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

Max. Marks: 35 **15 May 2023** **Duration: 3hrs.**

Instructions to the students:

1) There are seven 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 and other electronic gadgets are to be switched off and kept away from you; This time lap-tops are allowed without net connection; there is no recharging facility.
5) Any unfair means, if identified, will be sternly dealt with.
6) Data required are available in Text and/or Reference books.

1. a) Write the group multiplication table for C_{2V} point group. **[2]**
b) Based on symmetry principles classify the following molecules as **i)** dissymmetric or not **ii)** having zero or non-zero electric dipole moment (Justify your answers in one line; also write the point groups). **A)** Naphthalene ($C_{10}H_8$) **B)** SOClF **[2 x 2 = 4]**

2. Consider all the isomers of PF_4Cl and PF_3Cl_2 and identify their point groups. **[4]**

3. Determine the irreducible representation of each of the fundamental vibrations of ClF_3 molecule; classify these vibrations as IR and/or Raman active. **[5]**

4. Consider the electronic configuration of $\mathbf{e_g^3}$ in O_h symmetry. Derive the labels corresponding to the states of this configuration (hint: use direct product and then resolve). Further considering the D_{4h} point group and using the method descending symmetry try to assign the spin multiplicity values to these labels. **[5]**

5. Consider BF_3 molecule. Draw its structure. Identify its point group. Label the B-F σ bonds as σ_1, σ_2 etc. and apply the projection operators corresponding to all the irreducible representations of the point group on σ_1 and write the resultant SALCs**.** **[5]**

6. Consider the species $\mathbf{[NiCl_4]^{2-}}$ (Ni atomic number 28). Identify its point group. Now using T-S diagrams predict whether this species will show J-T distortion or not. Also predict the possible electronic spectral transitions**.** **[5]**

7. Consider the species $\mathbf{[Ni(H_2O)_6]^{2+}}$ (Ni atomic number 28). Identify its point group. Assume during electronic transitions vibrational couplings happen. If polarized light is used (polarized in x, y, z directions and z being one of the major axes direction), predict about the allowed/forbidden status of the transitions. **[5]**

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