Name:

Quiz 2

Chemistry 3BB3; Winter 2003

1. **Write the Schrödinger equation for the Hydrogen atom and do not use atomic units. That is, include the explicit dependence on $\hbar$, m_e, e, ε_0, etc. explicit.**

2. **Using separation of variables to simplify your result in Question 1, write the Schrödinger equation for the radial component of the hydrogen atom wave function. Do not use atomic units.**

3. **Write the energy formula for the one-electron atom with atomic number *Z*. You can use atomic units, if you want. Make sure your formula shows how the energy changes as the principle quantum number, *n*, increases.**

4. **For the state with principle quantum number, *n*, the orbital angular momentum quantum number, *l*, is restricted to the values**
   (a) $l = 0,1,2,\ldots,n$
   (b) $l = 1,2,\ldots,n$
   (c) $l = 0,1,2,\ldots,n-1$
   (d) $l = 1,2,\ldots,n-1$
   (e) $-n,-n+1,\ldots,n-1,n$
   (f) $-n+1,-n+2\ldots,n-2,n-1$
   (g) none of the above

5. **For the state with orbital angular momentum quantum number, *l*, the magnetic quantum number, *m*, is restricted to the values**
   (a) $m = 0,1,2,\ldots,l$
   (b) $m = 1,2,\ldots,l$
   (c) $m = 0,1,2,\ldots,l-1$
   (d) $m = 1,2,\ldots,l-1$
   (e) $-l,-l+1,\ldots,l-1,l$
   (f) $-l+1,-l+2\ldots,l-2,l-1$
   (g) none of the above

Name:

6. In the usual set of spherical coordinates (that is, $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, and $z = r\cos\theta$), the $5d_{z^2} \to 5d_{2z^2-x^2-y^2}$ orbital corresponds to what values for

The principle quantum number, *n* ____________

The orbital angular momentum quantum number, *l* ____________

The magnetic quantum number, *m* _______________

7. In the usual set of spherical coordinates (that is, $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, and $z = r\cos\theta$), the $6p_x$ orbital corresponds to what values for

The principle quantum number, *n* ____________

The orbital angular momentum quantum number, *l* ____________

The magnetic quantum number, *m* _______________

8. The radial eigenfunctions of the Hydrogen atom are most simply expressed in terms of

(a) The associated Legendre polynomials
(b) The Schrödinger polynomials
(c) The associated Lewis pair polynomials
(d) The generalized Jacobi functions
(e) The associated Laguerre polynomials
(f) The generalized Hermite Polynomials
(g) none of the above

9. The Schrödinger equation for a 2-electron, 2-atom molecule is written below, in atomic units. Cross out the terms that are ignored in the Born-Oppenheimer approximation.

$$\psi_e\left(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{R}_1,\boldsymbol{R}_2\right)\left(-\tfrac{\nabla^2_{\boldsymbol{R}_1}}{2M_1}-\tfrac{\nabla^2_{\boldsymbol{R}_2}}{2M_2}\right)\chi_n\left(\boldsymbol{R}_1,\boldsymbol{R}_2\right)+\chi_n\left(\boldsymbol{R}_1,\boldsymbol{R}_2\right)\left(-\tfrac{\nabla^2_{\boldsymbol{R}_1}}{2M_1}-\tfrac{\nabla^2_{\boldsymbol{R}_2}}{2M_2}\right)\psi_e\left(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{R}_1,\boldsymbol{R}_2\right)$$
$$-\frac{\nabla_{\boldsymbol{R}_1}\chi_n\left(\boldsymbol{R}_1,\boldsymbol{R}_2\right)\cdot\nabla_{\boldsymbol{R}_1}\psi_e\left(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{R}_1,\boldsymbol{R}_2\right)}{M_1}-\frac{\nabla_{\boldsymbol{R}_2}\chi_n\left(\boldsymbol{R}_1,\boldsymbol{R}_2\right)\cdot\nabla_{\boldsymbol{R}_2}\psi_e\left(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{R}_1,\boldsymbol{R}_2\right)}{M_2}$$
$$+\chi_n\left(\boldsymbol{R}_1,\boldsymbol{R}_2\right)\left(-\tfrac{\nabla^2_{\boldsymbol{r}_1}}{2}-\tfrac{\nabla^2_{\boldsymbol{r}_2}}{2}+\tfrac{Z_1Z_2}{|\boldsymbol{R}_1-\boldsymbol{R}_2|}-\tfrac{Z_1}{|\boldsymbol{r}_1-\boldsymbol{R}_1|}-\tfrac{Z_2}{|\boldsymbol{r}_1-\boldsymbol{R}_2|}-\tfrac{Z_1}{|\boldsymbol{r}_2-\boldsymbol{R}_1|}-\tfrac{Z_2}{|\boldsymbol{r}_2-\boldsymbol{R}_2|}+\tfrac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}\right)\psi_e\left(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{R}_1,\boldsymbol{R}_2\right)$$
$$=E\chi_n\left(\boldsymbol{R}_1,\boldsymbol{R}_2\right)\psi_e\left(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{R}_1,\boldsymbol{R}_2\right)$$

10. Using the following definitions,

$$\hat{T}_e \equiv -\tfrac{\nabla^2_{\boldsymbol{r}_1}}{2}-\tfrac{\nabla^2_{\boldsymbol{r}_2}}{2} \qquad \hat{T}_n \equiv -\tfrac{\nabla^2_{\boldsymbol{R}_1}}{2M_1}-\tfrac{\nabla^2_{\boldsymbol{R}_2}}{2M_2}$$
$$\hat{V}_{ee} \equiv \tfrac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|} \qquad \hat{V}_{nn} \equiv \tfrac{Z_1Z_2}{|\boldsymbol{R}_1-\boldsymbol{R}_2|}$$
$$\hat{V}_{ne} \equiv -\tfrac{Z_1}{|\boldsymbol{r}_1-\boldsymbol{R}_1|}-\tfrac{Z_2}{|\boldsymbol{r}_1-\boldsymbol{R}_2|}-\tfrac{Z_1}{|\boldsymbol{r}_2-\boldsymbol{R}_1|}-\tfrac{Z_2}{|\boldsymbol{r}_2-\boldsymbol{R}_2|}$$

the Schrödinger equation for the electrons, in the Born-Oppenheimer approximation, can be written as

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

What is the Schrödinger equation for the nuclei in the Born-Oppenheimer approximation?

Name:

Quiz 2

Chemistry 3BB3; Winter 2003

1. **Write the Schrödinger equation for the Hydrogen atom and do not use atomic units. That is, include the explicit dependence on $\hbar$, m_e, e, ε_0, etc. explicit.**

$$\left(-\frac{\hbar^2}{2m_e}\nabla^2 - \frac{Ze^2}{4\pi\varepsilon_0 r}\right)\Psi(r,\theta,\phi) = E\Psi(r,\theta,\phi)$$

2. **Using separation of variables to simplify your result in Question 1, write the Schrödinger equation for the radial component of the hydrogen atom wave function. Do not use atomic units.**

$$\left(-\frac{\hbar^2}{2m_e}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right) - \frac{Ze^2}{4\pi\varepsilon_0 r}\right)R_{n,l}(r) = E_n R_{n,l}(r)$$

3. **Write the energy formula for the one-electron atom with atomic number *Z*. You can use atomic units, if you want. Make sure your formula shows how the energy changes as the principle quantum number, *n*, increases.**

$$E = -\frac{Z^2}{2n^2}$$

4. **For the state with principle quantum number, *n*, the orbital angular momentum quantum number, *l*, is restricted to the values**
   (a) $l = 0,1,2,\ldots,n$
   (b) $l = 1,2,\ldots,n$
   (c) $l = 0,1,2,\ldots,n-1$
   (d) $l = 1,2,\ldots,n-1$
   (e) $-n,-n+1,\ldots,n-1,n$
   (f) $-n+1,-n+2\ldots,n-2,n-1$
   (g) none of the above

5. **For the state with orbital angular momentum quantum number, *l*, the magnetic quantum number, *m*, is restricted to the values**
   (a) $m = 0,1,2,\ldots,l$
   (b) $m = 1,2,\ldots,l$
   (c) $m = 0,1,2,\ldots,l-1$
   (d) $m = 1,2,\ldots,l-1$
   (e) $-l,-l+1,\ldots,l-1,l$
   (f) $-l+1,-l+2\ldots,l-2,l-1$
   (g) none of the above

Name:

6. **In the usual set of spherical coordinates (that is, $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, and $z = r\cos\theta$), the $5d_{z^2} \to 5d_{2z^2-x^2-y^2}$ orbital corresponds to what values for**

   The principle quantum number, n ______**5**______

   The orbital angular momentum quantum number, l ______**2**______

   The magnetic quantum number, m ______**0**_________

7. **In the usual set of spherical coordinates (that is, $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, and $z = r\cos\theta$), the $6p_x$ orbital corresponds to what values for**

   The principle quantum number, n _____**6**_______

   The orbital angular momentum quantum number, l _____**1**_______

   The magnetic quantum number, m **trick question; this is not an eigenfunction of $\hat{L}_z$**

8. **The radial eigenfunctions of the Hydrogen atom are most simply expressed in terms of**
   (a) The associated Legendre polynomials
   (b) The Schrödinger polynomials
   (c) The associated Lewis pair polynomials
   (d) The generalized Jacobi functions
   (e) The associated Laguerre polynomials
   (f) The generalized Hermite Polynomials
   (g) none of the above

9. **The Schrödinger equation for a 2-electron, 2-atom molecule is written below, in atomic units. Cross out the terms that are ignored in the Born-Oppenheimer approximation.**

$$\psi_e(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{R}_1,\boldsymbol{R}_2)\left(-\frac{\nabla^2_{\boldsymbol{R}_1}}{2M_1}-\frac{\nabla^2_{\boldsymbol{R}_2}}{2M_2}\right)\chi_n(\boldsymbol{R}_1,\boldsymbol{R}_2)+\cancel{\chi_n(\boldsymbol{R}_1,\boldsymbol{R}_2)\left(-\frac{\nabla^2_{\boldsymbol{R}_1}}{2M_1}-\frac{\nabla^2_{\boldsymbol{R}_2}}{2M_2}\right)\psi_e(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{R}_1,\boldsymbol{R}_2)}$$
$$-\cancel{\frac{\nabla_{\boldsymbol{R}_1}\chi_n(\boldsymbol{R}_1,\boldsymbol{R}_2)\cdot\nabla_{\boldsymbol{R}_1}\psi_e(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{R}_1,\boldsymbol{R}_2)}{M_1}}-\cancel{\frac{\nabla_{\boldsymbol{R}_2}\chi_n(\boldsymbol{R}_1,\boldsymbol{R}_2)\cdot\nabla_{\boldsymbol{R}_2}\psi_e(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{R}_1,\boldsymbol{R}_2)}{M_2}}$$
$$+\chi_n(\boldsymbol{R}_1,\boldsymbol{R}_2)\left(-\frac{\nabla^2_{\boldsymbol{r}_1}}{2}-\frac{\nabla^2_{\boldsymbol{r}_2}}{2}+\frac{Z_1Z_2}{|\boldsymbol{R}_1-\boldsymbol{R}_2|}-\frac{Z_1}{|\boldsymbol{r}_1-\boldsymbol{R}_1|}-\frac{Z_2}{|\boldsymbol{r}_1-\boldsymbol{R}_2|}-\frac{Z_1}{|\boldsymbol{r}_2-\boldsymbol{R}_1|}-\frac{Z_2}{|\boldsymbol{r}_2-\boldsymbol{R}_2|}+\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}\right)\psi_e(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{R}_1,\boldsymbol{R}_2)$$
$$=E\chi_n(\boldsymbol{R}_1,\boldsymbol{R}_2)\psi_e(\boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{R}_1,\boldsymbol{R}_2)$$

10. **Using the following definitions,**

$$\hat{T}_e \equiv -\frac{\nabla^2_{\boldsymbol{r}_1}}{2}-\frac{\nabla^2_{\boldsymbol{r}_2}}{2} \qquad \hat{T}_n \equiv -\frac{\nabla^2_{\boldsymbol{R}_1}}{2M_1}-\frac{\nabla^2_{\boldsymbol{R}_2}}{2M_2}$$
$$\hat{V}_{ee} \equiv \frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|} \qquad \hat{V}_{nn} \equiv \frac{Z_1Z_2}{|\boldsymbol{R}_1-\boldsymbol{R}_2|}$$
$$\hat{V}_{ne} \equiv -\frac{Z_1}{|\boldsymbol{r}_1-\boldsymbol{R}_1|}-\frac{Z_2}{|\boldsymbol{r}_1-\boldsymbol{R}_2|}-\frac{Z_1}{|\boldsymbol{r}_2-\boldsymbol{R}_1|}-\frac{Z_2}{|\boldsymbol{r}_2-\boldsymbol{R}_2|}$$

the Schrödinger equation for the electrons, in the Born-Oppenheimer approximation, can be written as

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

What is the Schrödinger equation for the nuclei in the Born-Oppenheimer approximation?

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

Name: