CHEM210 Assignment 2

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Question 1

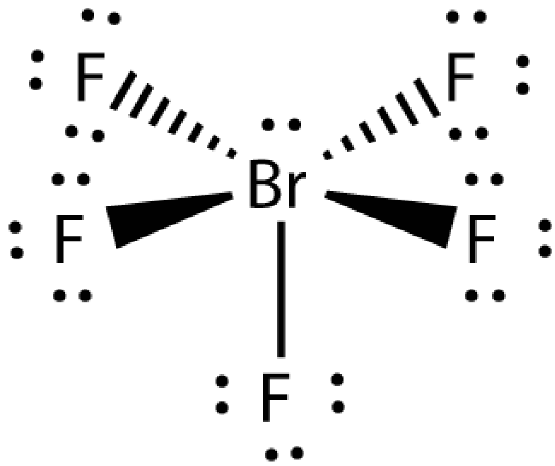
After calculating the number of valence electrons and drawing the Lewis dot structures of each molecule, we found the total regions of electron density by adding the number of bonded pairs (BP) and lone pairs (LP). The electronic and molecular geometries of each structure were then deduced.

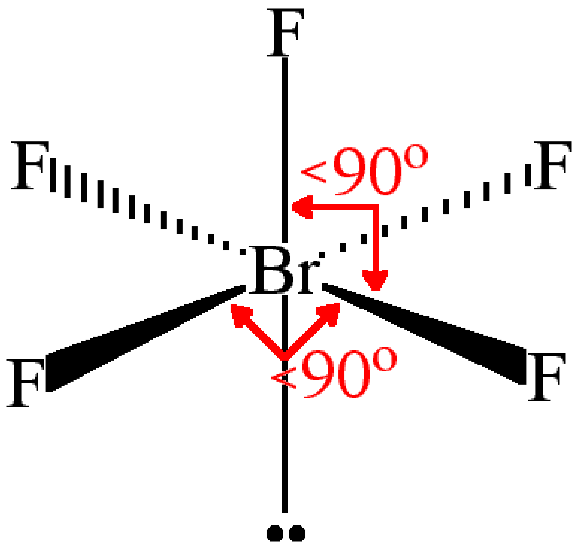
	Valence e^-	BP+LP	LP	Electronic	Molecular
ClO_2^-	20	4	2	Tetrahedral	Bent
ClF_4^+	34	5	1	Trigonal Bypyramid	Seesaw
ICl_4^-	36	6	2	Octahedral	Square Planar
NF_3	26	4	1	Tetrahedral	Trigonal Pyramid
SO_2	16	2	0	Linear	Linear

Question 2

	Valence e^-	BP+LP	LP	Electronic	Molecular
PF_5	40	5	0	Trigonal Bypyramid	Trigonal Bypyramid
CH_3I	14	4	0	Tetrahedral	Tetrahedral
BrF_5	42	6	1	Octahedral	Square Pyramid

We would expect BrF_5 to have bond angles that deviate from the ideal VSEPR values due to its single lone pair. Its molecular geometry is predicted to be square pyramidal, rather than the ideal octahedral structure. As shown below, the angles between bonded atoms are slightly less than 90°.


Br
F
F
F
F
F


F
F
F
Br
F
F
<90°
<90°

Question 3

Question 4

Electrons in a shell of lower principal quantum number, n, are in more compact orbitals that pack around the nucleus more tightly than electrons in large diffuse orbitals. When orbital size is small, the partial cancellation of attractive forces between the nucleus and incoming electrons is easier and screening is more effective. As orbital size increases as n increases, an electron's ability to screen decreases as there is more space to move around and avoid being *screened*.

Question 5

$$\begin{aligned}
&\int_0^a N^2 \left|\psi(x)\right|^2 \, dx = 1 \\
&\int_0^a N^2 \left|a(a-x)\right|^2 \, dx = 1 \\
&N^2 \int_0^a a^4 - 2a^3x + a^2x^2 \, dx = 1 \\
&N^2 \left[a^4x - a^3x^2 + \frac{a^2x^3}{3} \right]_0^a = 1 \\
&N^2 \left(\frac{a^5}{3} \right) = 1 \\
&N = \sqrt{\frac{3}{a^5}}
\end{aligned}$$

The normalized wavefunction is given by

$$\sqrt{\frac{3}{a^5}} \, a(a-x)$$

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Question 6

(a) (i)

$$\begin{aligned}
\psi(x) &= A\sin(Bx) \\
\frac{d}{dx}\psi(x) &= AB\cos(Bx) \\
\frac{d^2}{dx^2}\psi(x) &= -AB^2\sin(Bx) \\
&= -B^2\psi(x)
\end{aligned}$$

The corresponding eigenvalue is $-B^2$.

(ii)

$$\begin{aligned}\psi(x) &= C\cos(Bx)\\ \frac{d}{dx}\psi(x) &= -BC\sin(Bx)\\ \frac{d^2}{dx^2}\psi(x) &= -B^2C\cos(Bx)\\ &= -B^2\psi(x)\end{aligned}$$

The corresponding eigenvalue is $-B^2$.

(b) No, different values of A and C give the same eigenfunctions. The two eigenfunctions are degenerate since their eigenvalues are equal.

Question 7

Question 8