Revisit our last calculation on a macroscopic level:

Mix 0.100 mol H_2 + 0.200 mol D_2 + 0.0500 mol HD (+ Pt dust) in a box of volume V.

(a) Find Q at the start of the reaction

$$H_2 + D_2 \rightleftharpoons 2HD$$

$$Q = \frac{[HD]^2}{[H_2][D_2]} = \frac{\left(\frac{\text{mol HD}}{V}\right)^2}{\left(\frac{\text{mol } H_2}{V}\right)\left(\frac{\text{mol } D_2}{V}\right)} = \frac{(\text{mol HD})^2}{(\text{mol } H_2)(\text{mol } D_2)}$$

volumes always cancel for an isotope exchange reaction!

$$Q = \frac{(0.0500)^2}{(0.100)(0.200)} = 0.125$$

(b) Find K

Start by finding the equilibrium (i.e. most probable) amounts of each molecule:

mol H = 2(0.100 mol) + 0.0500 mol = 0.250 mol

mol D = 2(0.200 mol) + 0.0500 mol = 0.450 mol

0.700 mol atoms total

⇒ 0.350 mol molecules total

so $P_H = \left(\frac{0.250 \text{ mol}}{0.700 \text{ mol}}\right) = 0.357_1$

and $P_D = \left(\frac{0.450 \text{ mol}}{0.700 \text{ mol}}\right) = 0.642_9$

then $P_{H_2} = P_H P_H = (0.357_1)(0.357_1) = 0.127_5$

identical! (unlike with small #s)

$P_{D_2} = P_D P_D = (0.642_9)^2 = 0.413_3$

$P_{HD} = 1 - P_{H_2} - P_{D_2} = 1 - 0.127_5 - 0.413_3 = 0.459_2$

∴ mol H_2 = $(0.350 \text{ mol})(0.127_5) = 0.0446_{25}$ mol

mol D_2 = $(0.350 \text{ mol})(0.413_3) = 0.144_{66}$ mol

mol HD = $(0.350 \text{ mol})(0.459_2) = 0.160_{72}$ mol

and $K = \frac{(0.160_{72})^2}{(0.0446_{25})(0.144_{66})} = 4.00$ (look familiar?)

- $Q < K$ ⇒ rxn moves right to reach equil
- $Q \neq K$ ⇒ the initial distribution is less likely than the most probable distribution