24.12: The Gibbs Free Energy Change for Forming HI(g) from H_2(g) and I_2(g)

The standard Gibbs free energies of formation[1] for $HI\,(g)$ and $I_2\,(g)$ are $1.7\,\text{kJ mol}^{-1}$ and $19.3\,\text{kJ mol}^{-1}$, respectively. Calculation of the Gibbs free energy of this reaction from thermochemical data gives $\Delta_r G^o\,(298.15\,\text{K}) = -15.9\,\text{kJ}$. The difference between this value and the value calculated above is $0.3\,\text{kJ}$. The magnitude of this difference is consistent with the number of significant figures given for the tabulated thermochemical data. However, some error results because we have used the simplest possible quantum mechanical models for rotational and vibrational motions. The accuracy of the statistical–mechanical calculation can be increased by using models in which the vibrational oscillator does not follow Hooke's law exactly and in which the rotating molecule is not strictly rigid.