3. Kasap problem 1.4

$$E(r) = -\frac{ke^2M}{r} + \frac{B}{r^m}$$

$M = 1.763$

$B = 1.192\times10^{-104}\ Jm^9 = 7.442\times10^{-5}\ eV\,nm^9$

$m = 9$

$$\frac{dE}{dr} = \frac{ke^2M}{r_o^2} + \frac{-mB}{r_o^{m+1}} = \frac{ke^2M}{r_o^2} - \frac{9B}{r_o^{10}} = 0$$

$$r_o^8\, ke^2M - 9B = 0$$

$$r_o = \left(\frac{9B}{ke^2M}\right)^{1/8} = \left[\frac{9\times1.192\times10^{-104}\ Jm^9}{9\times10^9\ Nm^2/C^2\ (1.602\times10^{-19}C)^2\times1.763}\right]^{1/8} =$$

$$= \left(\frac{9\times1.192}{9\times(1.602)^2\times1.763}\right)^{1/8} \times 10^{(-104-9+38)/8} =$$

$$= 3.57\times10^{-10}\ m = \boxed{0.357\ nm = r_o}$$

note that $ke = 9\times10^{18}\ eV\,nm/C$

$$E(r_o) = -\frac{ke^2M}{r_o} + \frac{B}{r_o^m} = -\frac{(9\times10^{18}\ eV\,nm/C)(1.602\times10^{-19}C)\ (1.763)}{0.357\ nm} +$$

$$+ \frac{7.442\times10^{-5}\ eV\,nm^9}{(0.357\ nm)^9} =$$

$= -6.33$ eV per ion pair, or 3.17 eV per ion

the ionic cohesive energy per mole:

$$E_{cohesive} = 6.33\,eV\left(\frac{1.602\times10^{-19}\,J}{eV}\right)\left(\frac{6.022\times10^{23}}{1\ mol}\right) = 6.1\times10^5\ J/mol =$$

$= 610$ kJ/mol of $Cs^+$-$Cl^-$ ion pairs, which is close to the experimental value of 657 kJ/mol

the ionization energy of Cs: $E_{ionization} = 3.89\ eV$

the electron affinity of Cl: $E_{affinity} = -3.61\ eV$

the bond energy per pair of atoms:

$$E_{cohesive} - (E_{ionization} + E_{affinity}) = 6.33\ eV - 3.89\ eV + 3.61\ eV =$$

$$= 6.04\ eV$$

the atomic cohesive energy then is:

$$E_{cohesive}^{atomic} = 6.04\ eV \left(\frac{1.602 \times 10^{-19}\ J}{eV}\right)\left(\frac{6.022 \times 10^{23}}{mol}\right) = 582\ kJ/mol \text{ of } Cs\text{-}Cl \text{ atom pairs}$$

$$= 291\ kJ/mol \text{ of atoms}$$