

# Chem3140 Extra Practice

I. Provide the **total Reducible Representation** for the  $x, y, z$  rotational, translational, and vibrational modes of the following molecules:

1.  $\text{PF}_5$  ( $D_{3h}$ )

$D_{3h}$	E	$2C_3$	$3C_2$	$\sigma_h$	$2S_6$	$3\sigma_v$
	18		-2	4		4

2.  $\text{ClF}_3$  (F is axial,  $C_{2v}$ )

$C_{2v}$	E	$2C_2$	$C_2$	$2\sigma_v$	$2\sigma_d$
	18	2	-2	4	2

3.  $\text{C}_6\text{H}_{12}$  ("chair",  $D_{3d}$ )

$D_{3d}$	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$
	54	0	0	0	0	6

II. Determine the total Reducible Representation for the C-O stretching vibrations in the following molecules:

4.  $\text{Fe}(\text{CO})_5$  ( $D_{3h}$ )

$D_{3h}$	E	$2C_3$	$3C_2$	$\sigma_h$	$2S_6$	$3\sigma_v$
	5	2	1	3	0	3

5.  $\text{Cr}(\text{CO})_6$  ( $O_h$ )

$O_h$	E	$8C_3$	$6C_2$	$(6C_4, 3C_2)$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$
	6	0	0	2	2	0	0	4	2

III. **Vibrational Spectroscopy:** Determine the symmetry point group of the molecule *trans*- $\text{Cl}_2\text{SeF}_4$  (Se is central atom). Then, using the  $x, y,$  and  $z$  coordinates for each atom determine the reducible representation, reduce it, and classify the representations into translational, rotational, and vibrational modes and decide which modes will be IR-active.

*trans*- $\text{Cl}_2\text{SeF}_4$

$D_{2h}$	E	$(2C_4, C_2)$	$2C_2'$	$2C_2''$	i	$2S_4$	$\sigma_h$	$2\sigma_v$	$2\sigma_d$
	21	3	-3	-3	-1	-3	-1	5	3

$$2A_{1g} + A_{2g} + B_{1g} + B_{2g} + 2E_g + 3A_{2u} + B_{2u} + 4E_u$$

-  $A_{2u}$  (z) and  $-E_u$  (x,y) as translational modes

-  $A_{2g}$  ( $R_z$ ) and  $-E_g$  ( $R_x, R_y$ ) as rotational modes

$2A_{1g} + B_{1g} + B_{2g} + E_g + 2A_{2u} + B_{2u} + 3E_u$  vibrational modes (remaining)

Only 5 modes are IR active (5 peaks):  $2A_{2u}$  (z) +  $3E_u$  (x,y)

# Inorganic Chemistry Practice Exam Answers

**RD Boyd**



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