

9-5. (a) Total potential energy: $U(r) = -\frac{ke^2}{r} + E_{ex} + E_{ion}$ (Equation 9-1)

$$\text{attractive part of } U(r_0) = -\frac{ke^2}{r_0} = -\frac{1.44eV \cdot nm}{0.267nm} = -5.39eV$$

(b) The net ionization energy is:

$$E_{ion} = (\text{ionization energy of } Rb) - (\text{electron affinity of } Cl) \\ = 4.18eV - 3.62eV = 0.56eV$$

Neglecting the exclusion principle repulsion energy E_{ex} ,

$$\text{dissociation energy} = -U(r_0) = 5.39eV - 0.56eV = 4.83eV$$

(c) Including exclusion principle repulsion,

$$\text{dissociation energy} = 4.37eV - U(r_0) = 5.39eV - 0.56eV - E_{ex}$$

$$E_{ex} = 5.39eV - 4.37eV - 0.56eV = 0.46eV$$

9-6. $U_c = -\frac{ke^2}{r_0} + E_{ion} = -\frac{1.440eV \cdot nm}{0.282nm} + (4.34eV - 3.36eV) = -4.13eV$

The dissociation energy is $3.94eV$.

$$E_d = |U_c + E_{ex}| = 3.94eV = |-4.13eV + E_{ex}|$$

$$E_{ex} = 0.19eV \text{ at } r_0 = 0.282nm$$

9-12. Dipole moment $p_{ionic} = er_0$ (Equation 9-3)

$$= (1.609 \times 10^{-19} C)(0.0917nm)$$

$$= 1.47 \times 10^{-20} C \cdot nm \times 10^{-9} m / nm$$

$$= 1.47 \times 10^{-29} C \cdot m$$

if the HF molecule were a pure ionic bond. The measured value is $6.64 \times 10^{-29} C \cdot m$, so

$$\text{the } HF \text{ bond is } (6.40 \times 10^{-30} C \cdot m) / (1.47 \times 10^{-29} C \cdot m) = 0.44 \text{ or } 44\% \text{ ionic.}$$

9-19. (a) $NaCl$ is polar. The Na^+ ion is the positive charge center, the Cl^- ion is the negative

charge center.

(b) O_2 is nonpolar. The covalent bond involves no separation of charges, hence no polarization of the molecule.

9-21. $E_{0r} = \frac{\hbar^2}{2I}$ (Equation 9-14) where $I = \frac{1}{2}mr_0^2$ for a symmetric molecule.

$$E_{0r} = \frac{\hbar^2}{mr_0^2} = \frac{(\hbar c)^2}{mc^2 r_0^2} = \frac{(197.3 \text{ eV} \cdot \text{nm})^2}{(16 \text{ uc})^2 (931.5 \times 10^6 \text{ eV} / \text{uc}^2) (0.121 \text{ nm})^2} = 1.78 \times 10^{-4} \text{ eV}$$

9-22. For Co : $f = 6.42 \times 10^{13} \text{ Hz}$ (See Example 9-6)

$$E_v = (v + 1/2)hf \quad (\text{Equation 9-20})$$

(a) $E_1 - E_0 = 3hf/2 - hf/2 = hf$

$$= (4.14 \times 10^{-15} \text{ eV} \cdot \text{s}) (6.42 \times 10^{13} \text{ Hz})$$

$$= 0.27 \text{ eV}$$

(b) $\frac{n_1}{n_0} = e^{-(E_1 - E_0)/kT}$ (from Equation 8-2)

$$0.01 = e^{-(0.27)/(8.62 \times 10^{-5})}$$

$$\ln(0.01) = -(0.27 \text{ eV}) / (8.62 \times 10^{-5} \text{ eV} / \text{K}) T$$

$$T = \frac{-(0.27 \text{ eV})}{\ln(0.01) (8.62 \times 10^{-5} \text{ eV} / \text{K})}$$

$$T = 680 \text{ K}$$

9-23. For LiH : $f = 4.22 \times 10^{13} \text{ Hz}$ (from Table 9-7)

(a) $E_v = (v + 1/2)hf = E_0 = hf/2 = (4.14 \times 10^{-15} \text{ eV} \cdot \text{s}) (4.22 \times 10^{13} \text{ Hz}) / 2$

$$E_0 = 0.087 \text{ eV}$$

(b) $\mu = \frac{m_1 m_2}{m_1 + m_2}$ (Equation 9-17)

$$\mu = \frac{(7.0160 \text{ u})(1.0078 \text{ u})}{(7.0160 \text{ u}) + (1.0078 \text{ u})} = 0.8812 \text{ u}$$

$$(c) f = \frac{1}{2\pi} \sqrt{\frac{K}{\mu}} \quad (\text{Equation 9-21})$$

$$K = (2\pi f)^2 \mu = (2\pi)^2 (4.22 \times 10^{13} \text{ Hz})(0.8812)(1.66 \times 10^{-27} \text{ kg/u})$$

$$K = 117 \text{ N/m}$$

$$(d) E_n = n^2 h^2 / 8m r_0^2 \rightarrow r_0^2 = n^2 h^2 / 8m E_n$$

$$r_0 \approx h / (8m E_0)^{1/2}$$

$$r_0 \approx \frac{6.63 \times 10^{-34} \text{ J}\cdot\text{s}}{\left[8(0.8812u)(1.66 \times 10^{-27} \text{ kg/u})(0.087 \text{ eV})(1.60 \times 10^{-19} \text{ J/eV})\right]^{1/2}}$$

$$r_0 \approx 5.19 \times 10^{-11} \text{ m} = 0.052 \text{ nm}$$

$$9-25. (a) \mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{(39.1u)(35.45u)}{39.1u + 35.45u} = 18.6u$$

$$(b) E_{0r} = \frac{\hbar^2}{2I} \quad (\text{Equation 9-14}) \quad I = \mu r_0^2$$

$$E_{0r} = \frac{\hbar^2}{2\mu r_0^2} = \frac{(\hbar c)^2}{2\mu c^2 r_0^2} \rightarrow r_0^2 = \frac{(\hbar c)^2}{2\mu c^2 E_r}$$

$$\therefore r_0 = \frac{\hbar c}{(2\mu c^2 E_r)^{1/2}} = \frac{197.3 \text{ eV}\cdot\text{nm}}{\left[2(10.6 \mu c^2)(931.5 \times 10^6 \text{ eV}/\mu c^2)(1.43 \times 10^{-5} \text{ eV})\right]^{1/2}}$$

$$r_0 = 0.280 \text{ nm}$$

$$9-26. f = \frac{1}{2\pi} \sqrt{\frac{K}{\mu}} \quad (\text{Equation 9-21})$$

$$(a) \text{ For } H^{35}\text{Cl}: \mu = 0.980u \text{ and } f = 8.97 \times 10^{13} \text{ Hz}.$$

$$K = (2\pi f)^2 \mu = (2\pi)^2 (8.97 \times 10^{13} \text{ Hz})^2 (0.980u)(1.66 \times 10^{-27} \text{ kg/u}) = 517 \text{ N/m}.$$

(b) For $K^{79}\text{Br}$: $\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{(39.102u)(78.918u)}{39.102u + 78.918u} = 26.147u$ and

$$f = 6.93 \times 10^{12} \text{ Hz}$$

$$K = (2\pi f)^2 \mu = (2\pi)^2 (6.93 \times 10^{12} \text{ Hz})^2 (26.147u)(1.66 \times 10^{-27} \text{ kg/u}) = 82.3 \text{ N/m}$$

9-27. $E_{0r} = \hbar^2/2I$ Treating the Br atom as fixed,

$$I = m_H r_0^2 = (1.0078u)(1.66 \times 10^{-27} \text{ kg/u})(0.141 \text{ nm})^2$$

$$E_{0r} = \frac{(1.055 \times 10^{-34} \text{ J}\cdot\text{s})^2}{2(1.0078u)(1.66 \times 10^{-27} \text{ kg/u})(0.141 \text{ nm})^2 (10^{-9} \text{ m/nm})^2}$$

$$= 1.67 \times 10^{-22} \text{ J} = 1.04 \times 10^{-3} \text{ eV}$$

$$E_\ell = \ell(\ell+1)E_{0r} \text{ for } \ell = 0, 1, 2, \dots \quad (\text{Equation 9-13})$$

The four lowest states have energies:

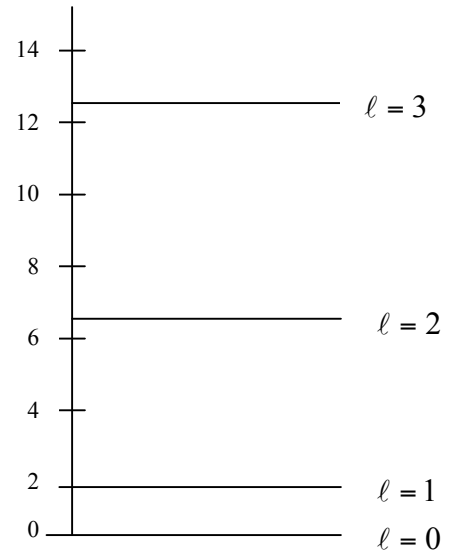
$$E_0 = 0$$

$$E_1 = 2E_{0r} = 2.08 \times 10^{-3} \text{ eV}$$

$$E_2 = 6E_{0r} = 6.27 \times 10^{-3} \text{ eV}$$

$$E_3 = 12E_{0r} = 12.5 \times 10^{-3} \text{ eV}$$

$$E_\ell \quad (\times 10^{-3} \text{ eV})$$



9-29. $E_{0r} = \frac{\hbar^2}{2I}$ where $I = \mu r_0^2$ (Equation 9-14)

$$\text{For } K^{35}\text{Cl: } \mu = \frac{(39.102u)(34.969u)}{39.102u + 34.969u} = 18.46u$$

$$\text{For } K^{37}\text{Cl: } \mu = \frac{(39.102u)(34.966u)}{39.102u + 34.966u} = 19.00u$$

$$r_0 = 0.267\text{nm for } KCl.$$

$$E_{0r}(K^{35}\text{Cl}) = \frac{(1.055 \times 10^{-34} \text{J}\cdot\text{s})^2}{2(18.46u)(1.66 \times 10^{-27} \text{kg}/u)(0.267 \times 10^{-9} \text{m})^2}$$

$$= 2.55 \times 10^{-24} \text{J} = 1.59 \times 10^{-5} \text{eV}$$

$$E_{0r}(K^{37}\text{Cl}) = \frac{(1.055 \times 10^{-34} \text{J}\cdot\text{s})^2}{2(19.00u)(1.66 \times 10^{-27} \text{kg}/u)(0.267 \times 10^{-9} \text{m})^2}$$

$$= 2.48 \times 10^{-24} \text{J} = 1.55 \times 10^{-5} \text{eV}$$

$$\Delta E_{0r} = 0.04 \times 10^{-5} \text{eV}$$

9-40. (a) Total potential energy: $U(r) = -\frac{ke^2}{r} + E_{ex} + E_{ion}$

the electrostatic part of $U(r)$ at r_0 is $-\frac{ke^2}{r_0} = -\frac{1.44\text{eV}\cdot\text{nm}}{0.24\text{nm}} = -6.00\text{eV}$

(b) The net ionization energy is:

$$E_{ion} = (\text{ionization energy of Na}) - (\text{electron affinity of Cl})$$

$$= 5.14\text{eV} - 3.62\text{eV} = 1.52\text{eV}$$

dissociation energy of $\text{NaCl} = 4.27\text{eV}$ (from Table 9-2)

$$4.27\text{eV} = -U(r_0) = 6.00\text{eV} - 1.52\text{eV} = 4.67\text{eV} - E_{ex}$$

$$E_{ex} = 6.00\text{eV} - 4.27\text{eV} - 1.52\text{eV} = 0.21\text{eV}$$

(c) $E_{ex} = \frac{A}{r^n}$ (Equation 9-2)

At $r_0 = 0.24\text{nm}$, $E_{ex} = 0.21\text{eV}$

At $r_0 = 0.14\text{nm}$, $U(r) = 0$ and $E_{ex} = \frac{ke^2}{r} - E_{ion} = 8.77\text{eV}$

$$\text{At } r_0 : E_{ex} = 0.21eV = \frac{A}{(0.24nm)^n} \rightarrow A = (0.21eV)(0.24nm)^n$$

$$\text{At } r = 0.14nm : E_{ex} = 8.77eV = \frac{A}{(0.14nm)^n} \rightarrow A = (8.77eV)(0.14nm)^n$$

Setting the two equations for A equal to each other:

$$\frac{(0.24nm)^2}{(0.14nm)^n} = \left(\frac{0.24}{0.14}\right)^2 = \left(\frac{8.77eV}{0.21eV}\right) \rightarrow (1.71)^n = 41.76$$

$$n \log 1.71 = \log 41.76$$

$$n = (\log 41.76) / (\log 1.71) = 6.96$$

$$A = 0.21eV (0.24nm)^n = 0.21eV (0.24nm)^{6.96} = 1.02 \times 10^{-5} eV \cdot nm^{6.96}$$

9-52. (a) $\frac{dU}{dr} = U_0 \left[-12a^{12}r^{-13} - 2(-6a^6)r^{-7} \right]$

For U_{\min} , $dU/dr = 0$, so $-12a^{12}r^{-6} + 12a^6 = 0 \rightarrow r^{-6} = a^{-6} \rightarrow r = a$

(b) For $U = U_{\min}$, $r = a$ then $U_{\min} = U_0 \left[\left(\frac{a}{a}\right)^{12} - 2\left(\frac{a}{a}\right)^6 \right] = (1 - 2)U_0 = -U_0$

(c) From Figure 9-8(b): $r_0 = 0.074nm (= a)$ $U_0 = 32.8eV$

(d)

r/r_0	$(r_0/r)^{12}$	$-2(r_0/r)^6$	U
0.85	7.03	-5.30	+56.7
0.90	3.5	-3.8	-9.8
0.95	1.85	-2.72	-28.5
1.00	1	-2.0	-32.8
1.05	0.56	-1.5	-30.8
1.10	0.32	-1.12	-26.2
1.15	0.19	-0.86	-22.0
1.20	0.11	-0.66	-18.0

