Name:

Quiz 1

Chemistry 3BB3; Winter 2006

When we performed the Born-Oppenheimer approximation for the Hydrogen molecule, we separated the Schrödinger equation for the molecule into an electronic Schrödinger equation and a nuclear Schrödinger equation.

1. **Write the electronic Schrödinger equation for the Hydrogen molecule in SI units, showing the dependence on $\hbar$, *e*, m_e, etc..**

2. **Write the nuclear Schrödinger equation for the Hydrogen molecule in SI units, showing the dependence on $\hbar$, *e*, m_e, etc..**

3. **The Born-Oppenheimer Approximation is expected to be *least* accurate for which of the following molecules**
   (a) F_2 (b) Cl_2 (c) Br_2 (d) I_2

4. **High-resolution spectra are often resolved to about .1 cm^{-1}. In order to accurately model such spectra, one needs to solve the Schrödinger equation with an accuracy of about**
   (a) 10^6 Hartree (c) 1 Hartree (e) 10^{-6} Hartree
   (b) 10^3 Hartree (d) 10^{-3} Hartree

5. **The atomic unit of length is called the**
   (a) Schrödinger (e) Slater (i) Franck
   (b) Heisenberg (f) Pauling (j) Condon
   (c) Copenhagen (g) Bohr (k) Angstrom
   (d) Dirac (h) Planck (l) Hartree

6. **The atomic unit of length is [GREATER THAN] *or* [LESS THAN] 10^{-10} meters.**
   (Circle the appropriate answer.)

Name:

7,8. Below, different components of the molecular Hamiltonian are written (in atomic units). Match these components with the equation for them. See the first line for an example of how to complete this problem. (Clearly some of the choices listed correspond to *none* of the physically relevant operators!)

__B__ nuclear kinetic energy

_____ electronic kinetic energy

_____ electron-electron repulsion energy

_____ electron-nuclear attraction energy

_____ nuclear-nuclear repulsion energy

A. $\sum_{\alpha=1}^{P-1}\sum_{\beta=\alpha+1}^{P}\frac{-Z_\alpha Z_\beta}{\left|\boldsymbol{R}_\alpha-\boldsymbol{R}_\beta\right|}$

B. $\sum_{\alpha=1}^{P}-\frac{1}{2M_\alpha}\nabla_\alpha^2$

C. $\sum_{i=1}^{N}-\frac{1}{2}\nabla_i^2$

D. $\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{-1}{\left|\boldsymbol{r}_i-\boldsymbol{r}_j\right|}$

E. $\sum_{\alpha=1}^{P}\sum_{i=1}^{N}\frac{-Z_\alpha}{\left|\boldsymbol{r}_i-\boldsymbol{R}_\alpha\right|}$

F. $\sum_{\alpha=1}^{P-1}\sum_{\beta=\alpha+1}^{P}\frac{Z_\alpha Z_\beta}{\left|\boldsymbol{R}_\alpha-\boldsymbol{R}_\beta\right|}$

G. $\sum_{\alpha=1}^{P}\frac{1}{2M_\alpha}\nabla_\alpha^2$

H. $\sum_{i=1}^{N}\frac{1}{2}\nabla_i^2$

I. $\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{1}{\left|\boldsymbol{r}_i-\boldsymbol{r}_j\right|}$

J. $\sum_{\alpha=1}^{P}\sum_{i=1}^{N}\frac{Z_\alpha}{\left|\boldsymbol{r}_i-\boldsymbol{R}_\alpha\right|}$

9,10. When we wrote the molecular Schrodinger equation using terms like those in the previous question, we were making several approximations. List *two* of the approximations.

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Quiz 1 KEY

Chemistry 3BB3; Winter 2006

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1. **Write the electronic Schrödinger equation for the Hydrogen molecule in SI units, showing the dependence on $\hbar$, *e*, m_e , etc..**

$$\left(\sum_{i=1}^{2} -\frac{\hbar^2}{2m_e}\nabla_i^2 + \frac{e^2}{4\pi\varepsilon_0\left|\boldsymbol{r}_1-\boldsymbol{r}_2\right|} + \sum_{\alpha=1}^{2}\sum_{i=1}^{2}\frac{-e^2}{4\pi\varepsilon_0\left|\boldsymbol{r}_i-\boldsymbol{R}_\alpha\right|} + \frac{e^2}{4\pi\varepsilon_0\left|\boldsymbol{R}_1-\boldsymbol{R}_2\right|}\right)\psi\ \ \boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{R}_1,\boldsymbol{R}_2$$
$$= U\ \ \boldsymbol{R}_1,\boldsymbol{R}_2\ \ \psi\ \ \boldsymbol{r}_1,\boldsymbol{r}_2;\boldsymbol{R}_1,\boldsymbol{R}_2$$

2. **Write the nuclear Schrödinger equation for the Hydrogen molecule in SI units, showing the dependence on $\hbar$, *e*, m_e , etc..**

$$\left(\sum_{\alpha=1}^{2} -\frac{\hbar^2}{2M_\alpha}\nabla_\alpha^2 + U\ \ \boldsymbol{R}_1,\boldsymbol{R}_2\ \right)\chi\ \ \boldsymbol{R}_1,\boldsymbol{R}_2\ \ = E\chi\ \ \boldsymbol{R}_1,\boldsymbol{R}_2$$

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   (c) Copenhagen
   (d) Dirac
   (e) Slater
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9,10. When we wrote the molecular Schrodinger equation using terms like those in the previous question, we were making several approximations. List *two* of the approximations.

gravitational forces are neglected

nuclear forces/interactions are neglected. (E.g., the "weak force" between electrons and nucleons is neglected)

relativistic effects are neglected

atomic nucleii are assumed to be infinitely small. (That is, atomic nuclei are assumed to be point charges. In the Born-Oppenheimer approximation, atomic nuclei are actually assumed to be infinitely massive point charges.)