Quiz 1 Feedback

- Avg: 87% (good job!), St. Dev.: 2.5

A) How many electrons can be described by the following quantum numbers:

n=4, l=2 [   ]

l = 2 means a d orbital, there are 5 4d orbitals, so 10 electrons can be described by n=4 and l=2

B) What are the values for n (principal quantum number) and l (angular momentum quantum number) for a 7h orbital?

n = [7]

l = [5]

s: l = 0   f: l = 3
p: l = 1   g: l = 4
d: l = 2   h: l = 5
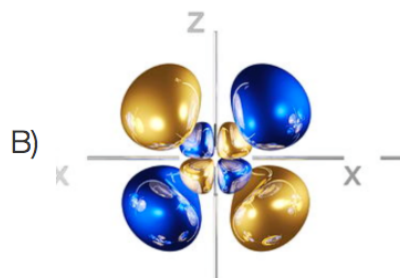
A) 5s

Angular nodes [ ]

Radial nodes [ ]

s: l = 0, zero angular nodes

n = 5, n-1 = 4 = total number of nodes. Radial nodes = 4

B)

Angular nodes [ ]

Radial nodes [ ]

This looks like a d orbital, there are 2 angular nodes along the depicted axes

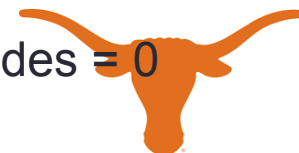Each 'branch' of the d orbital contains 2 lobes of different phases, this means there is 1 radial node.

C) A 4f orbital

Angular nodes [ ]

Radial nodes [ ]

f: l = 3, 3 angular nodes

n = 4, n-1 = 3 = total number of nodes. Radial nodes = 0

Select the best choice for the following:

A) Smallest radius: K^+, Ar, Cl^- | K+ ⬍

Each atom/ion contains same number of electrons, but K+ has most positive charge, will pull in electrons most tightly

K+	83 respondents	74 %	✔
Ar	22 respondents	20 %	
Cl-	6 respondents	5 %	
No Answer	1 respondents	1 %	

Ionization energy increases as you go across a period due to increasing Zeff
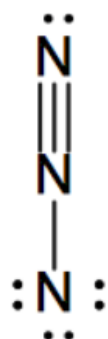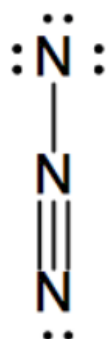
B) Highest ionization energy: Mo, Ru, Pd | Pd

When comparing ions of the same element, the most positively charged species will have the smallest radius, the least positively charged species will have the largest radius (see reasoning for 'A')

C) Largest radius: Fe^+, Fe^{2+}, Fe^{3+} | Fe+ ⬍

A) Which of the following structures would you predict to be favored for N_3^- ?
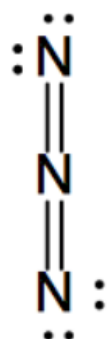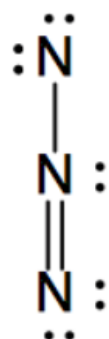
A   B   C   D

A/B: Formal charges of -2, +1, 0
D: One N does not have octet, formal charges 0 and -1

C: all Ns have octet, formal charges are +1 and -1

C

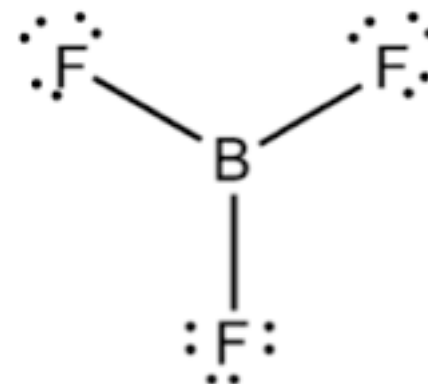|		
A		0 %
B	1 respondents	1 %
C	**89 respondents**	**79 %** ✔
D	15 respondents	13 %
A and B	5 respondents	4 %
A and C	1 respondents	1 %
B and D	1 respondents	1 %

B) In the Lewis dot structure for XeF4, how many lone pairs are found around the cen
atom?

2
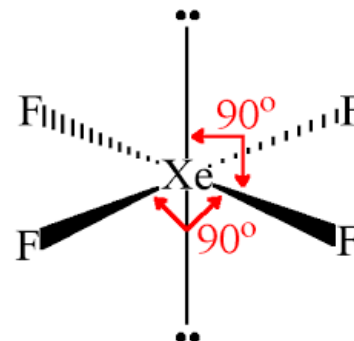
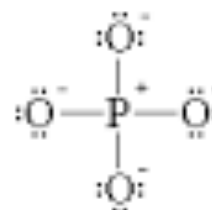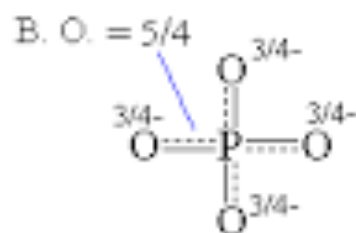D) What is the formal charge of boron in BF3 ?

0

C) What is the best description for the P-O bonds found in PO_4^{3-} ?

in between single and double ▲▼

B. O. = 5/4

single	5 respondents	4 %	
double	4 respondents	4 %	
triple		0 %	
both single and double	39 respondents	35 %	
in between single and double	64 respondents	**57 %**	

A) Compare the following bond angles in $SOCl_2$:

Cl-S-Cl [<] Cl-S-O

143 pm   207 pm
107.4°   96.5°
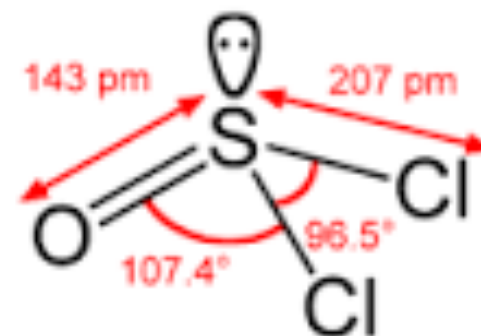
S=O double bond is more repulsive, pushes S-Cl bonds together

B) Which of the following structures corresponds to ICl_4^- ? (Note: any lone pairs in the molecule are not shown)

<	82 respondents	73 %	✔
=	17 respondents	15 %	
>	12 respondents	11 %	
No Answer	1 respondents	1 %	

B) Which of the following structures corresponds to ICl_4^- ? (Note: any lone pairs in the molecule are not shown)

A

B

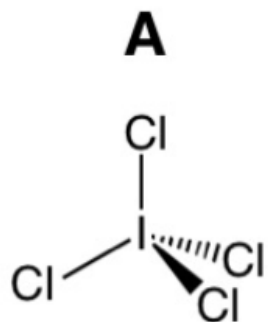$$\left[\begin{array}{c} :\ddot{C}l: \\ | \\ :\ddot{C}l - \overset{..}{\underset{..}{I}} - \ddot{C}l: \\ | \\ :\ddot{C}l: \end{array} \right]^{-}$$

C

Cl
|
Cl—I''''Cl
      Cl

Bond angles 109.5°

Cl—I—Cl
   Cl   Cl

Bond angles 90 and 180°

Cl''''I''''Cl
  Cl   Cl
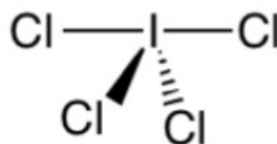
Bond angles 90 and 180°

C	⬍

option C puts two lone pairs the farthest away from each other,

Option B has 90° interaction between two lone pairs: BAD

A	8 respondents	7 %	
B	29 respondents	26 %	
C	75 respondents	**67** %	✔

C) What is the geometry of SF_6 ?

octahedral ▲▼

steric number 6, octahedral!

D) In KrF_2, what is the F-Kr-F bond angle?

180 ▲▼

:F—Kr—F:
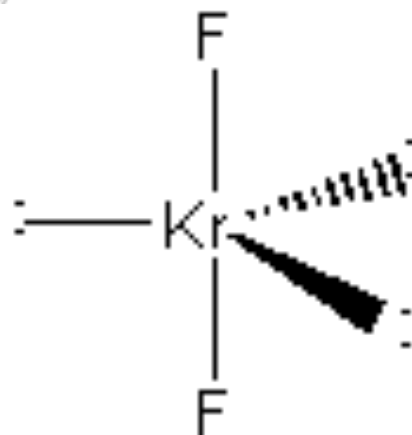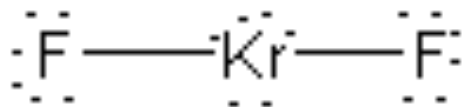
Quiz 2

- Find symmetry around Austin and UT!
- 4 pictures, each illustrating a different kind of symmetry operation

C_3, mirror planes

CH 431: SYMMETRY

MFT Chapter 4

Symmetry elements

- **Symmetry element:** a point, line, or plane in an object/molecule about which a symmetry operation can be performed
  - Inversion center (a point)
  - Rotation axis (line)
  - Mirror plane (plane)

Symmetry operations

- **Symmetry operation:** the actual action that is performed on the object
  - Inversion
  - Rotation
  - Reflection
  - Improper rotation

- When operation performed, object should look exactly the same as before
  - Every point is coincident with an identical point before the operation

Symmetry operations and elements

Symmetry operation	Symbol	Symmetry Element
Identity	E	none
Proper rotation	C_n	axis
Reflection	σ (sigma)	plane
Inversion	i	point
Improper rotation	S_n	none

Identity, E

- The identity operation is characteristic of every molecule
- This causes no change in the molecule

$$(x,y,z) \rightarrow (x,y,z)$$

Proper rotation, C_n

- A C_n is a rotation by 360°/n
- $C_n^n = E$ (For example, three C_3 rotations, C_3^3, results in original position of all points in object)

- Molecules can have multiple rotation axes (ex: snowflake)

- Principal rotation axis is the C_n with the highest value of n

Reflection, σ

- Molecule contains a mirror plane
- $(x,y,z) \rightarrow (x,-y,z)$ (reflection through the xz plane, σ_{xz})
- $\sigma^2 = E$

- σ_h = reflection across plane perpendicular to highest C_n
- σ_v = reflection across plane that contains (parallel) highest C_n, typically coincident with bonds in molecule
- σ_d = σ_v's that bisect bonds, adjacent C_2 axes etc. (d = diagonal)

Inversion, i

- A molecule has inversion symmetry if each point in a molecule can pass through center to the opposite side and still look the same

- $(x,y,z) \rightarrow (-x,-y,-z)$
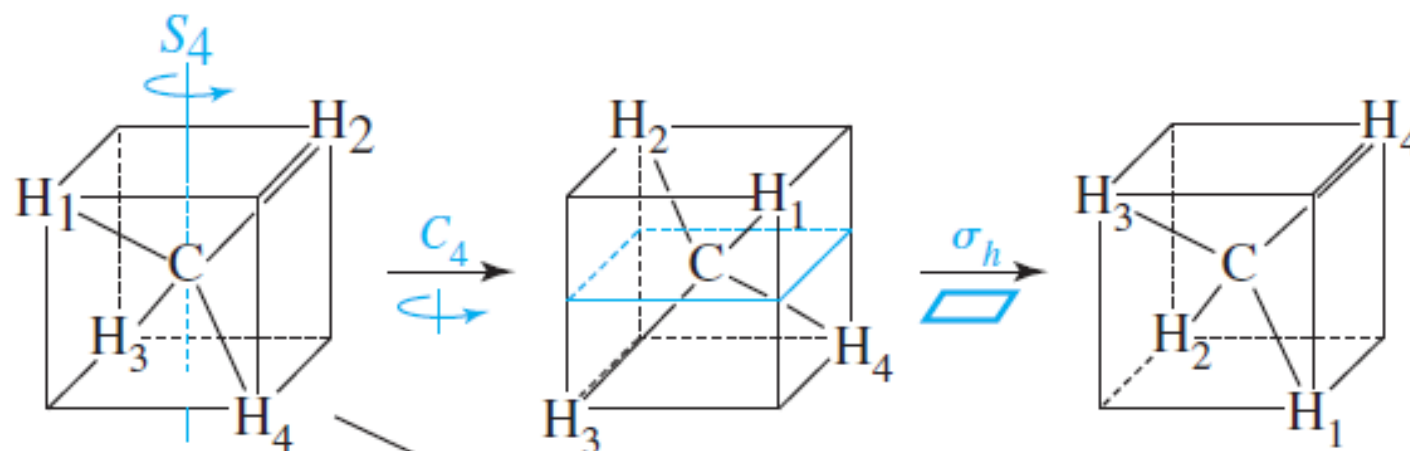- $i^2 = E$

- example: staggered ethane

Improper rotation, S_n

- An improper rotation is a rotation by 360°/n followed by a reflection in the plane perpendicular to the rotation axis

- $S_n = \sigma_h \cdot C_n$
- $S_2 = i$

- When n is even: 1) $S_n{}^n = E$

                                   2) There will be a collinear $C_{n/2}$

- When n is odd: $S_n{}^{2n} = E$

S$_4$ operation in methane