Problem Set 8

Due: 24 July 2020, 12.30 p.m.

Problem 1. The potential energy between a pair of atoms is often well described by the Lennard-Jones (or 6-12) potential $U(r) = U_0\left[\left(\frac{a}{r}\right)^{12} - \left(\frac{a}{r}\right)^{6}\right]$, where $U_0 > 0$ and a are constants. Find the interatomic equilibrium separation r_0 in terms of a. Find $U(r_0)$.

(2 points)

Problem 2. (a) Calculate the electrostatic potential energy of Na^+ and Cl^- ions at their equilibrium separation distance of 0.24 nm, assuming the ions to be point charges. (b) Find the energy corresponding to Pauli exclusion principle repulsion for NaCl. (c) Assuming that it may be described by the formula A/r^n, find the values of the constant A and the exponent n.

Please refer to the textbook for numerical values of the ionization energy of Na, electron affinity of Cl, dissociation energy of NaCl, and the equilibrium separation in NaCl. Additional information $\frac{e^2}{4\pi\varepsilon_0} = 1.44$ eV $\cdot$ nm, where e is the magnitude of the electron's charge, and ε_0 is the dielectric permittivity of vacuum.

(2 + 2 + 2 points)

Problem 3. The equilibrium separation of the atoms in the HF molecule is 0.0917 nm, and its measured electric dipole moment is 6.40×10^{-30} C·m. To what extent is the the bonding ionic? (give your answer in %)

(2 points)

Problem 4. Ionic bonding in the BaO molecule involves the transfer of two electrons from the Ba atom. If the equilibrium separation is 0.193 nm and the measured electric dipole moment is 26.7×10^{-30} C·m, to what extent is the bond actually ionic?

(2 points)

Problem 5. The hydrogen bonds linking the two helical strands of the DNA have bond strengths of about 0.3 eV, or approximately 15 percent of the strengths of the ionic/covalent bonds along the strands. (a) What is the wavelength of a photon with sufficient energy to break this bond? (b) In what part of the spectrum does this wavelength lie? (c) Since a significant intensity exists at this wavelength in the environment, why have not all the DNA hydrogen bonds long since broken?

(1 + 1 + 2 points)

Problem 6. The characteristic rotational energy $E_{\mathrm{rot}} = \hbar^2/2I$ for KCl is $1.43 \cdot 10^{-5}$ eV. (a) Find the reduced mass for the KCl molecule. (b) Find the separation distance of the K^+ and Cl^- ions.

(3/2 + 3/2 points)

Problem 7. The vibration frequency of the NO molecule is $5.63 \cdot 10^{13}$ Hz. Compute the force constant for NO.

(*3/2 points*)

Problem 8. For a molecule such as CO, which has a permanent electric dipole moment, radiative transitions obeying the selection rule $\Delta l = \pm 1$ between two rotational energy levels of the same vibrational energy state are allowed; that is the selection rule $\Delta \nu = \pm 1$ does not hold.

(a) Find the moment of inertia of CO, for which $r_0 = 0.113$ nm, and calculate the characteristic rotational energy E_{0r} in eV.

(b) Make an energy-level diagram for the rotational levels with $l = 0$ to $l = 5$ for some vibrational level. Label the energies in eV, starting with $E = 0$ for $l = 0$.

(c) Indicate on your diagram transitions that obey $\Delta l = -1$ and calculate the energy of photons emitted.

(d) Find the wavelength of the photon emitted for each transition in (c). In what region of the electromagnetic spectrum are these photons?

(*3/2 + 3/2 + 3/2 + 1 points*)