

1. (20%) Vibrational analysis for molecules gives the following representations:

(a) Reduce the representations of Γ_1 , Γ_2 and Γ_3 to their irreducible representations. (6%)

(b) For Γ_1 , also classify the irreducible representations into translational, rotational, and vibrational modes. (10%)

(c) For Γ_4 , which vibrational modes are infrared active? (4%)

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	-1	1	1	-1	R_z	
E'	2	-1	0	2	-1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	-1	-1	-1		
A_2''	1	1	-1	-1	-1	1	z	
E''	2	-1	0	-2	1	0	(R_x, R_y)	(xz, yz)
→ Γ_1	6	0	-2	-2	-2	2		

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		$(2z^2 - x^2 - y^2, x^2 - y^2)$
T_1	3	0	-1	1	-1		
T_2	3	0	-1	-1	1	(x, y, z)	(xy, xz, yz)
→ Γ_2	7	1	-1	1	1		

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	-1	R_z	
E_2	2	-1	0	(x, y) (R_x, R_y)	$(x^2 - y^2, xy)(xz, yz)$
→ Γ_3	3	0	1		
→ Γ_4	5	2	-1		

2. (10%) Determine the point groups for (a) H_3O^+ , (b) Acetylene, (c) Benzene, (d) Tetrachloroallene $\text{Cl}_2\text{C}=\text{C}=\text{Cl}_2$, and (e) The number 96.
3. (9%) Calculate the effective nuclear charge on a 5s, a 5p, and a 4d electron in an atom with a configuration of $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^2$.
4. (12%) For each of the following bonds, indicate which atom is more negative. (a) C-N, (b) N-O, (c) C-I, (d) O-Cl, (e) P-Br, and (f) S-Cl.
5. (10%) Use VSEPR theory to predict the shapes for the following structures:
(a) PH_3 , (b) PF_5 , (c) SF_6 , (d) ICl_3 , and (e) SnCl_2 .
6. (5%) Which of the molecules in problem 5 are polar?
7. (9%) Predict the number of unpaired electrons for each of the following: (a) A tetrahedral d^6 ion, (b) A square planar d^7 ion, (c) A coordination compound with a magnetic moment of 5.1 Bohr magnetons.
8. (9%) Give structural formula or draw structures for
(a) Sodium tetrachlorocobaltate(II), (b) Triammineaquadichlorocobalt(III) chloride, and (c) μ -Oxo-bis(pentaamminechromium(III)) ion.
9. (16%) Classify the following reactions into (I) Ligand Association (LA), (II) Ligand Dissociation (LD), (III) Oxidative Addition (OA), (IV) Reductive Elimination (RE), and (V) Migratory Insertion (MI):
For example, $\text{HRh}(\text{PPh}_3)_3 \rightarrow \text{HRh}(\text{PPh}_3)_2 + \text{PPh}_3$ Answer: LD
(a) $\text{CH}_3\text{-Co}(\text{CO})_4 \rightarrow \text{CH}_3(\text{CO})\text{Co}(\text{CO})_3$
(b) $\text{CH}_3(\text{CO})\text{Co}(\text{CO})_3 + \text{H}_2 \rightarrow \text{CH}_3(\text{CO})\text{Co}(\text{H})_2(\text{CO})_3$
(c) $\text{CH}_3(\text{CO})\text{Co}(\text{H})_2(\text{CO})_3 \rightarrow \text{CH}_3(\text{CO})\text{H} + \text{HCo}(\text{CO})_3$
(d) $\text{CH}_3\text{Co}(\text{H}_2\text{C}=\text{CH}_2)(\text{CO})_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{Co}(\text{CO})_3$