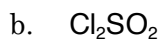


1. (8 pts. ea.) Draw Lewis structures for the following molecules.



1. _____

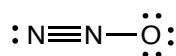
2. _____

3. _____

4. _____

2. a. (8 pts. ea.) Draw resonance structures for the following Lewis structure.

b. (6 pts. ea.) Rank the structures from lower (1) to higher (2, 3, etc) energy.



5. _____

6. _____

7. _____

8. _____

3. (8 pts. ea.) Determine the three-dimensional shapes of the following molecules and explain your choice (lone pairs not on the central atom have been omitted for clarity).

a.	b.
--	--

9. _____

10. _____

4. a. (6 pts.) An electron has the quantum numbers $n = 5$, $l = 2$, $m_l = 0$, $m_s = -1/2$. Is this an allowed state? If so, what is the orbital designation for this electron? If it is not, explain why it isn't.

b. (6 pts.) An electron has the quantum numbers $n = 2$, $l = 3$, $m_l = -1$, $m_s = +1/2$. Is this an allowed state? If so, what is the orbital designation for this electron? If it is not, explain why it isn't.

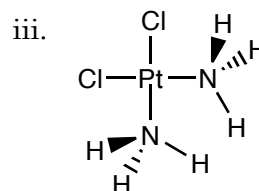
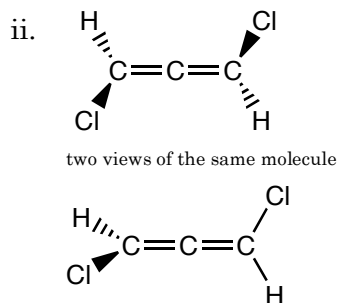
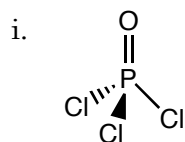
5. (10 pts.) Briefly describe how elements are formed from hydrogen and helium. You do not need to explain how all the elements are formed, highlights about how some of the elements are formed is sufficient; nevertheless, you'll want to make certain that some of the elements are lighter elements and some are heavier elements.
6. a. (10 pts.) Even though fluorine has more protons, neutrons and electrons than Li, it is smaller than Li. Explain this observation.
- b. (10 pts.) In general, as one moves from left to right across a period, it becomes more difficult to remove an electron from an atom. However, it is easier to remove an electron from an oxygen atom than it is to remove an electron from a nitrogen atom. Explain this observation.
7. (10 pts.) Describe the traits that Mendeleev's table and the current periodic table have in common. Describe how they differ. (Please don't tell me that Mendeleev's table had fewer elements on it, unless of course, you are describing how the appearance of the table has changed, thanks.)

8. (8 pts.) For the C_{3v} point group determine the irreducible representation for the following reducible representation (Γ).

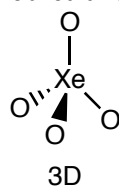
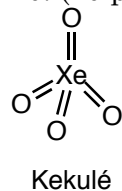
C_{3v}	E	2 C_3	3 σ_v
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0
Γ	5	2	-1

9. a. (4 pts. ea.) Determine the point groups of the following molecules.

b. (2 pts. ea.) Label the chiral molecules (character tables are attached to the back of this exam).



10. (10 pts.) Predict the number of Xe=O stretching bands if XeO_4 has the following structure.



a. Point group?

b. Reducible representation?

c. Irreducible representation?

d. Number of IR bands from Xe=O stretching?

Mendeleev's Table

Reihen	Gruppe I. — R ⁰	Gruppe II. — R ⁰	Gruppe III. — R ⁰	Gruppe IV. RH ⁴ R ⁰	Gruppe V. RH ⁵ R ⁰	Gruppe VI. RH ⁶ R ⁰	Gruppe VII. RH R ⁰	Gruppe VIII. — R ⁰
1	H=1							
2	Li=7	Be=9,4	B=11	C=12	N=14	O=16	F=19	
3	Na=23	Mg=24	Al=27,3	Si=28	P=31	S=32	Cl=35,5	
4	K=39	Ca=40	—=44	Ti=48	V=51	Cr=52	Mn=55	Fe=56, Co=59, Ni=59, Cu=63.
5	(Ca=63)	Zn=65	—=68	—=72	As=75	Se=78	Br=80	
6	Rb=85	Sr=87	?Yt=88	Zr=90	Nb=94	Mo=96	—=100	Ru=104, Rh=104, Pd=106, Ag=108.
7	(Ag=108)	Cd=112	In=113	Sn=118	Sb=122	Te=125	J=127	
8	Cs=133	Ba=137	?Di=138	?Ce=140	—	—	—	— — — —
9	(—)	—	—	—	—	—	—	
10	—	—	?Er=178	?La=180	Ta=182	W=184	—	Os=195, Ir=197, Pt=198, Au=199.
11	(Au=199)	Hg=200	Tl=204	Pb=207	Bi=208	—	—	
12	—	—	—	Th=231	—	U=240	—	— — — —

http://en.wikipedia.org/wiki/File:Mendelejevs_periodiska_system_1871.png

Slater's Rules for Determining Effective Nuclear Charge

$$Z_{\text{eff}} = Z - S$$

Where Z_{eff} = effective nuclear charge, Z = nuclear charge, and S = shielding constant

- list orbitals by n and l
(1s) (2s,2p) (3s,3p) (3d) (4s, 4p) (4d) (4f) (5s, 5p) (5d) (etc)
- electrons in groups to the right do not shield electrons to their left
- S can be determined for ns and np electrons
 - each electron in the same group contributes 0.35 to the value of S for other electrons in the same group
exception, 1s electron contributes 0.30
 - each electron in $n - 1$ groups contribute 0.85 to S
 - each electron in $n - 2$ groups contribute 1.00 to S
- for nd and nf
 - each electron in the same group contributes 0.35 to the value of S (same as 3a)
 - each electron in a group to the left contributes 1.00 to S

C ₂	E	C ₂		
A	1	1	R _x , R _y , R _z	x ² , y ² , z ² , xy
B	1	-1	x, y, z	xz, yz

C _{2h}	E	C ₂	<i>i</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 _{2v}	E	C ₂	σ _v (xz)	σ _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	2 C ₃	3 σ _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	2 C ₄	C ₂	2 σ _v	2 σ _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)

T _d	E	8 C ₃	3 C ₂	6 S ₄	6 σ _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)

D _{2h}	E	C ₂ (z)	C ₂ (y)	C ₂ (x)	i	σ _h (xy)	σ _d (xz)	σ _d (yz)		
A _g	1	1	1	1	1	1	1	1		x ² , y ² , z ²
B _{1g}	1	1	-1	-1	1	1	-1	-1	R _z	xy
B _{2g}	1	-1	1	-1	1	-1	1	-1	R _y	xz
B _{3g}	1	-1	-1	1	1	-1	-1	1	R _x	yz
A _u	1	1	1	1	-1	-1	-1	-1		
B _{1u}	1	1	-1	-1	-1	-1	1	1	z	
B _{2u}	1	-1	1	-1	-1	1	-1	1	y	
B _{3u}	1	-1	-1	1	-1	1	1	-1	x	

S ₄	E	C ₂	σ _v (xz)	σ _v (yz)		
A	1	1	1	1	z	x ² , y ² , z ²
B	1	1	-1	-1	R _z	xy
E	$\begin{bmatrix} 1 & i \\ 1 & - \end{bmatrix}$	$\begin{bmatrix} i & -1 \\ - & i \end{bmatrix}$	$\begin{bmatrix} -1 & -i \\ -1 & i \end{bmatrix}$	$\begin{bmatrix} -i & 1 \\ i & 1 \end{bmatrix}$	(x, y) (R _x , R _y)	(xz, yz)

number of irreducible representations of a given type needed = $1/\text{order} \sum_{\text{classes}} [(\# \text{ operations in class})(\chi \text{ of the irreducible representation})(\chi \text{ of the reducible representation})]$