$. One of the SALC corresponding to E_u representation (only functional form) is given by $\sigma_2 - \sigma_4$. Find the other partner.

- $(\sigma_2 + \sigma_4)$
 $(\sigma_2 - \sigma_1)$
 $(\sigma_1 - \sigma_3)$
 $(\sigma_1 + \sigma_2)$

No, the answer is incorrect.
Score: 0

Accepted Answers:
 $(\sigma_1 - \sigma_3)$