

Unit 9 - Week 7 - Molecular Vibrations: Normal modes and their symmetry aspects, Selection rules of fundamental vibrational transitions.

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.

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

Lecture 31

Lecture 32

Lecture 33

Lecture 34

Lecture 35

Feedback form 7

Quiz : Assignment 7

Solutions of Assignment 7

Text Transcripts

Week - 8 - Electronic Transitions

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Assignment 7

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

Due on 2020-03-18, 23:59 IST.

1) Consider ammonia molecule. Find all the Raman active modes (in terms of IRs)? 1 point

- $2A_1 + 2E$
 $2A_1$
 $3A_1 + A_2 + 4E$
 $A_1 + A_2 + E$

No, the answer is incorrect.
Score: 0

Accepted Answers:
 $2A_1 + 2E$

2) According to mutual exclusion rule _____ 1 point

- no Raman active vibration is IR active, for a centrosymmetric molecule
 no Raman active vibration is IR active, for any molecule
 Raman active vibrations must be IR active, for a centrosymmetric molecule
 Photon emission (fluorescence or phosphorescence) occurs in appreciable yield only from the lowest excited state of a given multiplicity.

No, the answer is incorrect.
Score: 0

Accepted Answers:
no Raman active vibration is IR active, for a centrosymmetric molecule

3) Consider methane molecule. Identify the symmetry corresponding to the vibration mode(s), which is/are only Raman active. 1 point

- T_1
 $E \text{ \& } A_2$
 $T_2 \text{ \& } E$
 $A_1 \text{ \& } E$

No, the answer is incorrect.
Score: 0

Accepted Answers:
 $A_1 \text{ \& } E$

4) Consider Trans - N_2F_2 molecule. Identify the symmetry corresponding to the vibration mode(s), which is/are only Raman active. 1 point

- $A_u \text{ \& } B_u$
 A_g
 $A_u, B_u \text{ \& } A_g$
 A_u

No, the answer is incorrect.
Score: 0

Accepted Answers:
 A_g

5) Consider Trans - N_2F_2 molecule. Identify the symmetry corresponding to the vibration mode(s), which is/are only IR active. 1 point

- $A_u \text{ \& } B_u$
 A_g
 $A_u, B_u \text{ \& } A_g$
 A_u

No, the answer is incorrect.
Score: 0

Accepted Answers:
 $A_u \text{ \& } B_u$

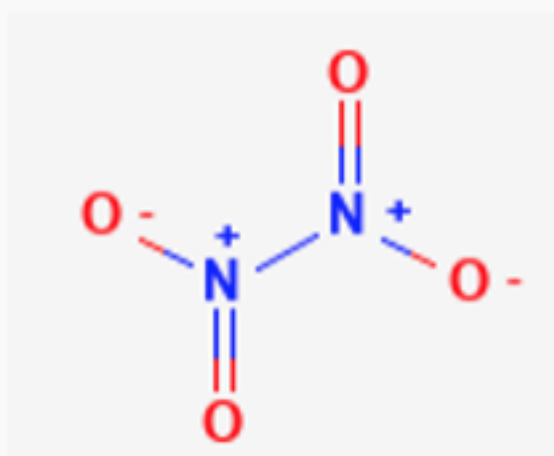
6) Write the symmetry of all the normal vibrational modes of water molecule?(taking molecular plane to be xz plane) 1 point

- $A_2 + B_1 + B_2$
 $A_1 + B_1 + B_2$
 $2A_1 + B_1$
 $2A_1 + B_2$

No, the answer is incorrect.
Score: 0

Accepted Answers:
 $2A_1 + B_1$

7) Consider N_2O_4 (D_{2h}). Identify the correct reducible representation for its vibrational normal modes. 1 point



- $3 A_g + 2 B_{1g} + B_{2g} + A_u + B_{1u} + 2 B_{2u} + 2 B_{3u}$
 $2 A_g + 2 B_{1g} + B_{2g} + A_u + B_{1u} + 2 B_{2u} + 3 B_{3u}$
 $2 A_g + 2 B_{1g} + B_{2g} + 2A_u + B_{1u} + 2 B_{2u} + 2 B_{3u}$
 $3 A_g + B_{1g} + B_{2g} + A_u + 2B_{1u} + 2 B_{2u} + 2 B_{3u}$

No, the answer is incorrect.
Score: 0

Accepted Answers:
 $3 A_g + 2 B_{1g} + B_{2g} + A_u + B_{1u} + 2 B_{2u} + 2 B_{3u}$

8) Consider N_2O_4 molecule. Identify the symmetry corresponding to the vibration mode(s), which is/are only IR active. 1 point

- $2 B_{1g} + B_{1u} + 2 B_{2u}$
 $3 A_g + A_u + B_{1u}$
 $B_{1u} + 2 B_{2u} + 2 B_{3u}$
 $2 B_{1g} + B_{2g} + A_u$

No, the answer is incorrect.
Score: 0

Accepted Answers:
 $B_{1u} + 2 B_{2u} + 2 B_{3u}$

9) Consider SF_6 molecule. Identify the symmetry corresponding to the vibration mode(s), which is/are only IR active. 1 point

- $2T_{1u}$
 A_{1g}, E_g, T_{2g}
 A_{1g}
 E_g, T_{2u}

No, the answer is incorrect.
Score: 0

Accepted Answers:
 $2T_{1u}$

10) A tetraatomic molecule has 6 vibrational normal modes. Three of them are only Raman active and the rest are only IR active. Based on these information, identify the correct molecule from the following 1 point

- trans- N_2F_2
 Cis- N_2F_2
 NH_3
 BN_3

No, the answer is incorrect.
Score: 0

Accepted Answers:
trans- N_2F_2