Quiz 2

Chemistry 3BB3; Winter 2005

1. **Write the Schrödinger Equation for the Hydrogen atom in atomic units. You may use the Born-Oppenheimer approximation.**

2. **In order to solve the Hydrogen atom, we used the solution of the following exactly solvable system**
   (a) particle in a box
   (b) harmonic oscillator
   (c) rigid rotor
   (d) Hückel Hamiltonian

(For #3 and #4). This fall, while I was in Europe, I rode the Thalys train from Brussels to Paris. Somewhere in Northern France, a highway ran beside the road. On the highway, there were some lorries (semi-trucks, 18-wheelers, etc.). Nearby, there were some trees. Suppose the train was going 300 km/hr, the lorries were going 40 km/hr, and the trees—well, they don't move at all.

3. **If I use this analogy to explain the motion of electrons and nuclei, which of the following sets gives the truest analogy. (Recall the notation X:Y :: A:B = X is to Y and A is to B)**
   (a) electrons : train :: nuclei : trees
   (b) electrons : train :: nuclei : lorries
   (c) electrons : lorries :: nuclei : train
   (d) electrons : lorries :: nuclei : trees
   (e) electrons : trees :: nuclei : train

4. **In this analogy, the Born-Oppenheimer approximation corresponds to making which of the following approximations:**
   (a) The trees, like the lorries, move at 40 km/hr.
   (b) The lorries, like the trees, do not move.

5. **Which of the following is *not* an approximations used in the electronic Hamiltonian we have been using in class?**
   (a) The effects of relativity are ignored.
   (b) Nuclear forces are ignored.
   (c) Interactions between electrons are ignored altogether.
   (d) Atomic nuclei are assumed to be a point charges.
   (e) The effects of gravity are ignored.

6. **Sometimes the energy of the atoms and molecules is reported not in Hartree, but in Rydberg.**

$$1 \text{ Hartree} = 2 \text{ Rydberg}$$

Which of the following is the correct formula for the ground state energy of the one-electron atom in units of Rydberg.

(a) $-\frac{Z}{2n}$

(b) $-\frac{Z^2}{2n}$

(c) $-\frac{Z}{2n^2}$

(d) $-\frac{Z^2}{2n^2}$

(e) $-\frac{Z}{n}$

(f) $-\frac{Z^2}{n}$

(g) $-\frac{Z}{n^2}$

(h) $-\frac{Z^2}{n^2}$

(i) $-\frac{2Z}{n}$

(j) $-\frac{2Z^2}{n}$

(k) $-\frac{2Z}{n^2}$

(l) $-\frac{2Z^2}{n^2}$

7-10: In class, we wrote that the Schrödinger equation for the molecule with *P* nuclei and *N* electrons could be written as

$$\left(\hat{T}_n + \hat{T}_e + V_{nn} + V_{ee} + V_{ne}\right)\Psi = E\Psi$$

Match the following operators to their mathematical definition and their "meaning" by filling in the table at the bottom of the page.

Meanings:

(a) nuclear-electron attraction energy operator

(b) nuclear-nuclear repulsion energy operator

(c) electron-electron repulsion energy operator

(d) nuclear kinetic energy operator

(e) electronic kinetic energy operator

Equations:

(i) $\sum_{\alpha=2}^{P}\sum_{\beta=1}^{\alpha-1}\frac{Z_\alpha Z_\beta e^2}{4\pi\varepsilon_0\left|\boldsymbol{R}_\beta - \boldsymbol{R}_\alpha\right|}$

(ii) $\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{e^2}{4\pi\varepsilon_0\left|\boldsymbol{r}_i - \boldsymbol{r}_j\right|}$

(iii) $-\sum_{\alpha=1}^{P}\sum_{i=1}^{N}\frac{Z_\alpha e^2}{4\pi\varepsilon_0\left|\boldsymbol{r}_i - \boldsymbol{R}_\alpha\right|}$

(iv) $\sum_{i=1}^{N}-\frac{\hbar^2}{2m_e}\nabla_i^2$

(v) $\sum_{\alpha=1}^{P}-\frac{\hbar^2}{2m_\alpha}\nabla_\alpha^2$

Operator	Equation	"meaning"
$\hat{T}_n$		
$\hat{T}_e$		
V_{nn}		
V_{ne}		

Quiz 2

Chemistry 3BB3; Winter 2005

1. **Write the Schrödinger Equation for the Hydrogen atom in atomic units. You may use the Born-Oppenheimer approximation.**

$$\left(-\frac{\nabla^2}{2}-\frac{Z}{r}\right)\Psi(\boldsymbol{r})=E\Psi(\boldsymbol{r})$$

2. **In order to solve the Hydrogen atom, we used the solution of the following exactly solvable system**
   (a) particle in a box
   (b) harmonic oscillator
   (c) rigid rotor
   (d) Hückel Hamiltonian

(For #3 and #4). This fall, while I was in Europe, I rode the Thalys train from Brussels to Paris. Somewhere in Northern France, a highway ran beside the road. On the highway, there were some lorries (semi-trucks, 18-wheelers, etc.). Nearby, there were some trees. Suppose the train was going 300 km/hr, the lorries were going 40 km/hr, and the trees—well, they don't move at all.

3. **If I use this analogy to explain the motion of electrons and nuclei, which of the following sets gives the truest analogy. (Recall the notation X:Y :: A:B = X is to Y and A is to B)**
   (a) electrons : train :: nuclei : trees
   (b) electrons : train :: nuclei : lorries
   (c) electrons : lorries :: nuclei : train
   (d) electrons : lorries :: nuclei : trees
   (e) electrons : trees :: nuclei : train

4. **In this analogy, the Born-Oppenheimer approximation corresponds to making which of the following approximations:**
   (a) The trees, like the lorries, move at 40 km/hr.
   (b) The lorries, like the trees, do not move.

5. **Which of the following is *not* an approximations used in the electronic Hamiltonian we have been using in class?**
   (a) The effects of relativity are ignored.
   (b) Nuclear forces are ignored.
   (c) Interactions between electrons are ignored altogether.
   (d) Atomic nuclei are assumed to be a point charges.
   (e) The effects of gravity are ignored.

6. Sometimes the energy of the atoms and molecules is reported not in Hartree, but in Rydberg.

$$1 \text{ Hartree} = 2 \text{ Rydberg}$$

Which of the following is the correct formula for the ground state energy of the one-electron atom in units of Rydberg.

(a) $-\dfrac{Z}{2n}$	(e) $-\dfrac{Z}{n}$	(i) $-\dfrac{2Z}{n}$
(b) $-\dfrac{Z^2}{2n}$	(f) $-\dfrac{Z^2}{n}$	(j) $-\dfrac{2Z^2}{n}$
(c) $-\dfrac{Z}{2n^2}$	(g) $-\dfrac{Z}{n^2}$	(k) $-\dfrac{2Z}{n^2}$
(d) $-\dfrac{Z^2}{2n^2}$	**(h)** $-\dfrac{Z^2}{n^2}$	(l) $-\dfrac{2Z^2}{n^2}$

7-10: In class, we wrote that the Schrödinger equation for the molecule with *P* nuclei and *N* electrons could be written as

$$\left(\hat{T}_n + \hat{T}_e + V_{nn} + V_{ee} + V_{ne}\right)\Psi = E\Psi$$

Match the following operators to their mathematical definition and their "meaning" by filling in the table at the bottom of the page.

Meanings:

(a) nuclear-electron attraction energy operator
(b) nuclear-nuclear repulsion energy operator
(c) electron-electron repulsion energy operator
(d) nuclear kinetic energy operator
(e) electronic kinetic energy operator

Equations:

(i) $\displaystyle\sum_{\alpha=2}^{P}\sum_{\beta=1}^{\alpha-1}\frac{Z_\alpha Z_\beta e^2}{4\pi\varepsilon_0\left|\boldsymbol{R}_\beta - \boldsymbol{R}_\alpha\right|}$

(ii) $\displaystyle\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{e^2}{4\pi\varepsilon_0\left|\boldsymbol{r}_i - \boldsymbol{r}_j\right|}$

(iii) $\displaystyle-\sum_{\alpha=1}^{P}\sum_{i=1}^{N}\frac{Z_\alpha e^2}{4\pi\varepsilon_0\left|\boldsymbol{r}_i - \boldsymbol{R}_\alpha\right|}$

(iv) $\displaystyle\sum_{i=1}^{N}-\frac{\hbar^2}{2m_e}\nabla_i^2$

(v) $\displaystyle\sum_{\alpha=1}^{P}-\frac{\hbar^2}{2m_\alpha}\nabla_\alpha^2$

Operator	**Equation**	**"meaning"**
$\hat{T}_n$	v	d
$\hat{T}_e$	iv	e
V_{nn}	i	b
V_{ne}	iii	a