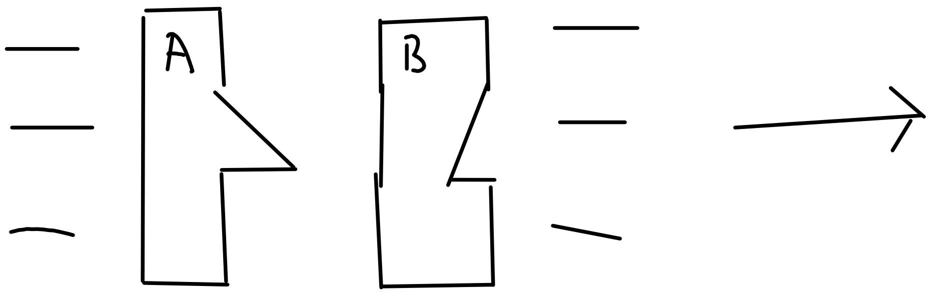
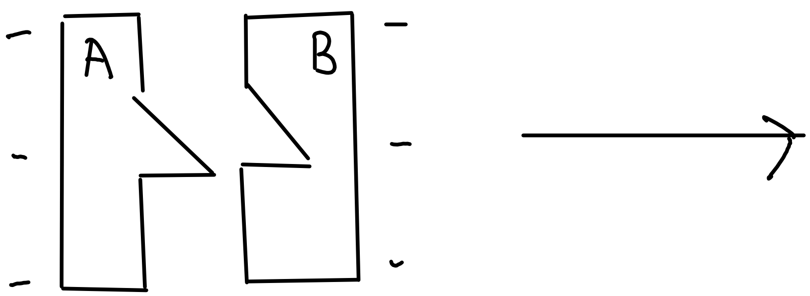
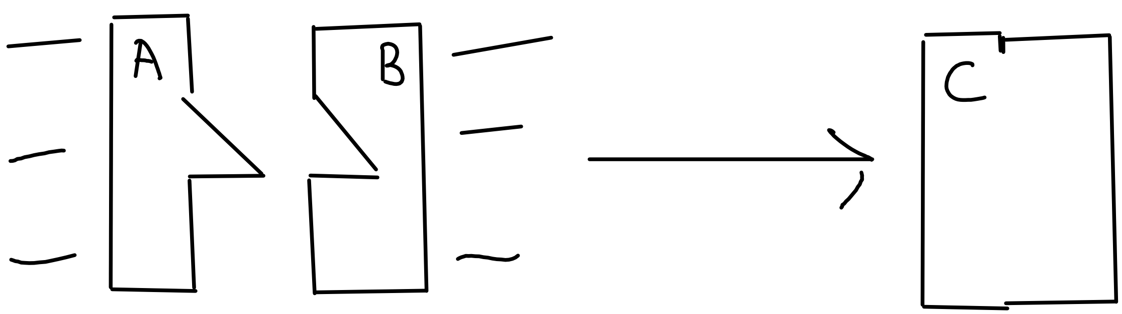


A collision like this - even an energetic one, would lead to NO REACTION, since the molecules are not aligned properly to react. This is particularly important for larger molecules (like biomolecules) where reactive parts of the molecule are small compared to the size of the whole molecule!



A collision where molecules don't hit each other very hard will not lead to a reaction. There isn't enough ENERGY available for the molecules to react with one another.



A collision where molecules hit each other with the correct orientation AND enough energy may lead to a reaction!

EXPLAINING SOME OF THE FACTORS

- Increasing the concentration of reactants increases THE NUMBER OF COLLISIONS that occur in a reaction mixture - increasing rate.

- Increasing SURFACE AREA provides more opportunities for reactant molecules to COLLIDE - increasing rate.

- Increasing temperature INCREASES THE ENERGY (and number) of collisions, since temperature is proportional to the average kinetic energy of molecules. More collisions will have the ACTIVATION ENERGY needed to react, so rate increases.

- Some catalysts work by bending reactant molecules into ORIENTATIONS favorable for reaction - making it easier for large molecules to react with one another.

... but what about this ACTIVATION ENERGY? Let's look at TRANSITION STATE THEORY

TRANSITION STATE THEORY

- States that when reactant molecules collide, they first form a TRANSITION STATE which then decomposes and/or loses energy to form product molecules.

- A TRANSITION STATE is a high-energy state: It may be an unstable combination of several reactant molecules or an excited (high energy) state of a single product molecule. The transition state breaks down and loses energy to form the products of the reaction.

- The ACTIVATION ENERGY is the energy required to form the transition state, and it acts as a barrier to reaction.

- We model the rate constant "k" using collision and transition state theory with the ARRHENIUS EQUATION:

$$\underset{\text{rate constant}}{k} = A \times e^{\frac{-E_a}{R \times T}}$$

Ea = ACTIVATION ENERGY

R = ideal gas constant

T = absolute temperature

A = frequency factor ... the fraction of collisions with the right orientation to react

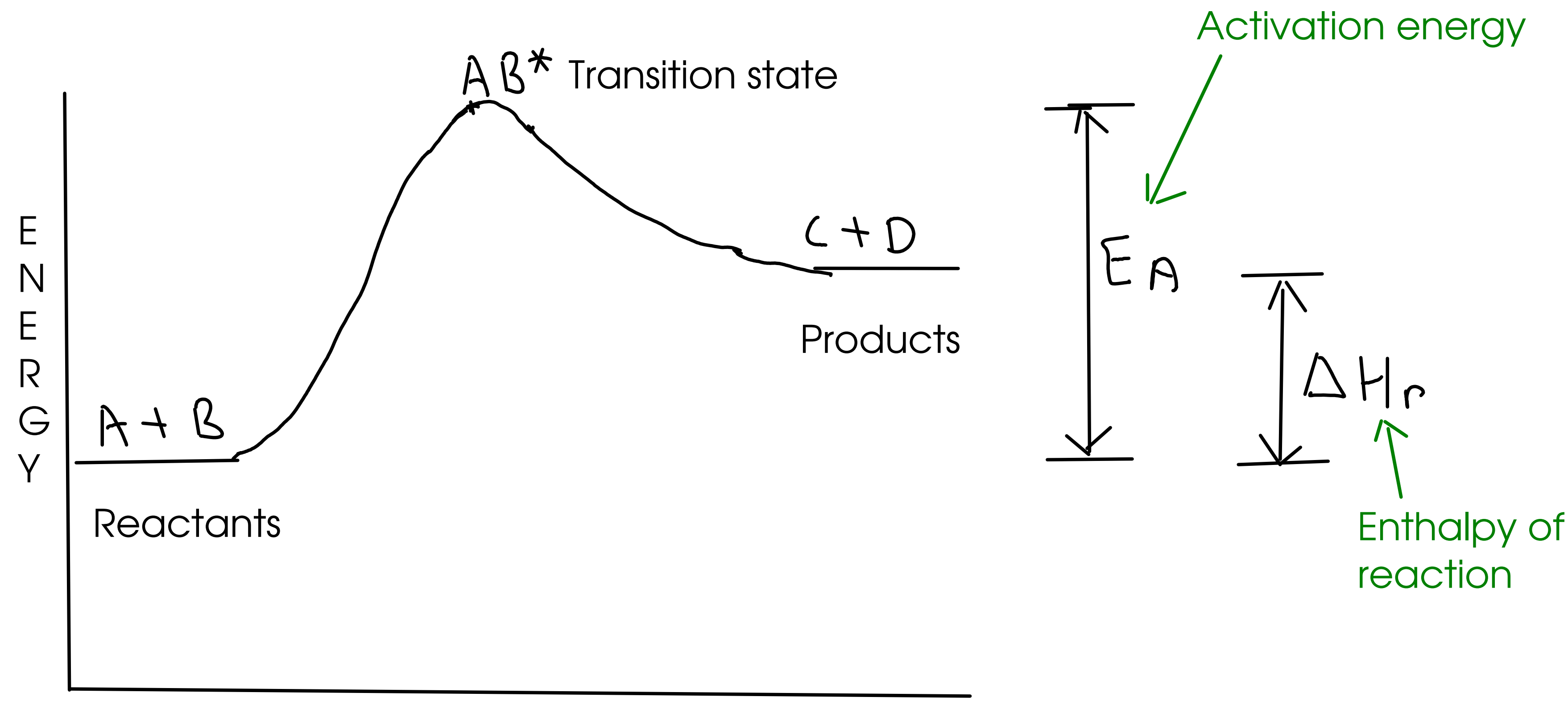
... this equation allows us to calculate the rate constant for different temperatures if we have values for "A" and "Ea". We can get these values by examining a reaction at two (or more) different temperatures.

ENERGY DIAGRAMS

- graphically, we can look at transition state theory via an ENERGY DIAGRAM

For an ENDOTHERMIC REACTION, the products have a higher energy than the reactants

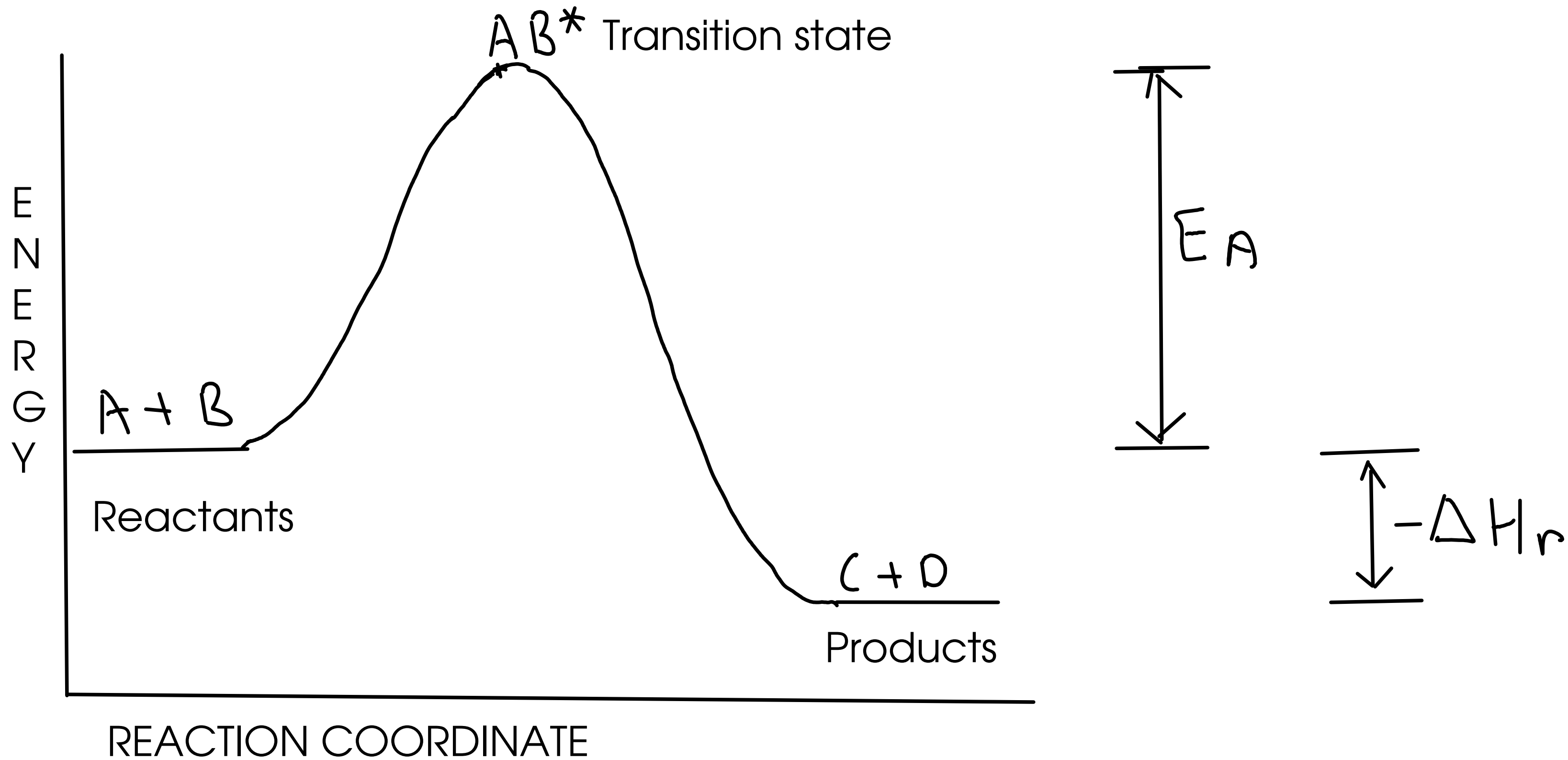
$A + B \rightarrow C + D$



REACTION COORDINATE
- a measure of how far the reaction has proceeded

For an EXOTHERMIC REACTION, the products have a lower energy than the reactants

$$A + B \rightarrow C + D$$

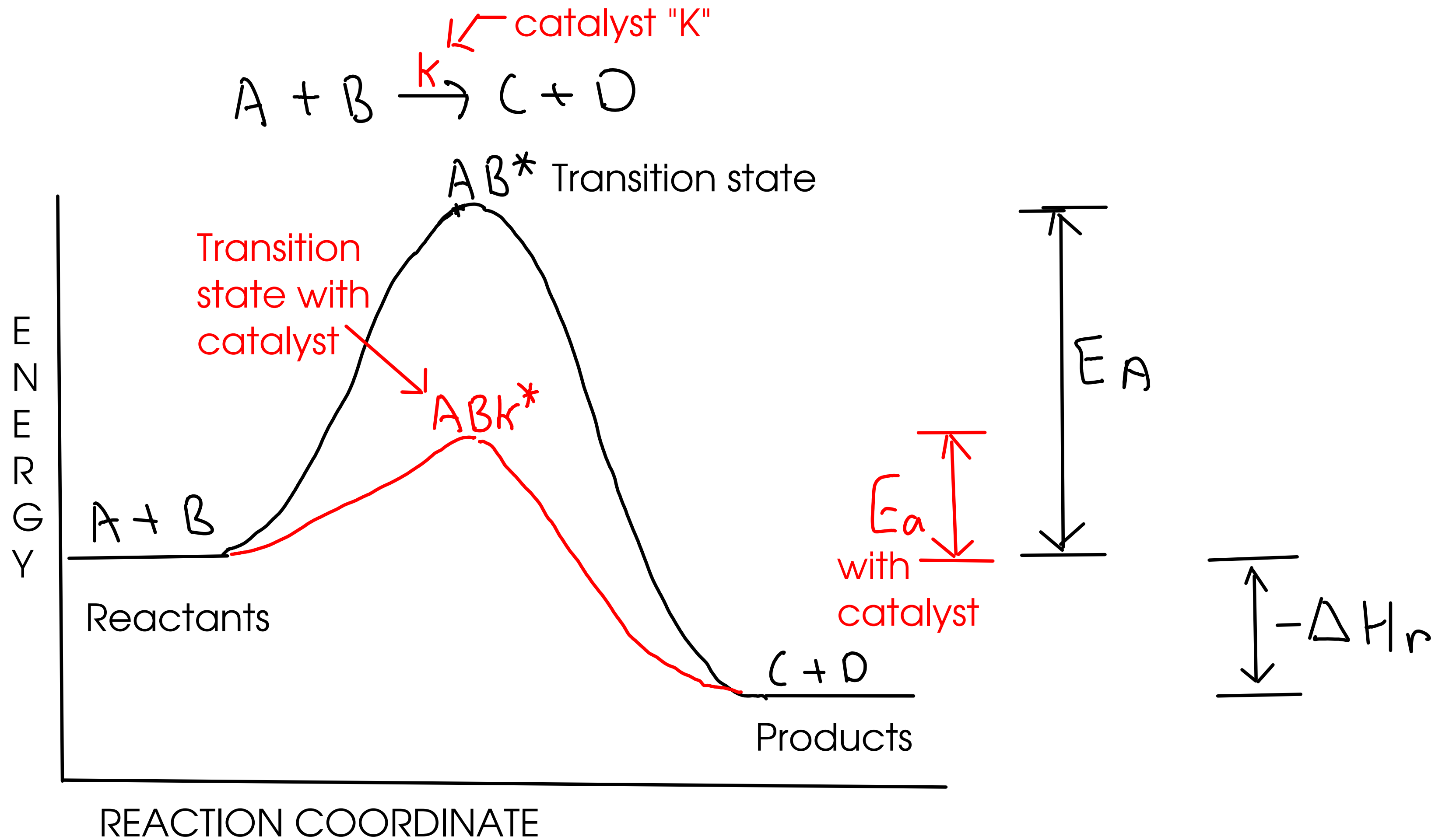


- Whether a reaction is endothermic OR exothermic, there is still an activation energy barrier that must be crossed in order to react.

- This explains why a pile of wood that's exposed to air doesn't just burst into flames. Even though the cdombustion of wood is EXOTHERMIC, there's still an activation energy barrier preventing the reaction from occurring without an initial input of energy - a "spark"!

CATALYSTS?

- So how does a catalyst fit into this picture? A catalyst LOWERS the activation energy for a reaction



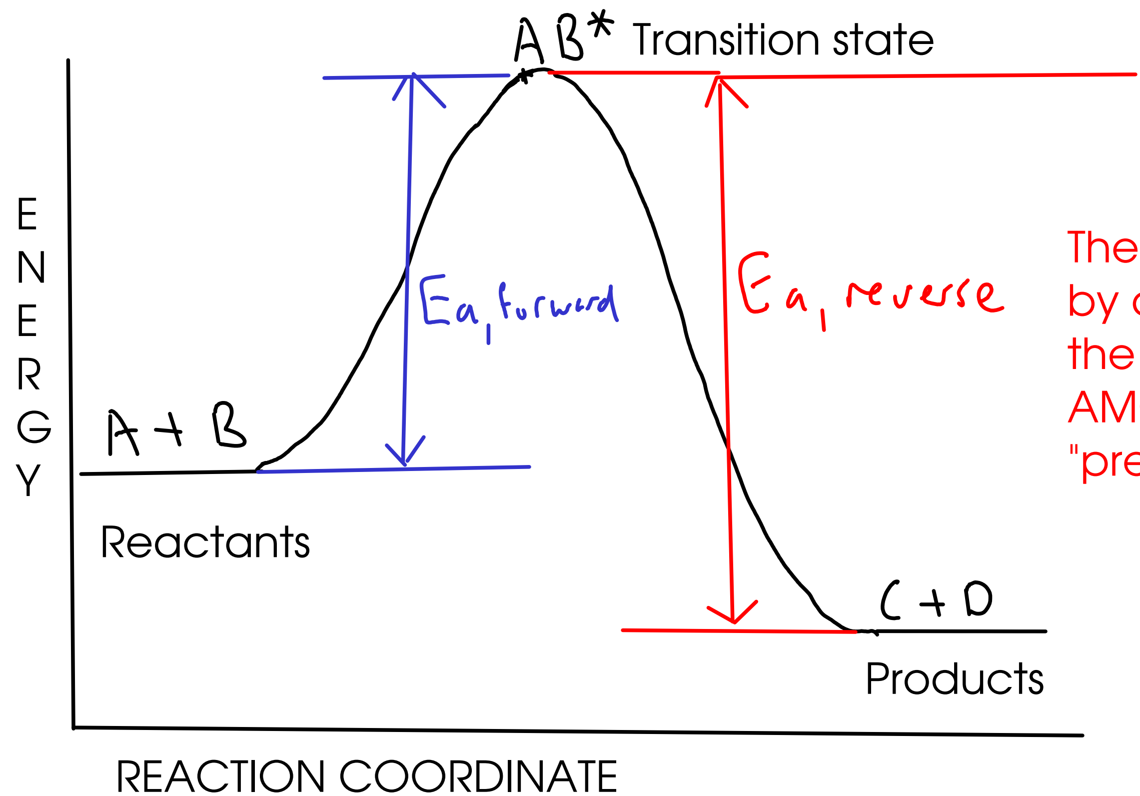
- The exact mechanism by which a catalyst lowers the energy of the transition state may be simple ... or complex. As we mentioned before, some catalysts hold molecules so that it's easier for reactants to come together, some react with reactant molecules to produce an intermediate that reacts more easily with other reactants to make the final product, etc.

WHAT KEEPS A REACTION FROM GOING BACKWARDS?

$A + B \rightarrow C + D$ (reactants → products) | $C + D \rightarrow A + B$ (reactants → products)

... what keeps the reaction on the right from occurring?

$$A + B \rightarrow C + D$$



The reverse reaction is "prevented" by an activation energy barrier - the same thing (if not the same AMOUNT of energy) that "prevents" the forward reaction!

So what really happens during a reaction? Both forward and reverse reactions occur!

$A + B \rightarrow C + D$

reactants   products

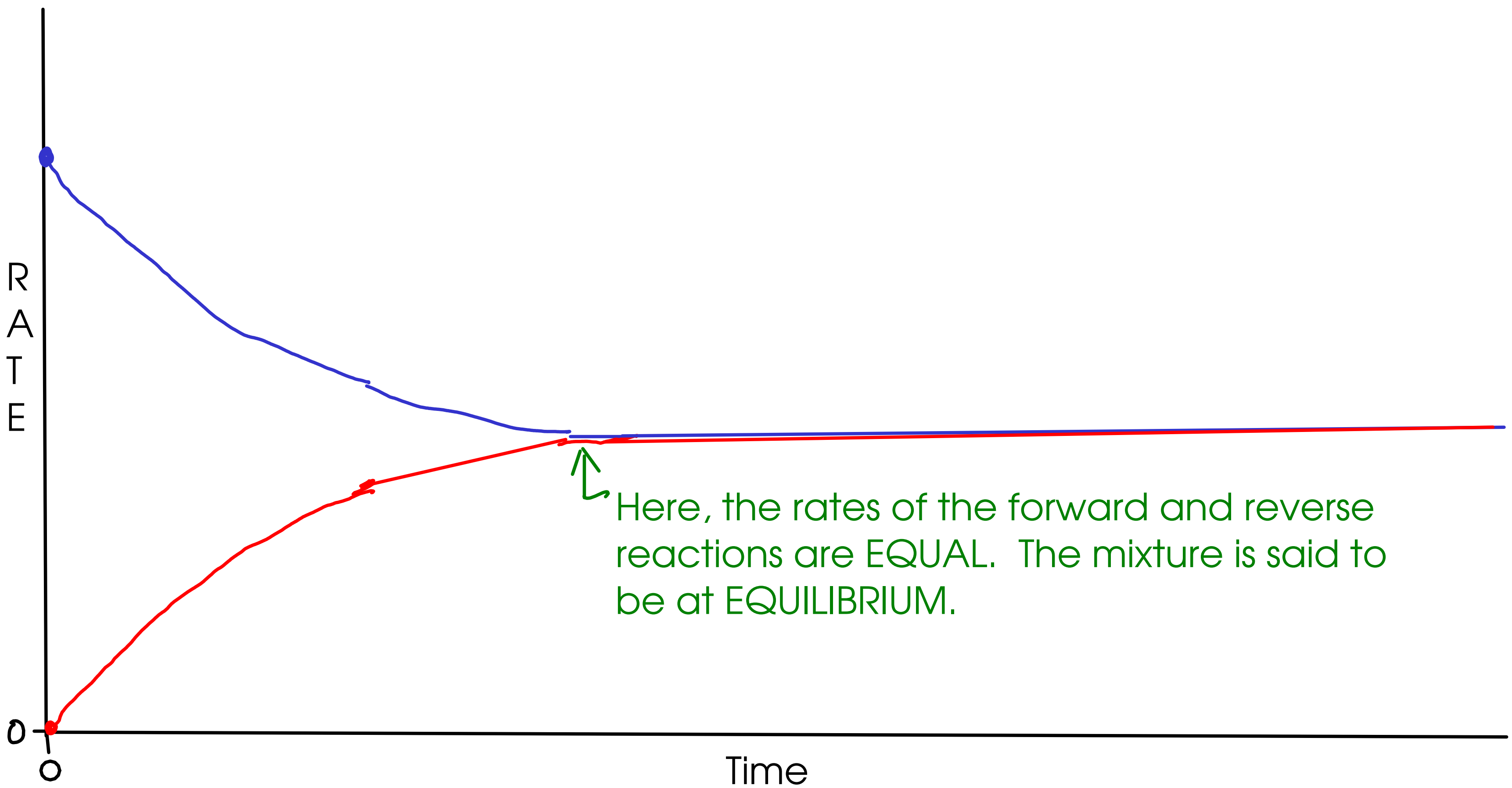
$Rate = k_F[A][B]$

$C + D \rightarrow A + B$

reactants   products

$Rate = k_r[C][D]$

- Let's look at the RATES of both the forward and reverse reactions over time.



- Initially, the mixture is all A and B. As C and D are formed, the rate of the reverse reaction increases while the rate of the forward reaction decreases. Eventually, these rates become equal.

- At EQUILIBRIUM, the concentrations of A, B, C, and D stop CHANGING. The reaction doesn't stop, but it appears stopped to an outside observer.

DESCRIBING EQUILIBRIUM

$$\underbrace{a}A + \underbrace{b}B \rightleftarrows \underbrace{c}C + \underbrace{d}D$$

Stoichiometric coefficients

- Double-headed arrow is often used to show that both the forward and reverse reactions are important.

[ ] : molar concentrations of reactants and products AT EQUILIBRIUM.

$$K_c = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

Equilibrium constant (concentration based)

- At equilibrium, the ratio above equals a constant number - the EQUILIBRIUM CONSTANT. The equilibrium constant depends on TEMPERATURE, but not on other factors.

- Not all reactants and products are included in the equilibrium constant expression!