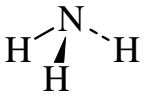
Chem 370 - Spring, 2019
Assignment 4 - Solutions

1. (a) NH_3

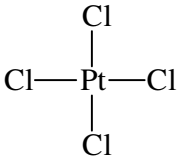


C_{3v}	E	$2C_3$	$3\sigma_v$
N_i	4	1	2
χ_i	3	0	1
Γ_{3n}	12	0	2

$$\Gamma_{3n} = 3A_1 + A_2 + 4E$$
$$\Gamma_{trans} = A_1 + E \quad \Gamma_{rot} = A_2 + E$$
$$\Gamma_{3n-6} = 2A_1 + 2E = 4 \text{ frequencies}$$

Infrared	4 ($2A_1 + 2E$)
Raman	4 ($2A_1 + 2E$)
Polarized	2 ($2A_1$)
Coincidences	4 ($2A_1 + 2E$)
Silent modes	0

(b) $PtCl_4^{2-}$

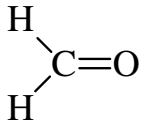


D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
N_i	5	1	1	3	1	1	1	5	3	1
χ_i	3	1	-1	-1	-1	-3	-1	1	1	1
Γ_{3n}	15	1	-1	-3	-1	-3	-1	5	3	1

$$\Gamma_{3n} = A_{1g} + A_{2g} + B_{1g} + B_{2g} + E_g + 2A_{2u} + B_{2u} + 3E_u$$
$$\Gamma_{\text{trans}} = A_{2u} + E_u \quad \Gamma_{\text{rot}} = A_{2g} + E_g$$
$$\Gamma_{3n\text{-}6} = A_{1g} + B_{1g} + B_{2g} + A_{2u} + B_{2u} + 2E_u = 7 \text{ frequencies}$$

Infrared	3 ($A_{2u} + 2E_u$)
Raman	3 ($A_{1g} + B_{1g} + B_{2g}$)
Polarized	1 (A_{1g})
Coincidences	0
Silent modes	1 (B_{2u})

(c) H_2CO

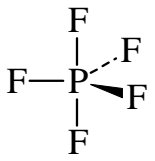


C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$
N_i	4	2	2	4
χ_i	3	-1	1	1
Γ_{3n}	12	-2	2	4

$$\Gamma_{3n} = 4A_1 + A_2 + 3B_1 + 4B_2$$
$$\Gamma_{\text{trans}} = A_1 + B_1 + B_2 \quad \Gamma_{\text{rot}} = A_2 + B_1 + B_2$$
$$\Gamma_{3n\text{-}6} = 3A_1 + B_1 + 2B_2 = 6 \text{ frequencies}$$

Infrared	6 ($3A_1 + B_1 + 2B_2$)
Raman	6 ($3A_1 + B_1 + 2B_2$)
Polarized	3 ($3A_1$)
Coincidences	6 ($3A_1 + B_1 + 2B_2$)
Silent modes	0

(d) PF_5

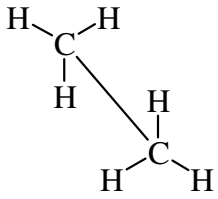


D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$
N_i	6	3	2	4	1	4
χ_i	3	0	-1	1	-2	1
Γ_{3n}	18	0	-2	4	-2	4

$$\Gamma_{3n} = 2A_1' + A_2' + 4E' + 3A_2'' + 2E''$$
$$\Gamma_{trans} = E' + A_2'' \qquad \Gamma_{rot} = A_2' + E''$$
$$\Gamma_{3n-6} = 2A_1' + 3E' + 2A_2'' + E'' = 8 \text{ frequencies}$$

Infrared	5 ($3E' + 2A_2''$)
Raman	6 ($2A_1' + 3E' + E''$)
Polarized	2 ($2A_1'$)
Coincidences	3 ($3E'$)
Silent modes	0

(e) C_2H_6 (staggered configuration)

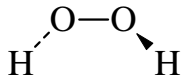


D_{3d}	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$
N_i	8	2	0	0	0	4
χ_i	3	0	-1	-3	0	1
Γ_{3n}	24	0	0	0	0	4

$$\Gamma_{3n} = 3A_{1g} + A_{2g} + 4E_g + A_{1u} + 3A_{2u} + 4E_u$$
$$\Gamma_{trans} = A_{2u} + E_u \quad \Gamma_{rot} = A_{2g} + E_g$$
$$\Gamma_{3n-6} = 3A_{1g} + 3E_g + A_{1u} + 2A_{2u} + 3E_u = 12 \text{ frequencies}$$

Infrared	5 ($2A_{2u} + 3E_u$)
Raman	6 ($3A_{1g} + 3E_g$)
Polarized	3 ($3A_{1g}$)
Coincidences	0
Silent modes	1 (A_{1u})

(f) H_2O_2

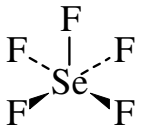


C_2	E	C_2
N_i	4	0
χ_i	3	-1
Γ_{3n}	12	0

$$\Gamma_{3n} = 6A + 6B$$
$$\Gamma_{trans} = A + 2B \quad \Gamma_{rot} = A + 2B$$
$$\Gamma_{3n-6} = 4A + 2B = 6 \text{ frequencies}$$

Infrared	6 ($4A + 2B$)
Raman	6 ($4A + 2B$)
Polarized	4 ($4A$)
Coincidences	6 ($4A + 2B$)
Silent modes	0

(g) SeF_5^-

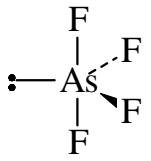


C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$
N_i	6	2	2	4	2
χ_i	3	1	-1	1	1
Γ_{3n}	18	2	-2	4	2

$$\Gamma_{3n} = 4A_1 + A_2 + 2B_1 + B_2 + 5E$$
$$\Gamma_{trans} = A_1 + E \quad \Gamma_{rot} = A_2 + E$$
$$\Gamma_{3n-6} = 3A_1 + 2B_1 + B_2 + 3E = 9 \text{ frequencies}$$

Infrared	6 ($3A_1 + 3E$)
Raman	9 ($3A_1 + 2B_1 + B_2 + 3E$)
Polarized	3 ($3A_1$)
Coincidences	6 ($3A_1 + 3E$)
Silent modes	0

(h) AsF_4^-

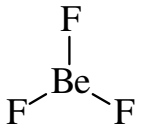


C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$
N_i	5	1	3	3
χ_i	3	-1	1	1
Γ_{3n}	15	-1	3	3

$$\Gamma_{3n} = 5A_1 + 2A_2 + 4B_1 + 4B_2$$
$$\Gamma_{trans} = A_1 + B_1 + B_2 \quad \Gamma_{rot} = A_2 + B_1 + B_2$$
$$\Gamma_{3n-6} = 4A_1 + A_2 + 2B_1 + 2B_2 = 9 \text{ frequencies}$$

Infrared	8 ($4A_1 + 2B_1 + 2B_2$)
Raman	9 ($4A_1 + A_2 + 2B_1 + 2B_2$)
Polarized	4 ($4A_1$)
Coincidences	8 ($4A_1 + 2B_1 + 2B_2$)
Silent modes	0

(i) BeF_3^-

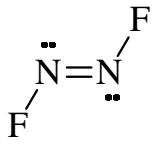


D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$
N_i	4	1	2	4	1	2
χ_i	3	0	-1	1	-2	1
Γ_{3n}	12	0	-2	4	-2	2

$$\Gamma_{3n} = A_1' + A_2' + 3E' + 2A_2'' + E''$$
$$\Gamma_{trans} = E' + A_2'' \quad \Gamma_{rot} = A_2' + E''$$
$$\Gamma_{3n-6} = A_1' + 2E' + A_2'' = 4 \text{ frequencies}$$

Infrared	3 ($2E' + A_2''$)
Raman	3 ($A_1' + 2E'$)
Polarized	1 (A_1')
Coincidences	2 ($2E'$)
Silent modes	0

(j) *trans*-FNNF

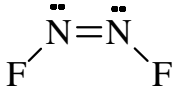


C_{2h}	E	C_2	i	σ_h
N_i	4	0	0	4
χ_i	3	-1	-3	1
Γ_{3n}	12	0	0	4

$$\Gamma_{3n} = 4A_g + 2B_g + 2A_u + 4B_u$$
$$\Gamma_{\text{trans}} = A_u + 2B_u \quad \Gamma_{\text{rot}} = A_g + 2B_g$$
$$\Gamma_{3n\text{-}6} = 3A_g + A_u + 2B_u = 6 \text{ frequencies}$$

Infrared	3 ($A_u + 2B_u$)
Raman	3 ($3A_g$)
Polarized	3 ($3A_g$)
Coincidences	0
Silent modes	0

(k) *cis*-FNNF

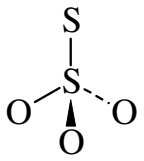


C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$
N_i	4	0	0	4
χ_i	3	-1	1	1
Γ_{3n}	12	0	0	4

$$\Gamma_{3n} = 4A_1 + 2A_2 + 2B_1 + 4B_2$$
$$\Gamma_{\text{trans}} = A_1 + B_1 + B_2 \quad \Gamma_{\text{rot}} = A_2 + B_1 + B_2$$
$$\Gamma_{3n\text{-}6} = 3A_1 + A_2 + 2B_2 = 6 \text{ frequencies}$$

Infrared	5 ($3A_1 + 2B_2$)
Raman	6 ($3A_1 + A_2 + 2B_2$)
Polarized	3 ($3A_1$)
Coincidences	5 ($3A_1 + 2B_2$)
Silent modes	0

(l) $S_2O_3^{2-}$



C_{3v}	E	$2C_3$	$3\sigma_v$
N_i	5	2	3
χ_i	3	0	1
Γ_{3n}	15	0	3

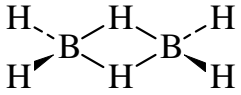
$\Gamma_{3n} = 4A_1 + A_2 + 5E$

$\Gamma_{trans} = A_1 + E \quad \Gamma_{rot} = A_2 + E$

$\Gamma_{3n-6} = 3A_1 + 3E = 6$ frequencies

Infrared	6 ($3A_1 + 3E$)
Raman	6 ($3A_1 + 3E$)
Polarized	3 ($3A_1$)
Coincidences	6 ($3A_1 + 3E$)
Silent modes	0

(m) B_2H_6



D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$
N_i	8	2	2	0	0	2	6	4
χ_i	3	-1	-1	-1	-3	1	1	1
Γ_{3n}	24	-2	-2	0	0	2	6	4

$$\Gamma_{3n} = 4A_g + 2B_{1g} + 3B_{2g} + 3B_{3g} + A_u + 4B_{1u} + 3B_{2u} + 4B_{3u}$$
$$\Gamma_{trans} = B_{1u} + B_{2u} + B_{3u} \qquad \Gamma_{rot} = B_{1g} + B_{2g} + B_{3g}$$
$$\Gamma_{3n-6} = 4A_g + B_{1g} + 2B_{2g} + 2B_{3g} + A_u + 3B_{1u} + 2B_{2u} + 3B_{3u}$$

Infrared	8 ($3B_{1u} + 2B_{2u} + 3B_{3u}$)
Raman	9 ($4A_g + B_{1g} + 2B_{2g} + 2B_{3g}$)
Polarized	4 ($4A_g$)
Coincidences	0
Silent modes	1 (A_u)