

Time: 2 hours

Chemistry 228
Final Exam

February 4, 2000

Name:

Number:

$$R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1} = 0.0821 \text{ L atm K}^{-1} \text{ mol}^{-1}$$

$$h = 6.63 \times 10^{-34} \text{ J s}$$

$$c = 3 \times 10^8 \text{ m s}^{-1}$$

$$R_H = 109678 \text{ cm}^{-1} = 2.18 \times 10^{-18} \text{ J}$$

$$m_e = 9.11 \times 10^{-31} \text{ kg}$$

$$e = 1.60 \times 10^{-19} \text{ C}$$

$$\text{First Bohr radius for H: } r = n^2 h^2 / Z 4 \pi^2 m_e e^2 = a_0 = 0.529 \text{ \AA}$$

$$\text{Energy of a Bohr orbit: } E = -2 \pi^2 m_e e^4 Z^2 / h^2 n^2$$

- (4%) Bohr postulated that the lines in the emission spectrum from hydrogen in highly excited states, such as $n = 20$, would not be observed under ordinary laboratory conditions. Using the Bohr model, calculate the ratio of the cross-sectional area of a hydrogen atom in the $n = 20$ state to that of one in the $n = 1$ state.

- (5%) The Balmer series ($n_i > 2 \rightarrow n_f = 2$) for atomic hydrogen occurs in the visible region of the spectrum. Which series in the emission spectrum of Be^{3+} has its lowest-energy line closest to the first line in the hydrogen Balmer series?

- (7%) Consider the molecule IF_3O_2 (with I as the central atom).
 - (a) Sketch all possible isomers.
 - (b) Assign point group designations to each isomer.

- (7%) Write ground state electron configurations of

- In^+ and In^{3+}

- Fe^{2+} and Fe^{3+}

- Cr^{3+} and Cr^{6+}

- (5%) What is the lanthanide contraction?

- (5%) Show Lewis structures for the following species keeping in mind resonance and formal charges.
 - SeO_3^{2-}
 - N_3^-
 - NO
 - SO_2

- (5%) For each of the following cases give the Lewis structure of a known chemical example.
 - a triatomic molecule with one unpaired electron
 - a triatomic molecule with two double bonds
 - a diatomic molecule with formal charge separation
 - a molecule or ion with four equivalent resonance structures

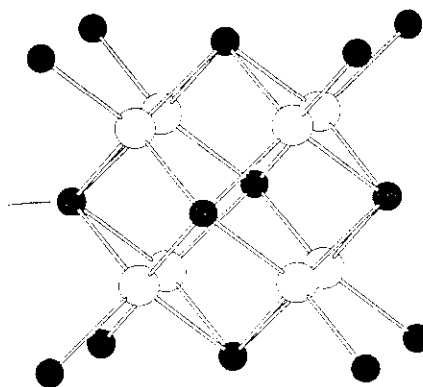
- (4%) How would you expect the X-O bond lengths to vary along the series SiO_4^{4-} , PO_4^{3-} , SO_4^{2-} , ClO_4^- ? Explain your reasoning.

- (5%) Use VSEPR theory to predict the molecular shapes of the following species.
 - ICl_4^-
 - I_3^-
 - SF_4
 - PH_3

- (7%) Consider the covalent molecule AsCl_5 .
 - To which point group does it belong?

 - Determine the infrared (IR) and Raman active modes. How many signals are observed in the IR and Raman spectra, respectively?

- (4%) Use the radius ratio to predict the coordination number of the calcium ions in the following ionic solids. ($r_{\text{Ca}^{2+}} = 1.00 \text{ \AA}$; $r_{\text{F}^-} = 1.33 \text{ \AA}$; $r_{\text{Cl}^-} = 1.67 \text{ \AA}$; $r_{\text{Br}^-} = 1.82 \text{ \AA}$)
 - CaF_2
 - CaCl_2
 - CaBr_2
- (5%) Which class(es) of compounds does the following figure represent? Give examples and explain.



- (5%) Draw the structures of chloric and chlorous acid and predict their pK_a values using Pauling's rules.

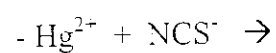
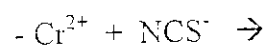
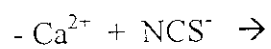
- (5%) An electrically conducting solution is produced when $AlCl_3$ is dissolved in acetonitrile (CH_3CN). Give formulas for the most probable conducting species.

- (6%) (a) The solid Lewis acid AlF_3 is not soluble in liquid HF. However, it dissolves if NaF is added to a mixture of AlF_3 and HF. Explain.

(b) When the solution in part (a) is treated with excess BF_3 , which is soluble in HF, AlF_3 precipitates. Explain.

- (6%) The thiocyanate anion NCS^- can form bonds with Lewis acids in two possible ways.

(a) Indicate in which way bonds are formed in the following cases:

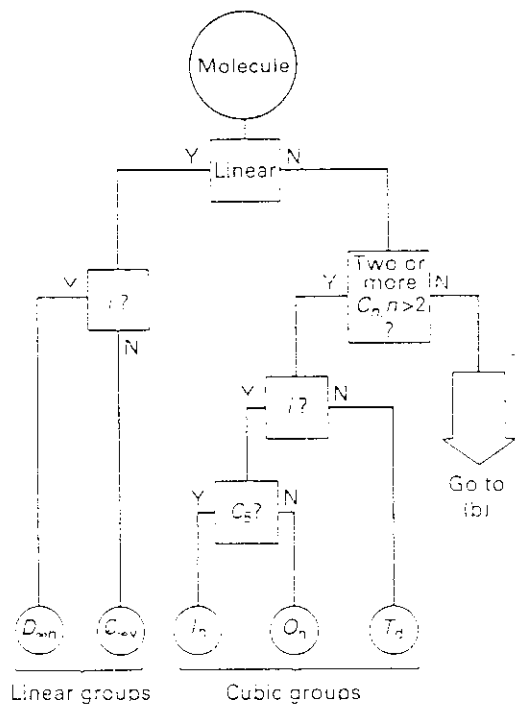


(b) How could infrared spectroscopy (IR) assist in determining which species has formed in (a)?

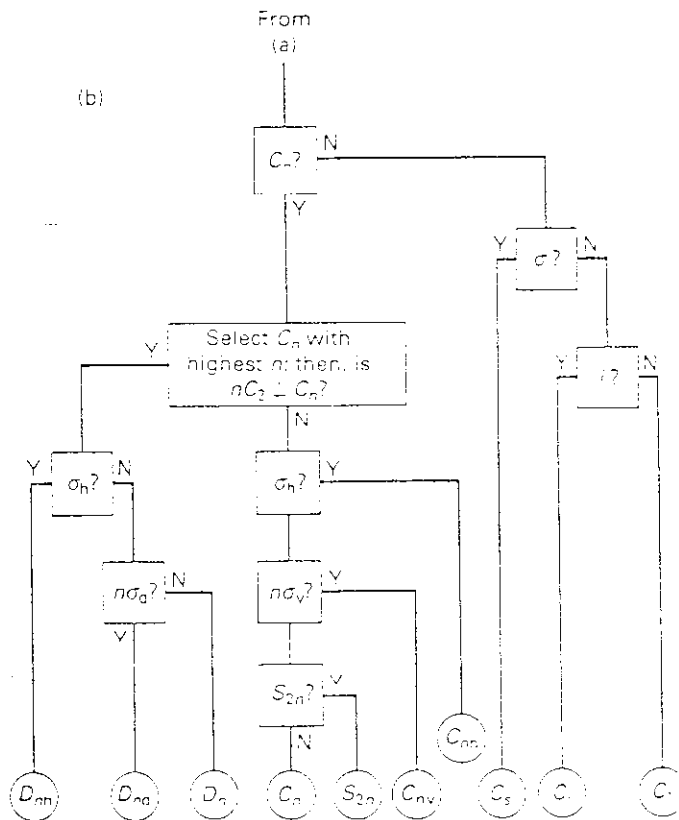
- (7%) Complete the following table on the basis of molecular orbital (MO) theory.

species	HOMO (e.g. $2\sigma_g$)	# of unpaired electrons	bond order
O_2^{2-}			
N_2			
CN^-			
HF			

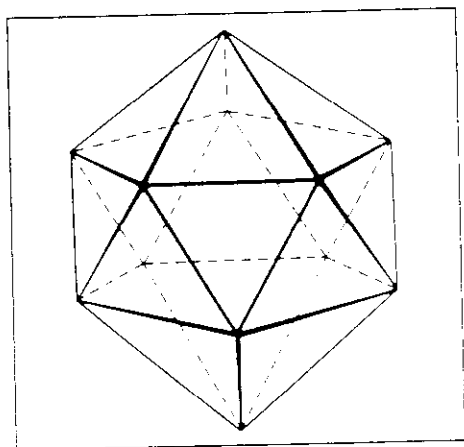
(a)



(b)



C



Character Tables[†]

I. GROUPS OF LOW SYMMETRY

C_1	E			
A	1			
C_2	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
C_3	E	i		
A_1	1	1	R_x, R_y, R_z	$x^2, y^2, z^2, xy, xz, yz$
A_2	1	-1	x, y, z	

2. C_n , C_{nv} AND C_{nh} GROUPS

The C_n groups

C_2	E	C_2		
A	1	1	z, R_z	x^2, y^2, z^2, xy
B	1	-1	x, y, R_x, R_y	yz, xz

[†] $i = \sqrt{-1}$; $\epsilon^* = \epsilon$ with $-i$ substituted for i .

C_1	E	C_3	C_3^2		
A	1	1	1	z, R_z	$x^2 + y^2, z^2$
E	$\begin{Bmatrix} 1 & \epsilon & \epsilon^* \\ & 1 & \epsilon \\ & & 1 \end{Bmatrix}$	ϵ	ϵ^*	$(x, y), (R_x, R_y)$	$(x^2 - y^2, xy), (yz, xz)$

$$\epsilon = e^{i2\pi/3}$$

C_4	E	C_4	C_2	C_4^3		
A	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
B	1	-1	1	-1		$x^2 - y^2, xy$
E	$\begin{Bmatrix} 1 & i & -1 & -i \\ & 1 & -1 & i \\ & & 1 & -i \\ & & & 1 \end{Bmatrix}$	i	-1	$-i$	$(x, y), (R_x, R_y)$	(yz, xz)

C_5	E	C_5	C_5^2	C_5^3	C_5^4		
A	1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
E_1	$\begin{Bmatrix} 1 & \epsilon & \epsilon^2 & \epsilon^{2*} & \epsilon^* \\ & 1 & \epsilon^* & \epsilon^2 & \epsilon \\ & & 1 & \epsilon & \epsilon^2 \\ & & & 1 & \epsilon^* \\ & & & & 1 \end{Bmatrix}$	ϵ	ϵ^2	ϵ^{2*}	ϵ^*	$(x, y), (R_x, R_y)$	(yz, xz)
E_2	$\begin{Bmatrix} 1 & \epsilon^2 & \epsilon^* & \epsilon & \epsilon^{2*} \\ & 1 & \epsilon^* & \epsilon & \epsilon^2 \\ & & 1 & \epsilon^* & \epsilon \\ & & & 1 & \epsilon^2 \\ & & & & 1 \end{Bmatrix}$	ϵ^2	ϵ^*	ϵ	ϵ^{2*}		$(x^2 - y^2, xy)$

$$\epsilon = e^{i2\pi/5}$$

C_6	E	C_6	C_3	C_2	C_3^2	C_6^5		
A	1	1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
B	1	-1	1	-1	1	-1		
E_1	$\begin{Bmatrix} 1 & \epsilon & -\epsilon^* & -1 & -\epsilon & \epsilon^* \\ & 1 & \epsilon^* & -\epsilon & -1 & -\epsilon^* \\ & & 1 & -\epsilon & 1 & -\epsilon^* \\ & & & 1 & -\epsilon & -\epsilon^* \end{Bmatrix}$	ϵ	$-\epsilon^*$	-1	$-\epsilon$	ϵ^*	$(x, y), (R_x, R_y)$	(xz, yz)
E_2	$\begin{Bmatrix} 1 & -\epsilon^* & -\epsilon & 1 & -\epsilon^* & -\epsilon \\ & 1 & -\epsilon & -\epsilon^* & 1 & -\epsilon^* \\ & & 1 & -\epsilon^* & -\epsilon & -\epsilon^* \\ & & & 1 & -\epsilon & -\epsilon^* \end{Bmatrix}$	$-\epsilon^*$	$-\epsilon$	1	$-\epsilon^*$	$-\epsilon$		$(x^2 - y^2, xy)$

$$\epsilon = e^{i\pi/3}$$

C_7	E	C_7	C_3^2	C_3	C_2	C_3	C_2		
A	1	1	1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
E_1	$\begin{Bmatrix} 1 & \epsilon & \epsilon^2 & \epsilon^3 & \epsilon^{3*} & \epsilon^{2*} & \epsilon^* \\ & 1 & \epsilon^* & \epsilon^{3*} & \epsilon^3 & \epsilon^2 & \epsilon \\ & & 1 & \epsilon^* & \epsilon & \epsilon^2 & \epsilon^{2*} \\ & & & 1 & \epsilon^* & \epsilon^3 & \epsilon^2 \\ & & & & 1 & \epsilon^* & \epsilon^3 \\ & & & & & 1 & \epsilon^* \end{Bmatrix}$	ϵ	ϵ^2	ϵ^3	ϵ^{3*}	ϵ^{2*}	ϵ^*	$(x, y), (R_x, R_y)$	(xz, yz)
E_2	$\begin{Bmatrix} 1 & \epsilon^2 & \epsilon^{3*} & \epsilon^* & \epsilon & \epsilon^3 & \epsilon^{2*} \\ & 1 & \epsilon^{3*} & \epsilon^* & \epsilon & \epsilon^3 & \epsilon^2 \\ & & 1 & \epsilon^* & \epsilon & \epsilon^3 & \epsilon^2 \\ & & & 1 & \epsilon^* & \epsilon^3 & \epsilon^2 \\ & & & & 1 & \epsilon^* & \epsilon^3 \\ & & & & & 1 & \epsilon^* \end{Bmatrix}$	ϵ^2	ϵ^{3*}	ϵ^*	ϵ	ϵ^3	ϵ^{2*}		$(x^2 - y^2, xy)$
E_3	$\begin{Bmatrix} 1 & \epsilon^3 & \epsilon^* & \epsilon^2 & \epsilon^{2*} & \epsilon & \epsilon^{3*} \\ & 1 & \epsilon^* & \epsilon^2 & \epsilon^{2*} & \epsilon & \epsilon^{3*} \\ & & 1 & \epsilon^2 & \epsilon^{2*} & \epsilon & \epsilon^{3*} \\ & & & 1 & \epsilon^2 & \epsilon^{2*} & \epsilon \\ & & & & 1 & \epsilon^2 & \epsilon^{2*} \\ & & & & & 1 & \epsilon^2 \end{Bmatrix}$	ϵ^3	ϵ^*	ϵ^2	ϵ^{2*}	ϵ	ϵ^{3*}		

$$\epsilon = e^{i2\pi/7}$$

C_8	E	C_8	C_4	C_2	C_4^3	C_4^2	C_4	C_4^3		
A	1	1	1	1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
B	1	-1	1	1	1	-1	-1	-1		
E_1	$\begin{Bmatrix} 1 & \epsilon & i & -1 & -i & -\epsilon^* & -\epsilon & \epsilon^* \\ & 1 & \epsilon^* & -i & -1 & -\epsilon & -\epsilon^* & \epsilon \\ & & 1 & -i & -1 & -\epsilon & -\epsilon^* & \epsilon \\ & & & 1 & -1 & -i & i & -i \\ & & & & 1 & -i & i & -i \\ & & & & & 1 & i & -i \end{Bmatrix}$	ϵ	i	-1	$-\epsilon^*$	$-\epsilon$	ϵ^*	$(x, y), (R_x, R_y)$	(xz, yz)	
E_2	$\begin{Bmatrix} 1 & i & -1 & 1 & -1 & -i & i & -i \\ & 1 & -i & -1 & -1 & i & -i & i \\ & & 1 & -1 & -1 & i & -i & i \\ & & & 1 & -1 & i & -i & i \\ & & & & 1 & i & -i & i \\ & & & & & 1 & i & i \end{Bmatrix}$	i	-1	-1	$-i$	i	$-i$		$(x^2 - y^2, xy)$	
E_3	$\begin{Bmatrix} 1 & -\epsilon & i & -1 & -i & \epsilon^* & \epsilon & -\epsilon^* \\ & 1 & -\epsilon^* & i & -1 & i & \epsilon & -\epsilon^* \\ & & 1 & i & -1 & i & \epsilon & -\epsilon^* \\ & & & 1 & -1 & i & \epsilon & -\epsilon^* \\ & & & & 1 & i & \epsilon & -\epsilon^* \\ & & & & & 1 & i & \epsilon \end{Bmatrix}$	$-\epsilon$	i	-1	ϵ^*	ϵ	$-\epsilon^*$			

$$\epsilon = e^{i\pi/4}$$

The C_{nv} groups

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

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	$(x, y), (R_x, R_y)$		$(x^2 - y^2, xy), (xz, yz)$

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$		
A_1	1	1	1	1	1	z	$x^2 - y^2, z^2$
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		xy
E	2	0	-2	0	0	$(x, y), (R_x, R_y)$	(xz, yz)

C_{5v}	E	$2C_5$	$2C_5^2$	$5\sigma_v$		
A_1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	-1	R_z	
E_1	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	$(x, y), (R_x, R_y)$	(xz, yz)
E_2	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0		$(x^2 - y^2, xy)$

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$		
A_1	1	1	1	1	1	1	z	$x^2 - y^2, z^2$
A_2	1	1	1	1	-1	-1	R_z	
B_1	1	-1	1	-1	1	-1		
B_2	1	-1	1	-1	-1	1		
E_1	2	1	-1	-2	0	0	$(x, y), (R_x, R_y)$	(xz, yz)
E_2	2	-1	-1	2	0	0		$(x^2 - y^2, xy)$

The C_{nh} groups

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	

C_{3h}	E	C_3	C_3^2	σ_h	S_6	S_6^5		
A'	1	1	1	1	1	1	R_z	$x^2 - y^2, z^2$
E'	$\left\{ \begin{array}{l} 1 \\ 1 \end{array} \right.$	$\left\{ \begin{array}{l} \epsilon \\ \epsilon^* \end{array} \right.$	$\left\{ \begin{array}{l} \epsilon^* \\ \epsilon \end{array} \right.$	$\left\{ \begin{array}{l} 1 \\ 1 \end{array} \right.$	$\left\{ \begin{array}{l} \epsilon \\ \epsilon^* \end{array} \right.$	$\left\{ \begin{array}{l} \epsilon^* \\ \epsilon \end{array} \right.$	(x, y)	$(x^2 - y^2, xy)$
A''	1	1	1	-1	-1	-1	z	
E''	$\left\{ \begin{array}{l} 1 \\ 1 \end{array} \right.$	$\left\{ \begin{array}{l} \epsilon \\ \epsilon^* \end{array} \right.$	$\left\{ \begin{array}{l} \epsilon^* \\ \epsilon \end{array} \right.$	$\left\{ \begin{array}{l} -1 \\ -1 \end{array} \right.$	$\left\{ \begin{array}{l} -\epsilon \\ -\epsilon^* \end{array} \right.$	$\left\{ \begin{array}{l} -\epsilon^* \\ -\epsilon \end{array} \right.$	(R_x, R_y)	(xz, yz)

$\epsilon = e^{2\pi i/3}$

3. D_n , D_{nd} , AND D_{nh} GROUPS

The D_n groups

D_2	E	$C_2(z)$	$C_2(y)$	$C_2(x)$			
A	1	1	1	1			x^2, y^2, z^2
B_1	1	1	-1	-1	z, R_z		xy
B_2	1	-1	1	-1	y, R_y		xz
B_3	1	-1	-1	1	x, R_x		yz
D_3	E	$2C_3$	$3C_2$				
A_1	1	1	1				$x^2 + y^2, z^2$
A_2	1	1	-1	z, R_z			
E	2	-1	0	$(x, y), (R_x, R_y)$			$(x^2 - y^2, xy), (xz, yz)$
D_4	E	$2C_4$	$C_2(=C_4^2)$	$2C_2'$	$2C_2''$		
A_1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	1	-1	-1	z, R_z	
B_1	1	-1	1	1	-1		$x^2 - y^2$
B_2	1	-1	1	-1	1		xy
E	2	0	-2	0	0	$(x, y), (R_x, R_y)$	(xz, yz)
D_5	E	$2C_5$	$2C_5^2$	$5C_2$			
A_1	1	1	1	1			$x^2 + y^2, z^2$
A_2	1	1	1	-1	z, R_z		
E_1	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	$(x, y), (R_x, R_y)$		(xz, yz)
E_2	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0			$(x^2 - y^2, xy)$
D_6	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$	
A_1	1	1	1	1	1	1	$x^2 + y^2, z^2$
A_2	1	1	1	1	-1	-1	z, R_z
B_1	1	-1	1	-1	1	-1	
B_2	1	-1	1	-1	-1	1	
E_1	2	1	-1	-2	0	0	$(x, y), (R_x, R_y)$
E_2	2	-1	-1	2	0	0	(xz, yz) $(x^2 - y^2, xy)$

The D_{nd} groups

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)
D_{3d}	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$	
A_{1g}	1	1	1	1	1	1	$x^2 + y^2, z^2$
A_{2g}	1	1	-1	1	1	-1	R_z
E_g	2	-1	0	2	-1	0	(R_x, R_y)
A_{1u}	1	1	1	-1	-1	-1	
A_{2u}	1	1	-1	-1	-1	1	z
E_u	2	-1	0	-2	1	0	(x, y)

D_{3d}	E	$2S_6$	$2C_4$	$2S_8$	C_2	$4C_2'$	$4\sigma_d$		
A_1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_2	1	1	1	1	1	-1	-1		
B_1	1	-1	1	-1	1	1	-1	z	$(x^2 - y^2, xy)$
B_2	1	-1	1	-1	1	-1	1		
E_1	2	$\sqrt{2}$	0	$-\sqrt{2}$	-2	0	0	(R_x, R_y)	(xz, yz)
E_2	2	0	-2	0	2	0	0		
E_3	2	$-\sqrt{2}$	0	$\sqrt{2}$	-2	0	0		

D_{3d}	E	$2C_2$	$2C_2'$	$5C_2$	i	$2S_{10}$	$2S_{10}$	$5\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_{2g}	1	1	1	-1	1	1	1	-1		
E_{1g}	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	(R_x, R_y)	(xz, yz)
E_{2g}	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0		
A_{1u}	1	1	1	1	-1	-1	-1	-1	z	$(x^2 - y^2, xy)$
A_{2u}	1	1	1	-1	-1	-1	-1	1		
E_{1u}	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	-2	$-2 \cos 72^\circ$	$-2 \cos 144^\circ$	0	(x, y)	
E_{2u}	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0	-2	$-2 \cos 144^\circ$	$-2 \cos 72^\circ$	0		

D_{3d}	E	$2S_{12}$	$2C_6$	$2S_4$	$2C_3$	$2S_{12}'$	C_2	$6C_2'$	$6\sigma_d$		
A_1	1	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_2	1	1	1	1	1	1	1	-1	-1		
B_1	1	-1	1	-1	1	-1	1	1	-1	z	$(x^2 - y^2, xy)$
B_2	1	-1	1	-1	1	-1	1	-1	1		
E_1	2	$\sqrt{3}$	1	0	-1	$-\sqrt{3}$	-2	0	0	(R_x, R_y)	(xz, yz)
E_2	2	1	-1	-2	-1	1	2	0	0		
E_3	2	0	-2	0	2	0	-2	0	0		
E_4	2	-1	-1	2	-1	$-\sqrt{3}$	2	0	0		
E_5	2	$-\sqrt{3}$	1	0	-1	$\sqrt{3}$	-2	0	0		

The D_{nh} groups

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$		
A_g	1	1	1	1	1	1	1	1	R_z	x^2, y^2, z^2
B_{1g}	1	1	-1	-1	1	1	-1	-1		
B_{2g}	1	-1	1	-1	1	-1	1	-1	R_x	xy
B_{3g}	1	-1	-1	1	1	-1	-1	1		
A_u	1	1	1	1	-1	-1	-1	-1	R_y	xz
B_{1u}	1	1	-1	-1	-1	-1	1	1		
B_{2u}	1	-1	1	-1	-1	1	-1	1	R_z	yz
B_{3u}	1	-1	-1	1	-1	1	1	-1		

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_6$	$3\sigma_v$		
A_1'	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_2'	1	1	-1	1	1	-1		
E'	2	-1	0	2	-1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	-1	-1	-1	z	(xz, yz)
A_2''	1	1	-1	-1	-1	1		
E''	2	-1	0	-2	1	0	(R_x, R_y)	

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1		$x^2 - y^2$
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1	(R_x, R_y)	xy
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1		(xz, yz)
E_{1g}	2	0	-2	0	0	2	0	-2	0	0		
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1	z	
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1		
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1	(x, y)	
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1		
E_{1u}	2	0	-2	0	0	-2	0	2	0	0		

D_{3h}	E	$2C_3$	$2C_2$	$3C_2$	σ_h	$2S_6$	$2S_6^5$	$3\sigma_v$		
A_1'	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_2'	1	1	1	-1	1	1	1	-1		(x, y)
E_1'	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	$(x^2 - y^2, xy)$	
E_2'	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0		
A_1''	1	1	1	1	-1	-1	-1	-1	z	
A_2''	1	1	1	-1	-1	-1	-1	1		(R_x, R_y)
E_1''	2	$2 \cos 72^\circ$	$2 \cos 144^\circ$	0	-2	$-2 \cos 72^\circ$	$-2 \cos 144^\circ$	0	(xz, yz)	
E_2''	2	$2 \cos 144^\circ$	$2 \cos 72^\circ$	0	-2	$-2 \cos 144^\circ$	$-2 \cos 72^\circ$	0		

D_{6h}	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$	i	$2S_6$	$2S_6^5$	σ_h	$3\sigma_d$	$3\sigma_v$		
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_{2g}	1	1	1	1	-1	-1	1	1	1	1	-1	-1		(x, y)
B_{1g}	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	(R_x, R_y)	(xz, yz)
B_{2g}	1	-1	1	-1	-1	1	1	-1	1	-1	-1	1		$(x^2 - y^2, xy)$
E_{1g}	2	1	-1	-2	0	0	2	1	-1	-2	0	0		
E_{2g}	2	-1	-1	2	0	0	2	-1	-1	2	0	0		
A_{1u}	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	z	
A_{2u}	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1		(x, y)
B_{1u}	1	-1	1	-1	1	-1	-1	1	-1	1	-1	-1	(x, y)	
B_{2u}	1	-1	1	-1	-1	1	-1	1	-1	1	1	-1		
E_{1u}	2	1	-1	-2	0	0	-2	-1	1	2	0	0		
E_{2u}	2	-1	-1	2	0	0	-2	1	1	-2	0	0		

D_{8h}	E	$2C_8$	$2C_4$	C_2	$4C_2'$	$4C_2''$	i	$2S_8$	$2S_8^3$	$2S_4$	σ_h	$4\sigma_d$	$4\sigma_v$		
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_{2g}	1	1	1	1	1	-1	-1	1	1	1	1	-1	-1		(x, y)
B_{1g}	1	-1	-1	1	1	1	-1	1	-1	1	1	1	-1	(R_x, R_y)	(xz, yz)
B_{2g}	1	-1	-1	1	1	-1	1	1	-1	1	1	-1	1		$(x^2 - y^2, xy)$
E_{1g}	2	$\sqrt{2}$	$-\sqrt{2}$	0	-2	0	0	2	$\sqrt{2}$	$-\sqrt{2}$	0	-2	0		
E_{2g}	2	0	0	-2	2	0	0	2	0	0	-2	2	0		
E_{3g}	2	$-\sqrt{2}$	$\sqrt{2}$	0	-2	0	0	2	$-\sqrt{2}$	$\sqrt{2}$	0	-2	0		
A_{1u}	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	-1	z	
A_{2u}	1	1	1	1	1	-1	-1	-1	-1	-1	-1	-1	1		(x, y)
B_{1u}	1	-1	-1	1	1	1	-1	-1	1	1	-1	-1	-1	(x, y)	
B_{2u}	1	-1	-1	1	1	-1	1	-1	1	1	-1	-1	1		
E_{1u}	2	$\sqrt{2}$	$-\sqrt{2}$	0	-2	0	0	-2	$-\sqrt{2}$	$\sqrt{2}$	0	2	0		
E_{2u}	2	0	0	-2	2	0	0	-2	0	0	2	-2	0		
E_{3u}	2	$-\sqrt{2}$	$\sqrt{2}$	0	-2	0	0	-2	$\sqrt{2}$	$-\sqrt{2}$	0	2	0		

4. LINEAR GROUPS

C_{nv}	E	$2C_n^{\phi}$...	∞C_2		
$A_1 \equiv \Sigma^+$	1	1	...	1	z	$x^2 + y^2, z^2$
$A_2 \equiv \Sigma^-$	1	1	...	-1	R_z	
$E_1 \equiv \Pi$	2	$2 \cos \phi$...	0	$(x, y), (R_x, R_y)$	(xz, yz)
$E_2 \equiv \Delta$	2	$2 \cos 2\phi$...	0		$(x^2 - y^2, xy)$
$E_3 \equiv \Phi$	2	$2 \cos 3\phi$...	0		
...		

D_{nh}	E	$2C_n^{\phi}$...	∞C_2	i	$2S_2^{\phi}$...	∞C_2	
Σ_g^+	1	1	...	1	1	1	...	1	$x^2 + y^2, z^2$
Σ_g^-	1	1	...	-1	1	1	...	-1	
Π_g	2	$2 \cos \phi$...	0	2	$-2 \cos \phi$...	0	(R_x, R_y)
Δ_g	2	$2 \cos 2\phi$...	0	2	$2 \cos 2\phi$...	0	(xz, yz)
...	$(x^2 - y^2, xy)$
Σ_u^+	1	1	...	1	-1	-1	...	-1	z
Σ_u^-	1	1	...	-1	-1	-1	...	1	
Π_u	2	$2 \cos \phi$...	0	-2	$2 \cos \phi$...	0	(x, y)
Δ_u	2	$2 \cos 2\phi$...	0	-2	$-2 \cos 2\phi$...	0	
...	

5. S_{2n} GROUPS

S_4	E	S_4	C_2	S_4^3		
A	1	1	1	1	R_z	$x^2 - y^2, z^2$
B	1	-1	1	-1	z	$x^2 - y^2, xy$
E	$\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}$	$\begin{pmatrix} i & -1 \\ -i & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & -i \\ -1 & i \end{pmatrix}$	$\begin{pmatrix} -i & 1 \\ i & 1 \end{pmatrix}$	$(x, y), (R_x, R_y)$	(xz, yz)

S_n	E	C_n	C_n^2	i	S_n^2	S_n	
A_2	1	1	1	1	1	1	R_z
E_2	$\begin{pmatrix} 1 & \epsilon \\ 1 & \epsilon^* \end{pmatrix}$	$\begin{pmatrix} \epsilon & \epsilon^* \\ \epsilon^* & \epsilon \end{pmatrix}$	$\begin{pmatrix} \epsilon^2 & \epsilon^{*2} \\ \epsilon^{*2} & \epsilon^2 \end{pmatrix}$	$\begin{pmatrix} 1 & -i \\ -1 & -i \end{pmatrix}$	$\begin{pmatrix} \epsilon & \epsilon^* \\ -\epsilon & -\epsilon^* \end{pmatrix}$	$\begin{pmatrix} \epsilon^* & \epsilon \\ \epsilon & \epsilon^* \end{pmatrix}$	(R_x, R_y)
A_1	1	1	1	-1	-1	-1	z
E_1	$\begin{pmatrix} 1 & \epsilon \\ 1 & \epsilon^* \end{pmatrix}$	$\begin{pmatrix} \epsilon & \epsilon^* \\ \epsilon^* & \epsilon \end{pmatrix}$	$\begin{pmatrix} \epsilon^2 & \epsilon^{*2} \\ \epsilon^{*2} & \epsilon^2 \end{pmatrix}$	$\begin{pmatrix} -1 & i \\ 1 & i \end{pmatrix}$	$\begin{pmatrix} -\epsilon & -\epsilon^* \\ \epsilon & \epsilon^* \end{pmatrix}$	$\begin{pmatrix} -\epsilon^* & -\epsilon \\ -\epsilon & -\epsilon^* \end{pmatrix}$	(x, y)

$\epsilon = e^{i2\pi/n}$

S_8	E	S_8	C_4	S_8^3	C_2	S_8^5	C_4^3	S_8^7	
A	1	1	1	1	1	1	1	1	R_z
B	1	-1	1	-1	1	-1	1	-1	z
E_1	$\begin{pmatrix} 1 & \epsilon \\ 1 & \epsilon^* \end{pmatrix}$	$\begin{pmatrix} \epsilon & \epsilon^* \\ \epsilon^* & \epsilon \end{pmatrix}$	$\begin{pmatrix} i & -i \\ -i & i \end{pmatrix}$	$\begin{pmatrix} -\epsilon^* & -\epsilon \\ -\epsilon & -\epsilon^* \end{pmatrix}$	$\begin{pmatrix} -1 & -\epsilon^* \\ -1 & -\epsilon \end{pmatrix}$	$\begin{pmatrix} -\epsilon & \epsilon^* \\ \epsilon^* & \epsilon \end{pmatrix}$	$\begin{pmatrix} -i & i \\ i & -i \end{pmatrix}$	$\begin{pmatrix} \epsilon^* & \epsilon \\ \epsilon & \epsilon^* \end{pmatrix}$	$(x, y), (R_x, R_y)$
E_2	$\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}$	$\begin{pmatrix} i & -1 \\ -i & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & -i \\ -1 & i \end{pmatrix}$	$\begin{pmatrix} -i & 1 \\ i & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & -\epsilon^* \\ 1 & -\epsilon \end{pmatrix}$	$\begin{pmatrix} 1 & \epsilon^* \\ 1 & \epsilon \end{pmatrix}$	$\begin{pmatrix} -1 & i \\ -1 & -i \end{pmatrix}$	$\begin{pmatrix} \epsilon & \epsilon^* \\ \epsilon^* & \epsilon \end{pmatrix}$	$(x^2 - y^2, xy)$
E_3	$\begin{pmatrix} 1 & \epsilon^* \\ 1 & \epsilon \end{pmatrix}$	$\begin{pmatrix} \epsilon^* & \epsilon \\ \epsilon & \epsilon^* \end{pmatrix}$	$\begin{pmatrix} -i & i \\ i & -i \end{pmatrix}$	$\begin{pmatrix} -\epsilon & -\epsilon^* \\ -\epsilon^* & -\epsilon \end{pmatrix}$	$\begin{pmatrix} -1 & \epsilon^* \\ -1 & \epsilon \end{pmatrix}$	$\begin{pmatrix} -1 & \epsilon \\ -1 & \epsilon^* \end{pmatrix}$	$\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}$	$\begin{pmatrix} \epsilon^* & \epsilon \\ \epsilon & \epsilon^* \end{pmatrix}$	(xz, yz)

$\epsilon = e^{i2\pi/8}$

6. TETRAHEDRAL, OCTAHEDRAL, AND ICOSAHEDRAL GROUPS

T	E	$4C_3$	$4C_3^2$	$3C_2$		
A	1	1	1	1		$x^2 + y^2 + z^2$
E	1	ϵ	ϵ^*	1		$(2z^2 - x^2 - y^2,$
	1	ϵ^*	ϵ	1		$x^2 - y^2)$
T	3	0	0	-1	$(R_x, R_y, R_z), (x, y, z)$	(xy, xz, yz)

$\epsilon = e^{(2\pi i)/3}$

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	
A_1	1	1	1	1	1	$x^2 + y^2 + z^2$
A_2	1	1	1	-1	-1	
E	2	-1	2	0	0	$(2z^2 - x^2 - y^2,$
						$x^2 - y^2)$
T_1	3	0	-1	1	-1	(R_x, R_y, R_z)
T_2	3	0	-1	-1	1	(x, y, z)
						(xy, xz, yz)

T_h	E	$4C_3$	$4C_3^2$	$3C_2$	i	$4S_6$	$4S_6^5$	$3\sigma_h$	
A_g	1	1	1	1	1	1	1	1	$x^2 + y^2 + z^2$
A_u	1	1	1	1	-1	-1	-1	-1	
E_g	1	ϵ	ϵ^*	1	1	ϵ	ϵ^*	1	$(2z^2 - x^2 - y^2,$
	1	ϵ^*	ϵ	1	1	ϵ^*	ϵ	1	$x^2 - y^2)$
E_u	1	ϵ	ϵ^*	1	-1	$-\epsilon$	$-\epsilon^*$	-1	
	1	ϵ^*	ϵ	1	-1	$-\epsilon^*$	$-\epsilon$	-1	
T_g	3	0	0	-1	3	0	0	-1	(R_x, R_y, R_z)
T_u	3	0	0	-1	-3	0	0	1	(x, y, z)
									(xy, xz, yz)

$\epsilon = e^{(2\pi i)/3}$

O	E	$6C_4$	$3C_2 (= C_4^2)$	$8C_3$	$6C_2$	
A_1	1	1	1	1	1	$x^2 + y^2 + z^2$
A_2	1	-1	1	1	-1	
E	2	0	2	-1	0	$(2z^2 - x^2 - y^2,$
						$x^2 - y^2)$
T_1	3	1	-1	0	-1	$(R_x, R_y, R_z), (x, y, z)$
T_2	3	-1	-1	0	1	(xy, xz, yz)

O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2(C=C)$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$	
A_{1g}	1	1	1	1	1	1	1	1	1	1	$x^2 + y^2 + z^2$
A_{2g}	1	1	-1	1	1	1	-1	1	1	-1	$(2z^2 - x^2 - y^2)$
E_g	2	-1	0	0	2	2	0	-1	2	0	(xy, xz, yz)
T_{1g}	3	0	-1	1	-1	3	1	0	1	-1	(R_x, R_y, R_z)
T_{2g}	3	0	1	-1	-1	3	1	0	-1	1	
A_{1u}	1	1	1	1	1	-1	1	-1	-1	-1	
A_{2u}	1	1	-1	1	1	-1	1	-1	-1	1	
E_u	2	-1	0	0	2	-2	0	1	-2	0	
T_{1u}	3	0	-1	1	-1	3	-1	0	1	1	(x, y, z)
T_{2u}	3	0	1	-1	-1	3	-1	0	1	-1	

I	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	
A	1	1	1	1	1	$x^2 + y^2 + z^2$
T_1	3	$\frac{1}{2}(1 + \sqrt{5})$	$\frac{1}{2}(1 - \sqrt{5})$	0	-1	$(x, y, z), (R_x, R_y, R_z)$
T_2	3	$\frac{1}{2}(1 - \sqrt{5})$	$\frac{1}{2}(1 + \sqrt{5})$	0	-1	
G	4	-1	1	1	0	$(xy, xz, yz, x^2 - y^2, 2z^2 - x^2 - y^2)$
H	5	0	0	1	1	

I_h	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	i	$12S_{10}$	$12S_6$	15σ	
A_g	1	1	1	1	1	1	1	1	1	$x^2 + y^2 + z^2$
T_{1g}	3	$\frac{1}{2}(1 + \sqrt{5})$	$\frac{1}{2}(1 - \sqrt{5})$	0	1	3	$\frac{1}{2}(1 - \sqrt{5})$	$\frac{1}{2}(1 + \sqrt{5})$	1	(R_x, R_y, R_z)
T_{2g}	3	$\frac{1}{2}(1 - \sqrt{5})$	$\frac{1}{2}(1 + \sqrt{5})$	0	1	3	$\frac{1}{2}(1 + \sqrt{5})$	$\frac{1}{2}(1 - \sqrt{5})$	1	
G_g	4	-1	1	1	0	4	-1	0	0	
H_g	5	0	0	1	1	5	0	-1	1	$(2z^2 - x^2 - y^2, x^2 - y^2, xy, xz, yz)$
A_u	1	1	1	1	1	1	1	1	-1	(x, y, z)
T_{1u}	3	$\frac{1}{2}(1 + \sqrt{5})$	$\frac{1}{2}(1 - \sqrt{5})$	0	1	3	$-\frac{1}{2}(1 + \sqrt{5})$	$-\frac{1}{2}(1 - \sqrt{5})$	1	
T_{2u}	3	$\frac{1}{2}(1 - \sqrt{5})$	$\frac{1}{2}(1 + \sqrt{5})$	0	1	-3	$\frac{1}{2}(1 + \sqrt{5})$	$\frac{1}{2}(1 - \sqrt{5})$	1	
G_u	4	-1	1	1	0	4	-1	0	0	
H_u	5	0	0	1	1	5	0	1	1	