Name:

Quiz 4

Chemistry 3BB3; Winter 2004

1. **Sketch the dependence of the effective nuclear charge of the Carbon atom versus the distance from the nucleus. Make sure you label the values of the effective nuclear charge at $r = 0$ and as $r \to \infty$.**

2. **Use your answer in problem 1 to argue why the 2p orbitals fills after the 2s orbital.**

The following terms enter into the Schrödinger equation for a 2-electron diatomic molecule. Use the following notation in problems 1 and 2.

$$\hat{V}_{nn} \equiv \frac{Z_1 Z_2}{|\boldsymbol{R}_1 - \boldsymbol{R}_2|} \qquad \hat{T}_e \equiv -\frac{\nabla^2_{\boldsymbol{r}_1}}{2} - \frac{\nabla^2_{\boldsymbol{r}_2}}{2}$$

$$\hat{V}_{ee} \equiv \frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} \qquad \hat{T}_n \equiv -\frac{\nabla^2_{\boldsymbol{R}_1}}{2M_1} - \frac{\nabla^2_{\boldsymbol{R}_2}}{2M_2}$$

$$\hat{V}_{ne} \equiv -\frac{Z_1}{|\boldsymbol{r}_1 - \boldsymbol{R}_1|} - \frac{Z_2}{|\boldsymbol{r}_1 - \boldsymbol{R}_2|} - \frac{Z_1}{|\boldsymbol{r}_2 - \boldsymbol{R}_1|} - \frac{Z_2}{|\boldsymbol{r}_2 - \boldsymbol{R}_2|}$$

3. **Using the preceding notation and your result from problem 2, write the Schrödinger equation for the electrons in the Born-Oppenheimer Approximation.**

4. **Using the preceding notation and your results from problems 2 and 3, write the Schrödinger equation for the nuclei in the Born-Oppenheimer Approximation.**

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5. What are the term symbols for a $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^2$ electron configuration.

6. List the terms from problem five in order of increasing energy.

7. What is the ground state term for a $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$ electron configuration?

8. What is the value of the total angular momentum quantum number, *J*, in the ground state term from problem seven. ($1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$ electron configuration)

9. The atomic unit of energy is the:

(a) Bohr.
(b) Schrödinger.
(c) Slater.
(d) Oppenheimer.
(e) Dirac.
(f) None of the above.

10. The atomic unit of length is the

(a) Bohr.
(b) Schrödinger.
(c) Slater.
(d) Oppenheimer.
(e) Dirac.
(f) None of the above.

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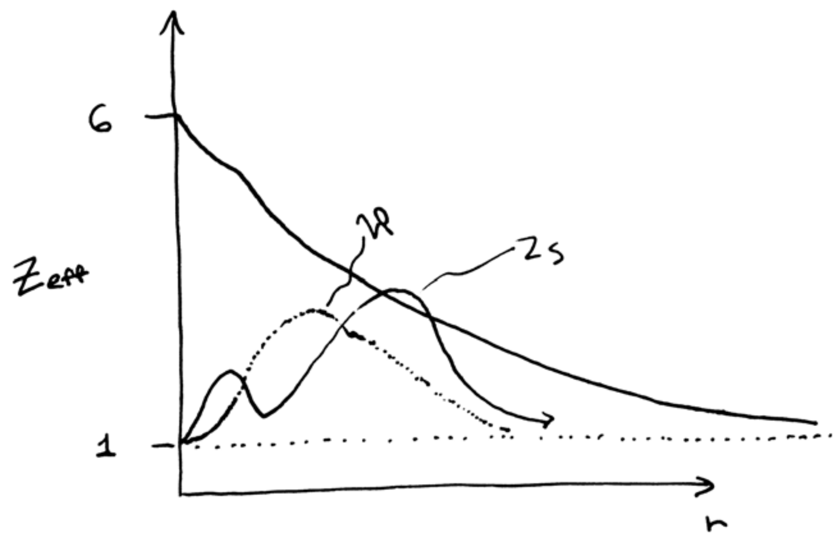
Chemistry 3BB3; Winter 2004

1. **Sketch the dependence of the effective nuclear charge of the Carbon atom versus the distance from the nucleus. Make sure you label the values of the effective nuclear charge at $r = 0$ and as $r \to \infty$.**



2. **Use your answer in problem 1 to argue why the 2p orbitals fills after the 2s orbital.**
The 2s orbital has some probability at the nucleus, where the effective nuclear charge is very large. The 2p orbital does not. Therefore, the an electron in a 2s orbital feels a greater effective nuclear charge than an electron in a 2p orbital. This makes the 2s orbital have a lower energy than the 2p orbital. Said differently, an electron in a 2p orbital is more effectively "shielded" because it has little density close to the nucleus. Thus, an electron in a 2p orbital generally has electrons "between" it and the nucleus (this is the essence of shielding). An electron in a 2s orbital is sometimes at, or very, very, close to the nucleus, which means that, on occasion, there will be no electrons between it and the nucleus. It is less shielding. The probabilities of observing an electron a distance *r* from the nucleus have been sketched in Figure 1, with hopes that this clarifies the picture.

The following terms enter into the Schrödinger equation for a 2-electron diatomic molecule. Use the following notation in problems 1 and 2.

$$\hat{V}_{nn} \equiv \frac{Z_1 Z_2}{|\boldsymbol{R}_1 - \boldsymbol{R}_2|} \qquad \hat{T}_e \equiv -\frac{\nabla^2_{\boldsymbol{r}_1}}{2} - \frac{\nabla^2_{\boldsymbol{r}_2}}{2}$$

$$\hat{V}_{ee} \equiv \frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} \qquad \hat{T}_n \equiv -\frac{\nabla^2_{\boldsymbol{R}_1}}{2M_1} - \frac{\nabla^2_{\boldsymbol{R}_2}}{2M_2}$$

$$\hat{V}_{ne} \equiv -\frac{Z_1}{|\boldsymbol{r}_1 - \boldsymbol{R}_1|} - \frac{Z_2}{|\boldsymbol{r}_1 - \boldsymbol{R}_2|} - \frac{Z_1}{|\boldsymbol{r}_2 - \boldsymbol{R}_1|} - \frac{Z_2}{|\boldsymbol{r}_2 - \boldsymbol{R}_2|}$$

3. **Using the preceding notation and your result from problem 2, write the Schrödinger equation for the electrons in the Born-Oppenheimer Approximation.**

$$\left(\hat{T}_e + V_{ne} + V_{ee} + V_{nn}\right)\psi(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{R}_1, \boldsymbol{R}_2) = U^{BO}(\boldsymbol{R}_1, \boldsymbol{R}_2)\psi(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{R}_1, \boldsymbol{R}_2)$$

4. **Using the preceding notation and your results from problems 2 and 3, write the Schrödinger equation for the nuclei in the Born-Oppenheimer Approximation.**

$$\left(\hat{T}_n + U^{BO}(\boldsymbol{R}_1, \boldsymbol{R}_2)\right)\chi(\boldsymbol{R}_1, \boldsymbol{R}_2) = E^{BO}\chi(\boldsymbol{R}_1, \boldsymbol{R}_2)$$

Name:

5. What are the term symbols for a $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^2$ electron configuration.

			M_L		
M_S	**4**	**3**	**2**	**1**	**0**
1		$\lvert \psi_2\alpha \quad \psi_1\alpha \rvert$	$\lvert \psi_2\alpha \quad \psi_0\alpha \rvert$	$\lvert \psi_2\alpha \quad \psi_{-1}\alpha \rvert$ $\lvert \psi_1\alpha \quad \psi_0\alpha \rvert$	$\lvert \psi_2\alpha \quad \psi_{-2}\alpha \rvert$ $\lvert \psi_1\alpha \quad \psi_{-1}\alpha \rvert$
1	$\lvert \psi_2\alpha \quad \psi_2\beta \rvert$	$\lvert \psi_2\alpha \quad \psi_1\beta \rvert$ $\lvert \psi_2\beta \quad \psi_1\alpha \rvert$	$\lvert \psi_2\alpha \quad \psi_0\beta \rvert$ $\lvert \psi_2\beta \quad \psi_0\alpha \rvert$ $\lvert \psi_1\alpha \quad \psi_1\beta \rvert$	$\lvert \psi_2\alpha \quad \psi_{-1}\beta \rvert$ $\lvert \psi_2\beta \quad \psi_{-1}\alpha \rvert$ $\lvert \psi_1\alpha \quad \psi_0\beta \rvert$ $\lvert \psi_1\beta \quad \psi_0\alpha \rvert$	$\lvert \psi_2\alpha \quad \psi_{-2}\beta \rvert$ $\lvert \psi_2\beta \quad \psi_{-2}\alpha \rvert$ $\lvert \psi_1\alpha \quad \psi_{-1}\beta \rvert$ $\lvert \psi_1\beta \quad \psi_{-1}\alpha \rvert$ $\lvert \psi_0\alpha \quad \psi_0\beta \rvert$

In this table, the microstates "struck out" for each term are color coded. ψ_{m_l} denotes the *d* orbital with angular momentum m_l. α is associated with $m_s = \frac{1}{2}$; β is associated with $m_s = -\frac{1}{2}$

${}^3F$, ${}^3P$, ${}^1G$, ${}^1D$, ${}^1S$

6. List the terms from problem five in order of increasing energy.
The terms are already listed in increasing order of energy, ${}^3F$, ${}^3P$, ${}^1G$, ${}^1D$, ${}^1S$. (That's why I gave you the prescription I did; you always get the terms in order this way).

7. What is the ground state term for a $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$ electron configuration?
${}^3F$

8. What is the value of the total angular momentum quantum number, *J*, in the ground state term from problem seven. ($1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$ electron configuration)
Since the shell is more than half-filled, we want the largest possible value fo *J*. That gives: $J_{\max} = L + S = 3 + 1 = 4$.

9. The atomic unit of energy is the:
(a) Bohr.
(b) Schrödinger.
(c) Slater.
(d) Oppenheimer.
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