

Chem3140 Extra Practice

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

1. PF_5 (D_{3h})

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

2. 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. C_6H_{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	$2C_3$	$3C_2$	σ_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*- Cl_2SeF_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- Cl_2SeF_4

D_{2h}	E	$(2C_4, C_2)$	$2C_2'$	$2C_2''$	i	$2S_4$	σ_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)

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