

Birla Institute of Technology & Science, Pilani (Raj)
Pilani Campus
II Semester, 2022-2023
CHEM G541 Chemical Applications of Group Theory
Mid Semester Test (Open Book)

Max. Marks: 35

16 March 2023

Duration: 1 hr. 30 min.

Instructions to the student:

- 1) There are six questions in total; answer all the questions.
- 2) Write brief answers to the point with proper justification.
- 3) Start answering each question on a fresh page and answer all parts of a question together.
- 4) Open book test. Textbook, Ref. books, class notes, and printed slides are allowed. However, exchange of these materials is not allowed. Mobile phones, lap-tops etc. are to be switched off and kept away from you.
- 5) Any unfair means, if deducted, will be sternly dealt with.
- 6) Data required are available in Text and/or Reference books. Character Tables available with the invigilator can be borrowed for a short period of time.

1. a) Write the Group Multiplication Table for the group of order five. Show that only one such table is possible. [2 + 1 = 3]
b) What are the "square" and "cube" of S_4^3 in S_4 point group? [2]

 2. a) Write the structures of the isomers of dichlorobenzene, and identify their point groups. Based on symmetry predict whether these molecules will have dipole moment or not. [3]
b) Consider Ammonia; one by one the hydrogens are replaced by different substituents. Among the compounds NH_3 , NH_2A , $NHAB$, $NABC$ which is/are dissymmetric; Explain based on symmetry. [3]

 3. a) Systematically deduce the point groups of the following species:
i) $[PtCl_4]^{2-}$ ii) cis $[PtCl_2Br]^{2-}$ iii) trans $[PtCl_2Br_2]^{2-}$ iv) cis $[PtCl_2Br_2]^{2-}$ [4]
b) What will be the highest value of degeneracy for the levels of i) a square planar molecule and ii) a square pyramidal molecule. [2]

 4. a) Identify the classes and subgroups of D_3 . A reducible representation of this point group has the character 6 for identity operation and the character 0 for all other operations. Resolve this reducible representation into irreducible representations. [4]
b) Identify any one molecule for each of the following characteristics. [2]
i) with σ_h ii) without σ_h iii) with σ_d iv) without σ_d

 5. Consider the complex ion $[CoF_6]^{3-}$. Based on symmetry principles identify the atomic orbitals of Co which after hybridization will be suitable to form σ bonds with F species. [6]

 6. a) How many normal modes of vibrations are there for $[CoF_6]^{3-}$? Out of these normal modes how many are stretching vibrations and how many are bending vibrations? [2]
b) Determine the irreducible representations of all the normal modes of vibrations of HOF molecule. Classify these modes as IR and/or Raman active modes. Show these modes pictorially by using arrows. [4]
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