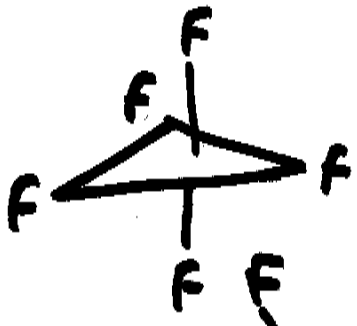
SOME GOOD PRACTICE QUESTIONS

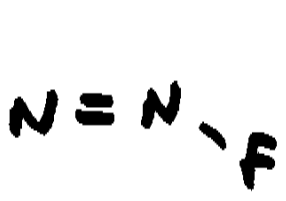
GIVE THE POINT GROUP, Γ_{3N}, AND THE SYMMETRIES OF THE FUNDAMENTAL VIBRATIONS FOR

1) ONCl 

C_s

2) PF_5 

D_{3h}

3) trans - N_2F_2 

4) NH_3

STATE WHICH VIBRATIONS ARE IR & RAMAN ACTIVE (POLARIZED OR DEPOLARIZED) AND WHICH WILL BE COINCIDENT (IF ANY)

(50) (K 1)

SYMMETRY PROBLEM SET KEY

1. ONCl ; BENT PLANAR, C_s (E, σ_h)

C_s	E	σ_h		
A'	1	1	x, y R_z	x^2, y^2, z^2, xy
A''	1	-1	z, R_x, R_y	yz, xz
$\sqrt{\Gamma_{xyz}}$	3	1		
# UNMOVED ATOMS	3	3		
$\sqrt{\Gamma_{3N}}$	9	3		

USING REDUCTION FORMULA

$$a_{A'} = \frac{1}{2}\left\{1.1.9 + 1.1.3\right\} = 6 \Rightarrow 6A'$$

$$a_{A''} = \frac{1}{2}\left\{1.1.9 + 1(-1)(+3)\right\} = 3 \Rightarrow 3A''$$

So $\Gamma_{3N} = 6A' + 3A''$

THE $\Gamma_{TRANS} = 2A' + A''$

$\Gamma_{ROT} = A' + 2A''$

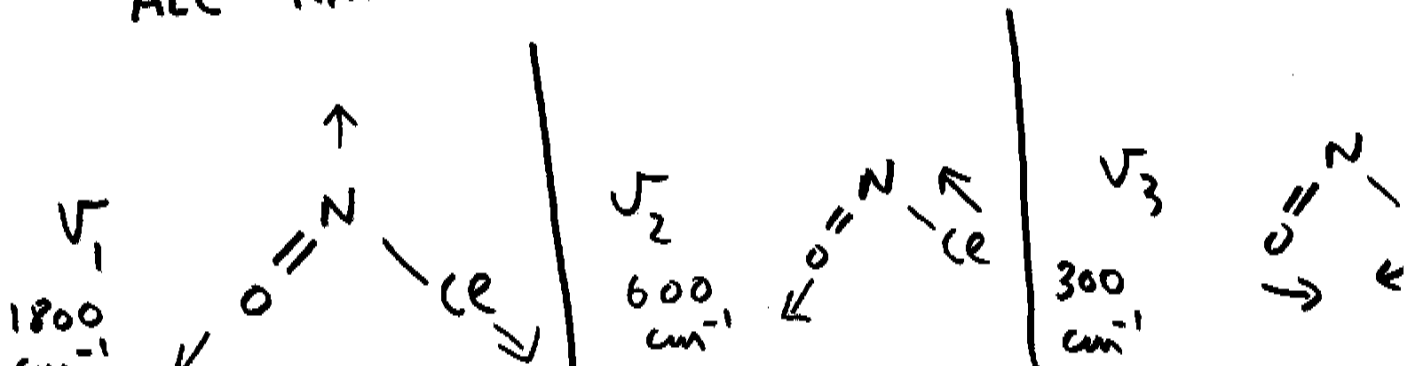
$\therefore \Gamma_{VIB} = 3A'$

THREE FUNDAMENTAL VIBRATIONS

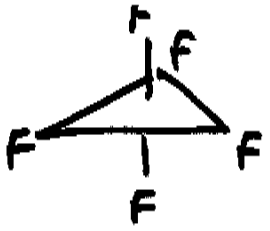
ALL A' TYPE

ALL I.R. ACTIVE

ALL RAMAN ACTIVE AND POLARIZED



(32) KJ

2. PF_5^-  D_{3h},

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$	
A_1'	1	1	1	1	1	1	
A_2'	1	1	−1	1	1	−1	R_z
E'	2	−1	0	2	−1	0	x, y
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
Γ_{xyz}	3	0	−1	1	−2	1	
# UN-MOVED ATOMS	6	3	2	4	1	4	
Γ_{3N}	18	0	−2	4	−2	4	

THE REDUCTION FORMULA WILL GIVE...

$$\Gamma_{3N} = 2A_1' + A_2' + 4E' + 3A_2'' + 2E''$$

AND THE CHARACTER TABLE FOR D_{3h} WILL GIVE

$$\Gamma_{TRANS} = E' + A_2''$$

$$\Gamma_{ROT} = A_2' + E''$$

$$\therefore \Gamma_{VIB} = 2A_1' + 3E' + 2A_2'' + E''$$

(39) ks

FROM WHICH

IR ACTWE : ONLY E' AND A_2'' ARE ACTWE

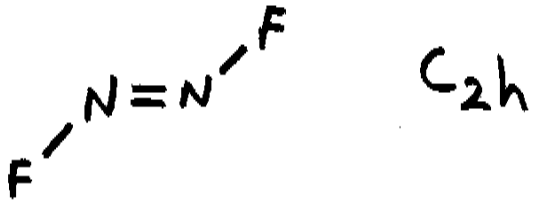
SO YOU WILL GET 5 FUNDAMENTAL BANDS IN THE IR SPECTRUM $(3E', 2A_2'')$

RAMAN A_1', E', E'' ARE RAMAN ACTIVE

SO YOU WILL GET 6 FUNDAMENTALS $(2A_1', 3E' \text{ AND } E'')$ A_1' AND E' (POLARIZED

THREE BANDS WILL BE COINCIDENT IN THE IR AND RAMAN (THE THREE E' BANDS)

35 K6

3.  C_{2h}

C_{2h}	E	C_2	i	σ_h		
A_g	1	1	1	1	R_z	x^2, y^2, z^2, xy
B_g	1	−1	1	−1	R_x R_y	xz, yz
A_u	1	1	−1	−1	z	
B_u	1	−1	−1	1	x, y	
Γ_{xyz}	3	−1	−3	1		
# UN-MOVED ATOMS	4	0	0	4		
Γ_{3N}	12	0	0	4		

THE REDUCTION FORMULA GIVES

$$\Gamma_{3N} = 4A_g + 2B_g + 2A_u + 4B_u$$

AND $\Gamma_{ROT} = 2B_g + A_g$

$\Gamma_{TRANS} = A_u + 2B_u$

So $\Gamma_{VIB} = 3A_g + A_u + 2B_u$

IR ACTIVE : 3 BANDS : $A_u + 2B_u$.

RAMAN ACTIVE: 3 BANDS : $3A_g$ (ALL POLARIZED)

NONE ARE COINCIDENT.

4. NH_3 : C_{3V}

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	−1	0	$(x,y)\ (R_x, R_y)$	x^2-y^2, xy xz, yz.
Γ_{XYZ}	3	0	1		
#UNMOVED ATOMS	4	1	2		
Γ_{3N}	12	0	2		

THE REDUCTION FORMULA GIVES

$$\Gamma_{3N} = 3A_1 + A_2 + 4E \qquad \Gamma_{ROT} = A_2 + E$$

$$\Gamma_{VIB} = 2A_1 + 2E \qquad \Gamma_{TRANS} = A_1 + E$$

ALL IR & RAMAN ACTIVE (& POLARIZED)