statistical physics → reaction kinetics ★★

Reaction of Hydrogen Isotopes

Consider the following reaction between isotopes of the hydrogen molecule:

$$H_2 + D_2 \to HD + HD.$$

Recall that D is a hydrogen atom with an extra neutron in the nucleus. This means that the mass of the nucleus is doubled.

This is a very special chemical reaction: we can compute its equilibrium constant $K(T)$ from *first principles* given only a single number: the photons absorbed by the HD covalent bond have wavelength 2.62 μm. Of course, we'll make a few assumptions: the key one here is that the chemical bond is approximately a harmonic oscillator, and that the "spring constant" of the oscillator is the same for all 3 molecules.

(a) Compute the ground state energy of the harmonic oscillator of each molecule given the data above. You should express your answer numerically.

(b) Argue that if each molecule is in its ground state, the only differences in energy are due to the differences you found in part (a).

(c) What is the energy of this reaction per H_2 molecule? Does this reaction tend to proceed forward or backward at low temperature?

(d) Next, compare the entropy of the final products to the initial products. Argue that $\Delta S = k_B \log 4$ for this reaction.

(e) Combining the previous parts, find a numerical formula for $K(T)$ as a function of T.

(f) Empirically, we know that $K(300\text{ K}) \approx 3$. Does your theoretical formula match up with this?