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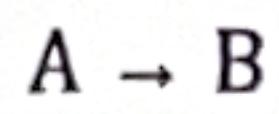
HW3.1 – Equilibrium Constants

Equilibrium Simulation #1

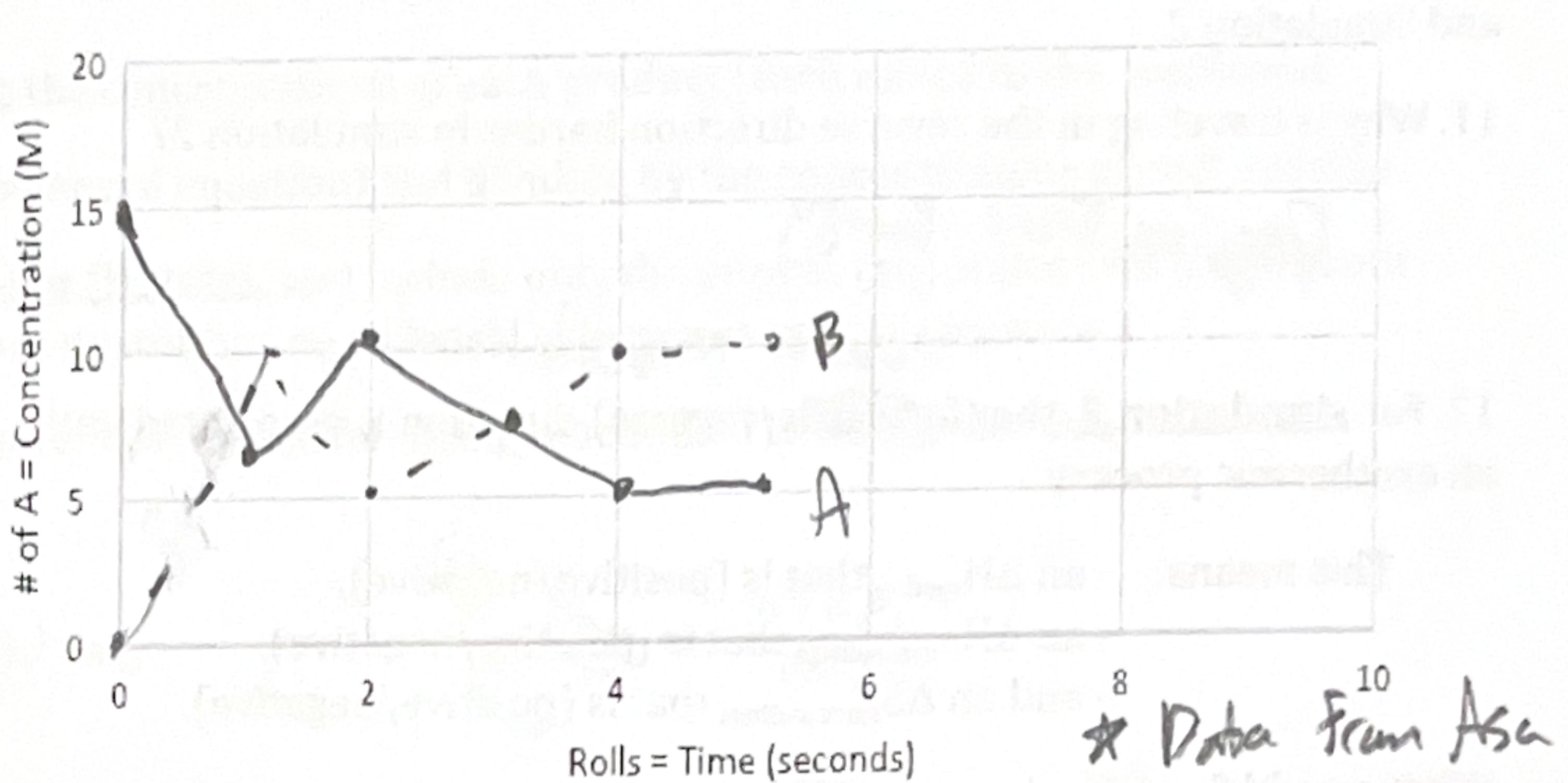
1. Simulation Rules: Plot **both**

A and B as a function of time:

- All molecules start as A; each person represents 1M of A.
- Everyone rolls dice simultaneously to simulate one second of time.
- If an A rolls an even number,



- If a B rolls an odd number,



2. What is the forward reaction rate ($A \rightarrow B$) as a function of [A]? $R_{fwd} = \frac{1}{2}[A]$

3. What is the reverse reaction rate ($B \rightarrow A$) as a function of [B]? $R_{rev} = \frac{1}{2}[B]$

4. At equilibrium, what is the relationship between R_{fwd} and R_{rev} ? $B/A = 1$

5. Combine these three expressions and solve for $[B] / [A]$: ([Products] / [Reactants]): 1

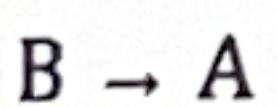
Equilibrium Simulation #2

6. Rules:

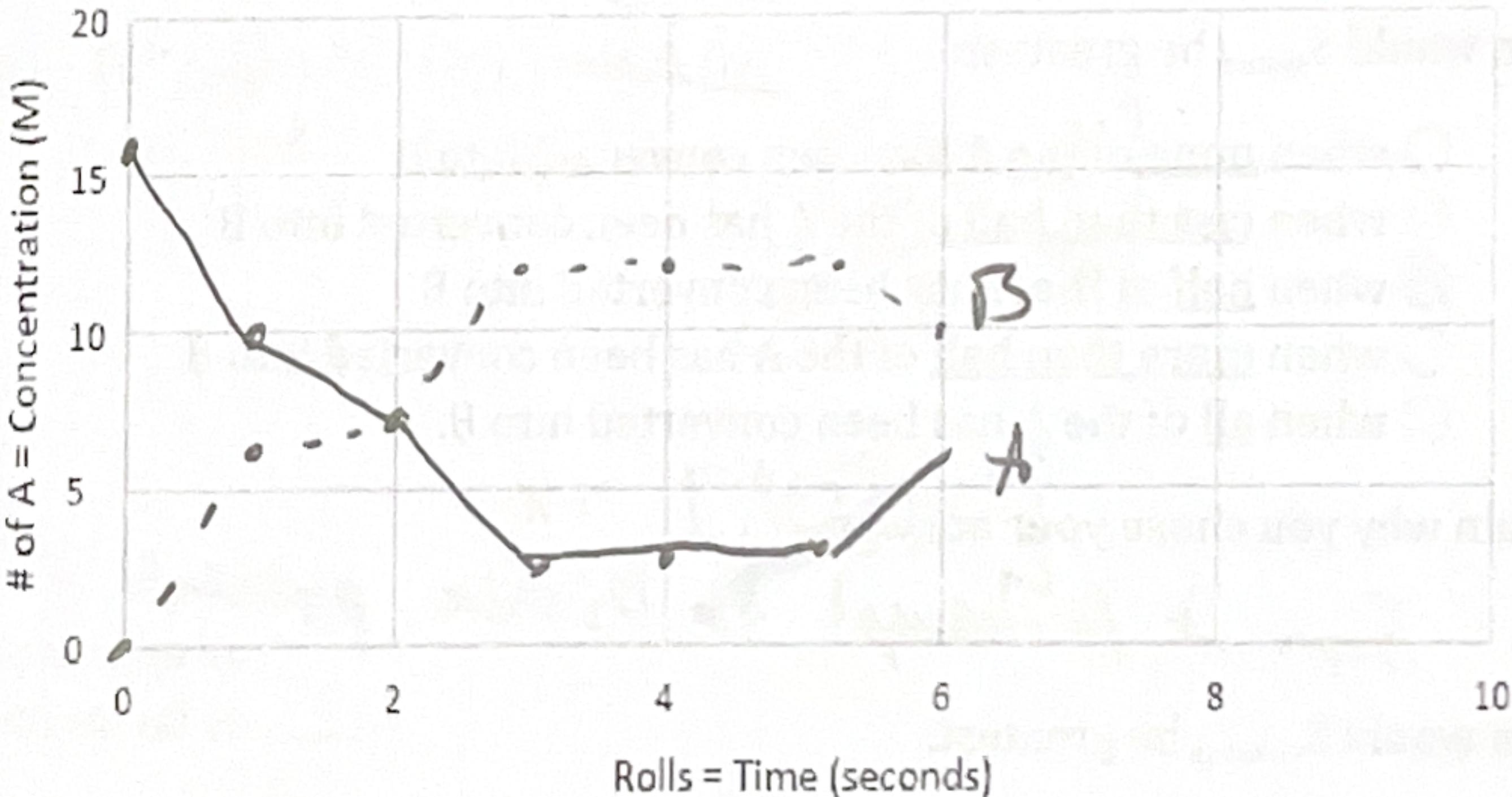
- If an A rolls an even number,



- If a B rolls the number 1,



Plot **both** A and B as a function of time:



7. What is the forward reaction

rate ($A \rightarrow B$) as a function of [A]? $R_{fwd} = \frac{1}{2}[A]$

8. What is the reverse reaction rate ($B \rightarrow A$) as a function of [B]? $R_{rev} = \frac{[B]}{6}$

9. If $R_{fwd} = R_{rev}$, what is $[B] / [A]$ ([Products] / [Reactants])? 3

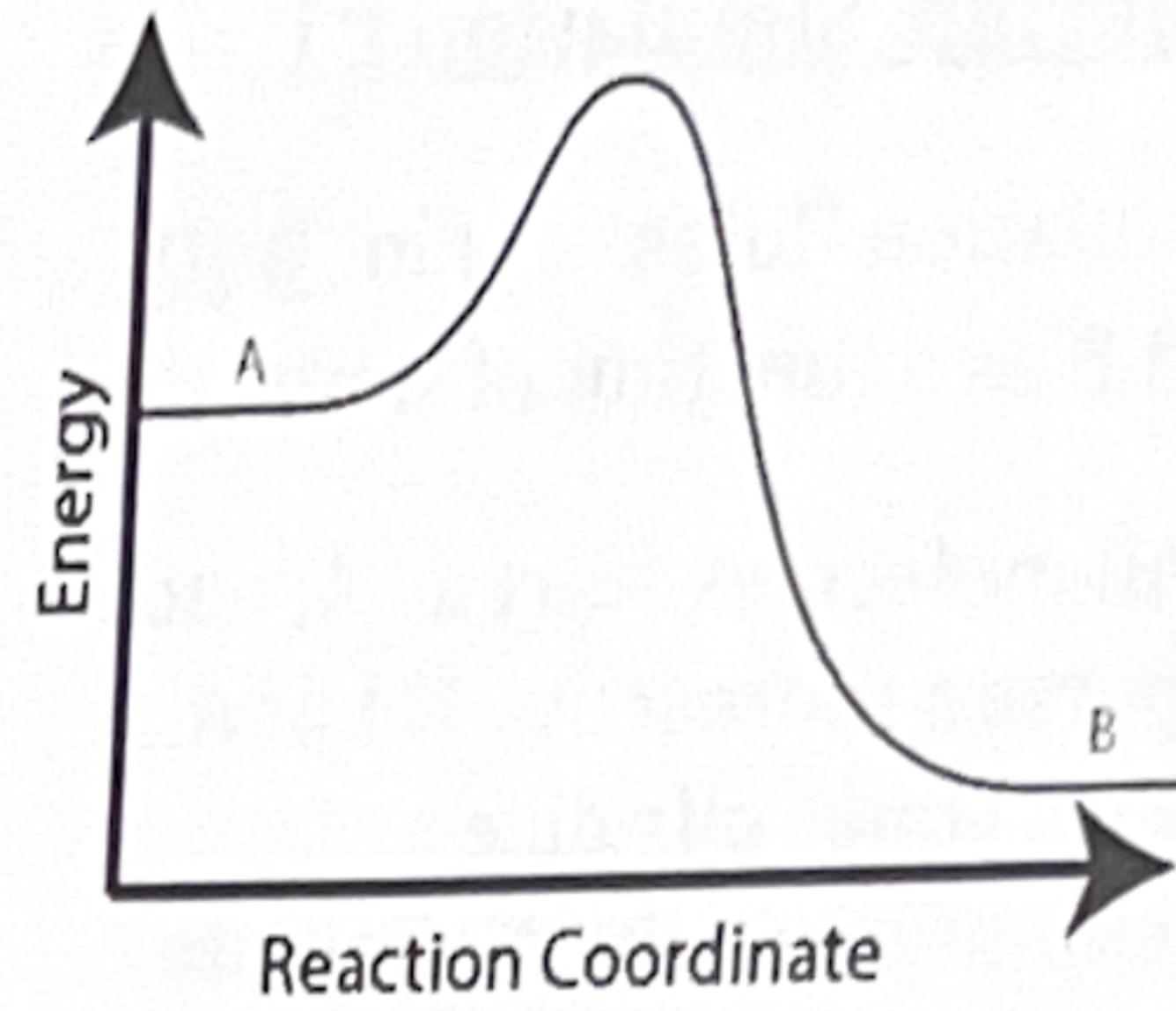
This ratio - [Products] / [Reactants] - is called K, the **equilibrium constant**. Let's think for a moment about how K relates to entropy.

Simulation 2

10. Label the two diagrams at right as corresponding with Simulation 1 and Simulation 2.

11. Why is traveling in the reverse direction harder in simulation 2?

Requires more energy
lower probabilities ($k_A < k_B$)



12. For **simulation 2**, the (forwards/reverse) direction is associated with an exothermic process

This means:

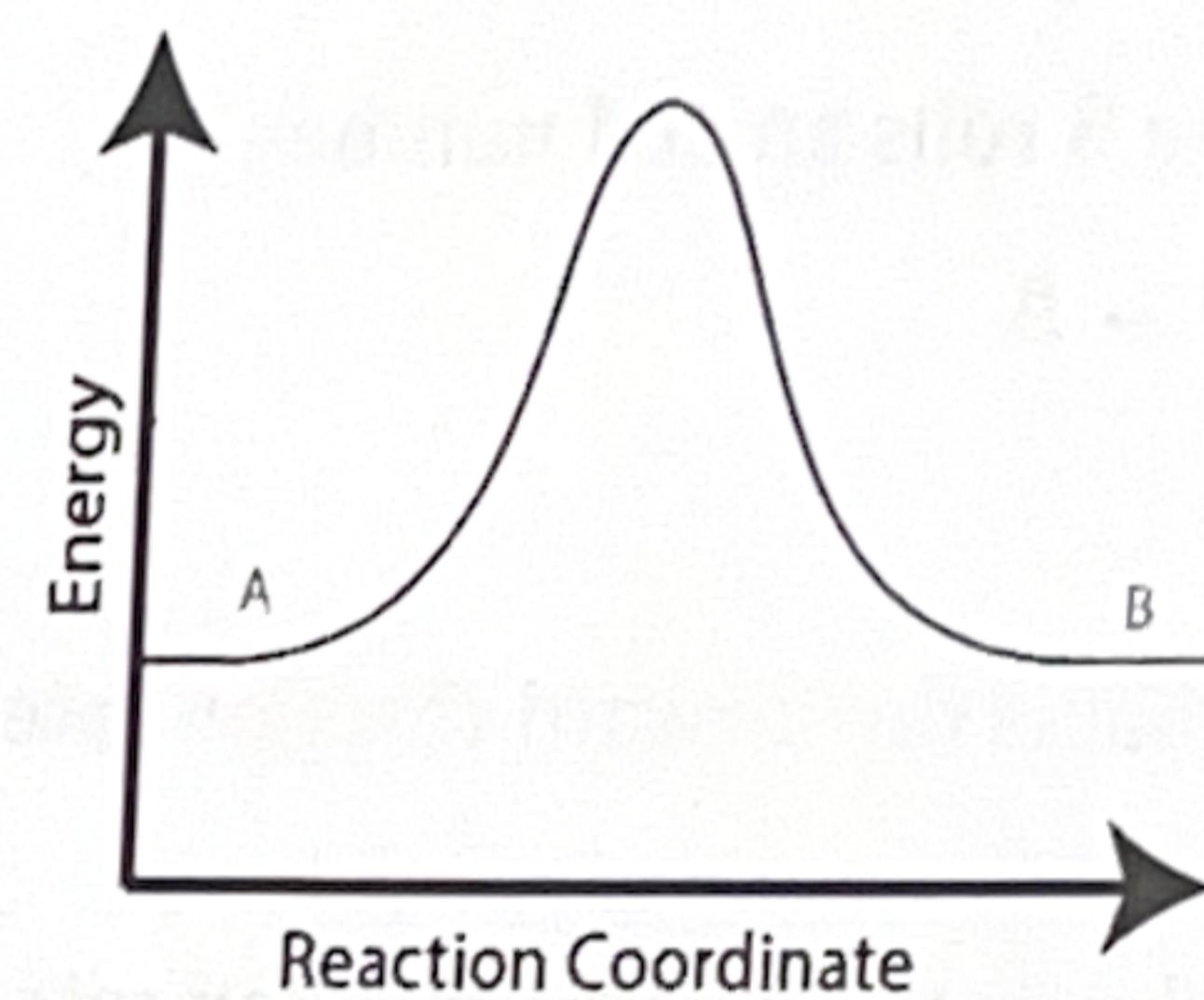
- an ΔH_{system} that is (positive/negative),
- an $\Delta H_{\text{surroundings}}$ that is (positive/negative),
- and an $\Delta S_{\text{surroundings}}$ that is (positive/negative).

When would $S_{\text{surroundings}}$ be greatest?

- when none of the A has been converted into B
- when less than half of the A has been converted into B
- when half of the A has been converted into B
- when more than half of the A has been converted into B
- when all of the A has been converted into B.

Explain why you chose your answer:

$A \rightarrow B$ releases energy \rightarrow more energy in surroundings



When would S_{system} be greatest?

- when none of the A has been converted into B
- when less than half of the A has been converted into B
- when half of the A has been converted into B
- when more than half of the A has been converted into B
- when all of the A has been converted into B.

Explain why you chose your answer:

Some of A changed to B, more particles

When would S_{universe} be greatest:

- when none of the A has been converted into B
- when less than half of the A has been converted into B
- when half of the A has been converted into B
- when more than half of the A has been converted into B
- when all of the A has been converted into B.

Explain why you chose your answer:

$R_{\text{ext}} = \text{more entropy}$

Equilibrium Constant

The equilibrium constant, K, for a reaction $m A + n B \rightarrow x C + y D$ has the form $K = [\text{Products}] / [\text{Reactants}]$

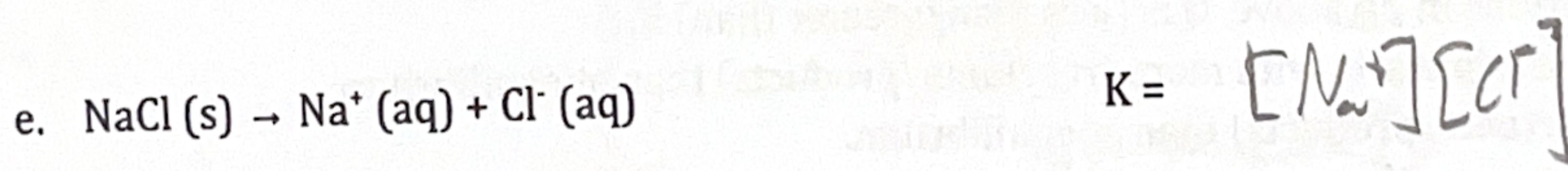
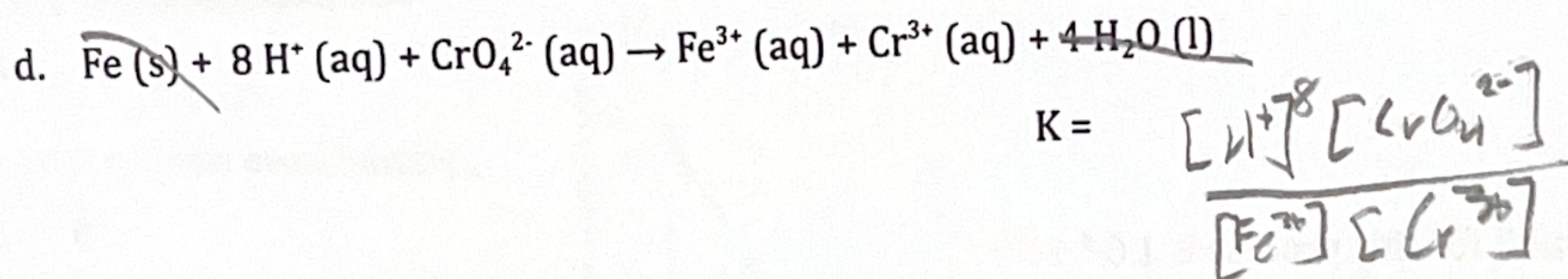
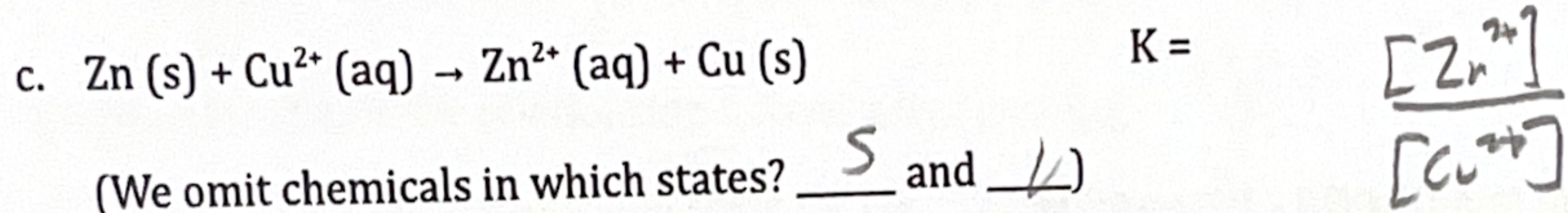
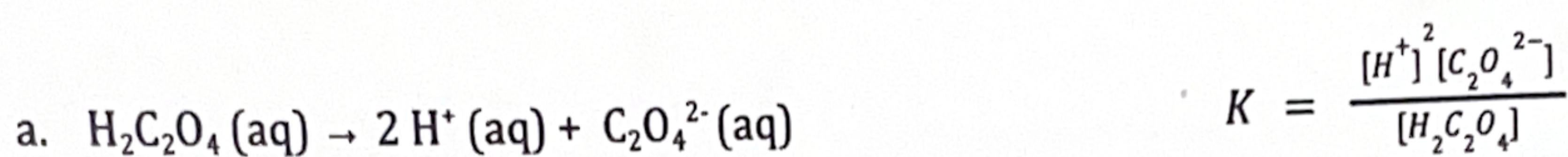
Or,

$$K = [C]^x [D]^y / [A]^m [B]^n$$

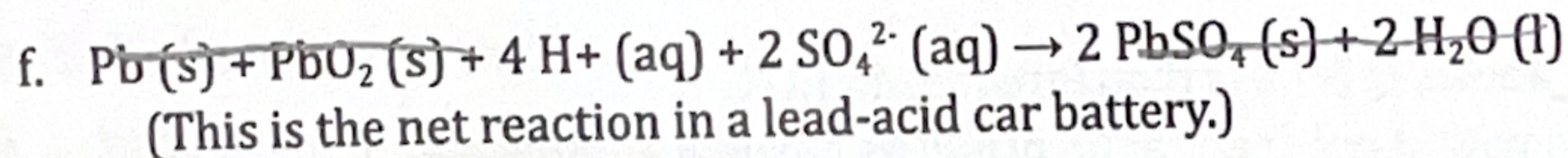
... multiplying the concentrations of each product (each raised to the coefficient from the balanced equation) and dividing by the concentrations of each reactant.

However, we omit the chemicals in (s) or (l) states, and include only the ones in (aq) states (We'll talk about gases below.) If the numerator or denominator has no chemical substances in it, it's equal to 1.

13. Write the equilibrium constant expression for the following reactions: (1a is done for you)



(If the numerator or denominator has no chemical substances in it, it's equal to 1.)

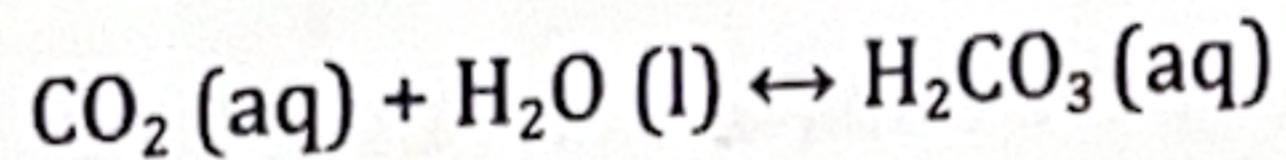


$$K = \frac{1}{[\text{H}^+]^4 [\text{SO}_4^{2-}]^2}$$

We can plug in any quantities (not just the equilibrium values) into the equilibrium constant expression, and find the reaction quotient Q, for any starting concentrations of compound.

Although Q (the reaction quotient), which describes where the reaction currently is, changes, K (the equilibrium constant), which describes where the reaction is going to, doesn't. Put another way: If a reaction is like a road trip, Q is like your current location, which constantly changes, and K is like your final destination, which doesn't change.

For the dissolving of carbon dioxide in water to form carbonic acid:



14. Write the expression for Q (or K) in terms of concentrations:

$$K = \frac{[\text{H}_2\text{CO}_3]}{[\text{CO}_2]}$$

15. Calculate the value of Q under the conditions...

a. $[\text{CO}_2] = 2 \times 10^{-3} \text{ M}$ and $[\text{H}_2\text{CO}_3] = 0 \text{ M}$

$$Q = \underline{\quad 0 \quad}$$

b. $[\text{CO}_2] = 0.5 \times 10^{-3} \text{ M}$ and $[\text{H}_2\text{CO}_3] = 1.5 \times 10^{-3} \text{ M}$

$$Q = \underline{\quad 3 \quad}$$

16. The actual value of K for this process is 1.6×10^{-2} .

a. Under the conditions in 2a above, Q is (less than/greater than) K, meaning the system starts with more (reactants/products) than at equilibrium, and fewer (reactants/products) than at equilibrium.

In order to reach equilibrium, the reaction will need to form more (reactants/products). We can also describe this the reaction going (forwards/backwards), or as the reaction shifting (to the left/to the right).

b. Under the conditions in 2b above, Q is (less than/greater than) K, meaning the system starts with more (reactants/products) than at equilibrium, and fewer (reactants/products) than at equilibrium.

In order to reach equilibrium, the reaction will need to form more (reactants/products). We can also describe this the reaction going (forwards/backwards), or as the reaction shifting (to the left/to the right).