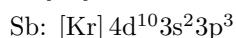
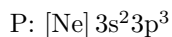
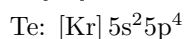
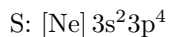
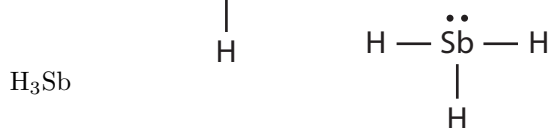
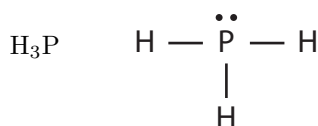
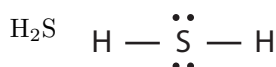


Solutions to assignment 5

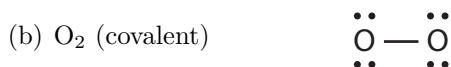
1. The elements H, S, Te, P, and Sb have electronic configurations:



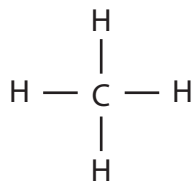
H has one electron to share. S and Te are eager to pick up two additional electrons in their p orbitals. P and Sb are looking for three additional electrons in their p orbitals. This leads to



2. (a) $\text{Ca}^{2+} + 2\text{Cl}^- \leftrightarrow \text{CaCl}_2$ (ionic)



- (c) CH_4 (covalent)



3. The Leonard-Jones potential is

$$U(r) = U_0(a^{12}r^{-12} - 2a^6r^{-6}).$$

- (a) Its derivative

$$\begin{aligned} \frac{dU(r)}{dr} &= U_0(a^{12}(-12r^{-13}) - 2a^6(-6r^{-7})) \\ &= -12\frac{U_0a^6}{r^7} \left(\frac{a^6}{r^6} - 1 \right) \end{aligned}$$

vanishes when $dU/dr|_{r=r_{\min}} = 0$; this occurs when $r_{\min} = a$.

- (b) The minimum value of the potential is

$$U(r_{\min}) = U_0 \times (1 - 2) = -U_0.$$

(c) The figure is offset from the energy zero by an amount $\lim_{r \rightarrow \infty} U(r) = U_{\infty} = -27.2 \text{ eV}$. Matching the figure and the Leonard-Jones potential gives

$$U(r) = U_0 \left[\left(\frac{a}{r} \right)^{12} - 2 \left(\frac{a}{r} \right)^6 \right] + U_{\infty},$$

with $r_0 = 0.074 \text{ nm}$, $U_0 = 4.5 \text{ eV}$. Observe that $U(r_{\min}) = -U_0 + U_{\infty} = -4.5 - 27.2 = -31.9 \text{ eV}$.

4. The size of the unit cell is $V_{\text{cell}} = (2R)^3 = 8R^3$. The occupied space is one eighth of each of eight spheres; i.e., $V_{\text{cell}} = 8 \times \frac{1}{8} \times \frac{4}{3}\pi R^3 = \frac{4}{3}\pi R^3$. Hence,

$$\frac{V_{\text{sphere}}}{V_{\text{cell}}} = \frac{\frac{4}{3}\pi R^3}{8R^3} = \frac{\pi}{6} = 0.524.$$

