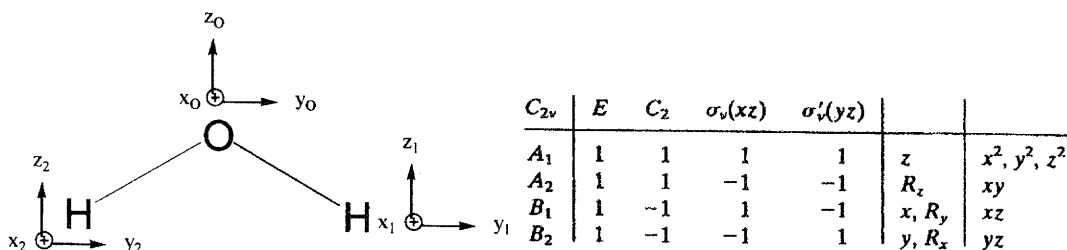科目： 無機化學　　　　　　系所組：化學系碩士班甲組

1) For the free V^{3+} ion, please give an answer to each of the following questions.(5pt each)

    (a) a list of all possible term symbol.

    (b) Which term from (a) is the ground state?

    (c) How many microstates are there for ^3P energy term?

    (d) The L value for the ^1G energy term?

2)   Setting the coordinates of water molecule as follow: (20pt)

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

    Determine the IR active vibration mode of water molecule.

3) For the anion of cyclopentadiene $C_5H_5^-$, use C_5 point group to find the wave functions of pi system in E_1 representation on the basis of p_1, p_2, p_3, p_4 and p_5.(where p_i refers to p_z orbital on the i-th C atom.) # The wave functions have to be normalized. Real number coefficients should be used. (20pt)

C_5	E	C_5	C_5^2	C_5^3	C_5^4	$\varepsilon = \exp(2\pi i/5)$	
A	1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
E_1	$\begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$	$\begin{matrix} \varepsilon \\ \varepsilon^* \end{matrix}$	$\begin{matrix} \varepsilon^2 \\ \varepsilon^{2*} \end{matrix}$	$\begin{matrix} \varepsilon^{2*} \\ \varepsilon^2 \end{matrix}$	$\begin{matrix} \varepsilon^* \\ \varepsilon \end{matrix}$	$(x, y), (R_x, R_y)$	(yz, xz)
E_2	$\begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$	$\begin{matrix} \varepsilon^2 \\ \varepsilon^{2*} \end{matrix}$	$\begin{matrix} \varepsilon^* \\ \varepsilon \end{matrix}$	$\begin{matrix} \varepsilon \\ \varepsilon^* \end{matrix}$	$\begin{matrix} \varepsilon^{2*} \\ \varepsilon^2 \end{matrix}$		$(x^2 - y^2, xy)$

4) (a) What is Jahn-Teller effect? (2pt) (b) In the case of a Mn^{3+} ion in an O_h coordinate field, please draw the energy levels before and after Jahn-Teller distortion (z-out). (3pt) (c) In a z-out Jahn-Teller distortion, if the energy difference between dx^2-y^2 and dz^2 is 2β, how much extra stabilization energy will this distorted complex obtain in compared with perfect O_h field? (5pt)

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5) A molecule has D_{2d} symmetry. Would $p_x \rightarrow d_{xy}$ be an allowed or forbidden transition?(10pt)

D_{2d}	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$		
A_1	1	1	1	1	1		$x^2 + y^2,\ z^2$
A_2	1	1	1	−1	−1	R_z	
B_1	1	−1	1	1	−1		$x^2 - y^2$
B_2	1	−1	1	−1	1	z	xy
E	2	0	−2	0	0	$(x, y),$ (R_x, R_y)	(xz, yz)

6) Please draw the structure of the following compound: (2pt each)

　　(a) $Co_2(CO)_8$ (b) $Ni(CO)_4$ (c) $Fe_2(CO)_9$ (d) $Fe_3(CO)_{12}$ (e) $Ir_4(CO)_{12}$

7) Write the mechanism of Wilkinson's catalyst. (10pt)