

CHEM 3420: Physical Chemistry II — Spring 2009

Homework 5

Due in Class: Monday, February 23, 2009

1. In a hydrogen atom, the $2s$ and $2p$ orbitals have the same energy. However, in a boron atom, the $2s$ orbital has a lower energy than the $2p$. Explain this in terms of the shape of the orbitals.
2. Classify the following wave functions as symmetric, antisymmetric, or neither in the exchange of electrons 1 and 2:

(a) $[\psi_{1s}(1)\psi_{2s}(2) + \psi_{2s}(1)\psi_{1s}(2)][\alpha(1)\beta(2) - \beta(1)\alpha(2)]$

(b) $[\psi_{1s}(1)\psi_{2s}(2) + \psi_{2s}(1)\psi_{1s}(2)]\alpha(1)\alpha(2)$

(c) $[\psi_{1s}(1)\psi_{2s}(2) + \psi_{2s}(1)\psi_{1s}(2)][\alpha(1)\beta(2) + \beta(1)\alpha(2)]$

(d) $[\psi_{1s}(1)\psi_{2s}(2) - \psi_{2s}(1)\psi_{1s}(2)][\alpha(1)\beta(2) - \beta(1)\alpha(2)]$

3. A more exact solution to the Schrödinger Equation for the hydrogen atom is obtained if the coordinate system is placed at the center of the mass of the atom rather than at the nucleus. In that case, the energy levels for a one-electron atom or ion of nuclear charge Z is given by:

$$E_n = \frac{Z^2 \mu e^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2}$$

where μ is the reduced mass of the atom. The masses of an electron, proton, and a tritium (^3H or T) nucleus are given by 9.1094×10^{-31} kg, 1.6726×10^{-27} kg, and 5.0074×10^{-27} kg, respectively.

Calculate the frequency of the $n = 1 \rightarrow n = 4$ transition in H and T to five significant figures. Which of the following transitions could the frequencies correspond to: $1s \rightarrow 4s$, $1s \rightarrow 4p$, or $1s \rightarrow 4d$.