Assignment 6

Due date for submitting this assignment has passed.

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

Unit 8 - Week 6 - Projection operator, concept of Symmetry Adapted Linear Combination (SALC), concept of Linear Combination of Atomic Orbitals (LCAO), LCAO-MO, Hückel Approximations and Introduction to Normal Mode of Vibration.

Course outline

How does an MPTE student improve their mark?

Week 1: Introduction to Group Theory, Symmetry Elements, Symmetry Operations and Group Theory

Week 2: Generation of Symmetry Operations from Symmetry Elements, then Group Analysis, Rotation between molecular symmetry and crystallographic symmetries and their correspondences.

Week 3: Introduction to Molecular Vibrations, Harmonic Oscillator and Normal Modes of Vibration.

Week 4: Symmetry and Group Theory, Introduction to Molecular Vibrations, Description of Character Table, Group Theorems and their correspondences.

Week 5: Introduction to Molecular Vibrations, Transformation of the irreducible representation, Description of Character Table, Group Theorems and their correspondences.

Week 6: Introduction to Molecular Vibrations, Transformation of the irreducible representation, Description of Character Table, Group Theorems and their correspondences.

Week 7: Molecular Vibrations, Normal modes and their symmetry properties, Molecular vibration normal modes, fundamentals vibrations transitions.

Test Vouchers

DOWNLOAD VOUCHERS

Assignment 6

The due date for submitting this assignment has passed.

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

No. the answer is incorrect. Score: 0

1. Consider OCS molecule (point group $D_{3h}$). What will be the SLC corresponding to its irreducible representation $(j=6)$ function?

   Accepted Answer:
   
   $\mathbf{6}$

   No. the answer is incorrect. Score: 0

2. Total number of the vibrational degrees of freedom for OCS molecule is

   Accepted Answer:
   
   12

   No. the answer is incorrect. Score: 0

3. The number of vibrational degrees of freedom that the molecule CO$_2$ can have is

   Accepted Answer:
   
   6

   No. the answer is incorrect. Score: 0

4. Consider $\text{H}_2\text{O}$ molecule (point group $C_{2v}$). The reducible representation formed using $\text{H}, \text{O}$ bond as basis functions, can be reduced to $\mathbf{2} + \mathbf{2}'$. What will be the SLC corresponding to its irreducible representation $(j=2)$ function?

   Accepted Answer:
   
   $\mathbf{2}'$

   No. the answer is incorrect. Score: 0

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

   Accepted Answer:
   
   6

   No. the answer is incorrect. Score: 0

6. Under Hückel approximation, what does $1s^2$ become when $1s$ and $2s$ are adjacent?

   Accepted Answer:
   
   $s^2$

   No. the answer is incorrect. Score: 0

7. Under Hückel approximation, what does $1s^2$ become when $1s$ and $2s$ are adjacent?

   Accepted Answer:
   
   $s^2$

   No. the answer is incorrect. Score: 0

8. Under Hückel approximation, what does $1s^2$ become when $1s$ and $2s$ are adjacent?

   Accepted Answer:
   
   $s^2$

   No. the answer is incorrect. Score: 0

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

   Accepted Answer:
   
   7

   No. the answer is incorrect. Score: 0

10. Consider $\text{CS}_2$ molecule (point group $D_{2d}$). A representation made by considering the $\text{C} - \text{S}$ bond as basis functions, can be reduced to $\mathbf{4} + \mathbf{2}$. What will be the SLC corresponding to its irreducible representation $(j=4)$ function?

   Accepted Answer:
   
   $\mathbf{4}$

   No. the answer is incorrect. Score: 0

11. Under Hückel approximation, what does $1s^2$ become when $1s$ and $2s$ are adjacent?

   Accepted Answer:
   
   $s^2$

   No. the answer is incorrect. Score: 0

12. Under Hückel approximation, what does $1s^2$ become when $1s$ and $2s$ are adjacent?

   Accepted Answer:
   
   $s^2$

   No. the answer is incorrect. Score: 0

13. Under Hückel approximation, what does $1s^2$ become when $1s$ and $2s$ are adjacent?

   Accepted Answer:
   
   $s^2$

   No. the answer is incorrect. Score: 0

14. Under Hückel approximation, what does $1s^2$ become when $1s$ and $2s$ are adjacent?

   Accepted Answer:
   
   $s^2$

   No. the answer is incorrect. Score: 0