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.

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 + B_{1g} + B_{2u} + B_{3u}. What will be the SALC corresponding to B3u representation (only functional form)? ***1 point***

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

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. What will be the SALC corresponding to A_{1g} representation (only functional form)? ***1 point***

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

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 ***1 point***

- 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 ***1 point***

- 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 point***

- 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'1representation (only functional form)? ***1 point***

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

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? ***1 point***

- 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? ***1 point***

- 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 ***1 point***

- 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 Eu representation (only functional form) is given by $\sigma_2 - \sigma_4$. Find the other partner. ***1 point***

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

No, the answer is incorrect.
Score: 0
Accepted Answers:
$(\sigma_1 - \sigma_3)$