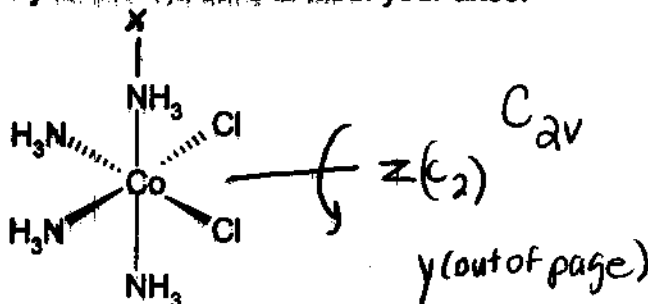


Group Theory

1. (12 marks)

- a) Determine the reducible representation of motion for the following complex and factor out the symmetry labels. Be sure to label your axes!



- b) What are the symmetry labels for the rotational, translational, and vibrational motions?
 c) Which vibrational motions are IR active? Which are Raman active?

(see next page)

2. (12 marks)

- a) The symmetry labels of the vibrational motions for PdCl_4 (square planar) are:

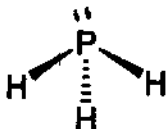
D_{4h}

$$\Gamma_{\text{vib}} = a_{1g} + b_{1g} + b_{2g} + a_{2u} + b_{2u} + 2e_u$$

Determine the symmetry labels for the stretching, bending, and rocking vibrations. Don't forget to label your axes!

3. (15 marks)

- a) Determine the symmetry-labeled σ -bonding molecular orbital (MO) scheme for phosphine. Be sure to label your axes!



C_{3v}

- b) Using projections of the Hydrogen 1s orbitals, determine the normalized and orthogonal wavefunctions for the linear combination of atomic orbitals (LCAOs) of the hydrogen orbitals.
 c) Draw the LCAOs

1a)

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$
	21	1x $\begin{pmatrix} z \rightarrow \cos 0 \\ y \rightarrow \cos 180 \\ x \rightarrow \cos 180 \end{pmatrix}$	3	5
	21	-1	3	5

$$a_1 \Rightarrow \frac{1}{4} (21 - 1 + 3 + 5)$$

$$= \frac{28}{4} = 7a_1$$

$$a_2 \Rightarrow \frac{1}{4} (21 - 1 - 3 - 5)$$

$$= \frac{12}{4}$$

$$= 3a_2$$

$$b_1 \Rightarrow \frac{1}{4} (21 + 1 + 3 - 5)$$

$$= \frac{20}{4} = 5b_1$$

$$b_2 \Rightarrow \frac{1}{4} (21 + 1 - 3 + 5)$$

$$= \frac{24}{4} = 6b_2$$

$$\Gamma_{\text{mot}} = 7a_1 + 3a_2 + 5b_1 + 6b_2 \quad (21 \text{ motions } \checkmark)$$

b) $\Gamma_{\text{rot}} = a_2 + b_1 + b_2$
 $\Gamma_{\text{trans}} = a_1 + b_1 + b_2$

$$\Gamma_{\text{vib}} = 6a_1 + 2a_2 + 3b_1 + 4b_2$$

(3N - 6 vib \checkmark)

c) IR: $6a_1 + 3b_1 + 4b_2$

Raman: $6a_1 + 2a_2 + 3b_1 + 4b_2$

2. D_{4h}

E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	$6h$	$2\sigma_v'$	$6d$
$\Gamma_{\text{Pt-Cl}}$	4	0	0	2	0	0	0	4	2
$\Gamma_{\text{Cl-Pt-Cl}}$	4	0	0	0	2	0	0	4	0
Γ_{stretch}	$a_{1g} + b_{1g} + e_u$								
Γ_{bend}				a_{1g}	$b_{2g} + e_u$				
Γ_{rock}								$a_{2u} + b_{2u}$	

impossible!

