Indian Institute of Technology, Kharagpur

Time: 3 Hours	Full Marks: 50	No. of students: 56
End Semester Examination	Autumn, 2012-2013	Department: Chemistry

Subject: **CY41007 GROUP THEORY FOR CHEMISTS**

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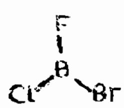
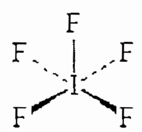
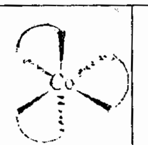
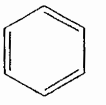
1. **Answer all questions.**
2. **If specified, answers <u>MUST be tabulated in the format shown</u> followed by the details of calculations, if any.**

Q.1. Complete the following tables in your answer script. 5+5=10

a.

Symmetry point group	Schönflies notation
(i) Non-rotational group with a center of inversion	
(ii) Cubic group without a center of inversion	
(iii) Single axis rotational group of order n with σ_h	
(iv) Group obtained by adding inversion i to C_3	
(v) Group generated by S_n axis (n odd)	

b.

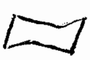
Molecule					
Number of σ_v planes in the molecule					

Q.2. Write down the symmetry point groups of the following molecules in the tabular format shown.

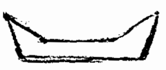
Molecule	Symmetry point group

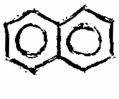
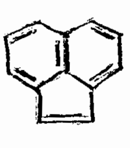
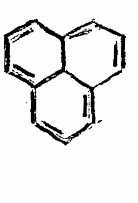
1X10=10

(i) MX_3 trigonal planar (undistorted); (ii) MX_3 trigonal planar (distorted by lifting M out of plane)

(iii)  (iv) 

(v) 

(vi)  (vii) 

(viii)  (ix)  (x) 

Q.3. Describe in brief the implied symmetry properties of the irreducible representations on the basis of their Mulliken symbols. 1X5=5

(i) A_g in C_{2h}
(ii) E_u in D_{3d}
(iii) A''_2 in D_{3h}
(iv) B_{1g} in D_{4h}
(v) E' in D_{3h}

Q.4. For the point group C_{2h}, answer the following questions. In each case, **briefly** state any rule/theorem that you may be using to obtain the answer, 25

(i) Write down the complete list of symmetry operations in this point group. 2

(ii) Obtain the group multiplication table. 2

(iii) Show that there are four classes in this group. List the members of each class. 2

(iv) Fill in the empty boxes in the character table given below. 2

C_{2h}				
A_g	1	1	1	1
B_u	1			
A_u	1			
B_g	1			

(v) Consider a general vector, $\vec{v}$ whose base is at (0,0,0) and whose tip is at *(x,y,z)* in the point group C_{2h}. Derive the set of four 3X3 transformation matrices that constitute the reducible representation, Γ_m by which $\vec{v}$ transforms. 4

(vi) Show that the group of matrices comprising Γ_m is homomorphic with the group C_{2h}. 2

(vii) Reduce Γ_m into its irreducible representations by block diagonalization. 2

(viii) Write the reducible representation of characters, Γ_v that corresponds to the matrix representation Γ_m. 2

(ix) Show that Γ_v reduces to the same irreducible representations as Γ_m. 4

(x) Using the results from above, obtain the symmetry adapted basis function for the irreducible representation A_u. 3