Reaction Mechanisms

Section 6.6
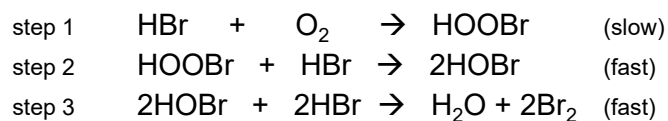
Homework

Recall…

- Collision theory

- Rate laws describe the relationship between a change in reactant concentration, and rate of reaction
  - Exponents are experimentally-determined and DO NOT come from the coefficients in the chemical equation.

$4 HBr + O_2 \rightarrow 2 H_2O + 2 Br_2$

- extremely unlikely this can happen in one step
- **Too many molecules need to collide simultaneously, with correct alignment!**

- Complicated reactions are thought to occur in several *smaller steps*
  - smaller steps are called **elementary steps**

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step 1	$HBr + O_2 \rightarrow HOOBr$	(slow)
step 2	$HOOBr + HBr \rightarrow 2HOBr$	(fast)
step 3	$2HOBr + 2HBr \rightarrow H_2O + 2Br_2$	(fast)

$4 HBr + O_2 \rightarrow 2 H_2O + 2 Br_2$

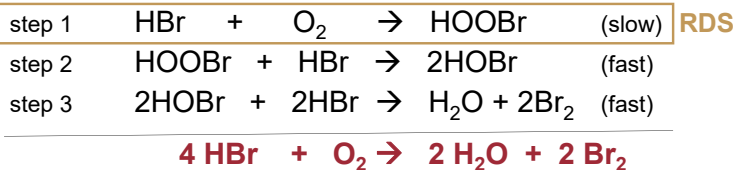In this reaction, HOOBr and HOBr are **reaction intermediates**:
- transient molecules, formed as products of elementary steps
- react further to give the observable products
- are never seen as products of the reaction

A **reaction mechanism** is a best guess of how a reaction actually occurs.

- made up of the series of elementary steps that sums to the overall reaction

- supported by underlined experimental evidence

- For a reaction that occurs in multiple steps, the overall rate is determined by *the slowest step.*

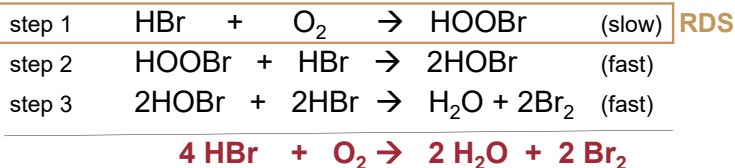- The slowest step is called the **rate determining step (RDS).**

step 1	HBr	+	O_2	$\rightarrow$	HOOBr	(slow)	**RDS**
step 2	HOOBr	+	HBr	$\rightarrow$	2HOBr	(fast)	
step 3	2HOBr	+	2HBr	$\rightarrow$	H_2O + $2Br_2$	(fast)	

4 HBr + O_2 $\rightarrow$ 2 H_2O + 2 Br_2

The rate law equation can be DIRECTLY linked to the rate determining step.

For a multi-step mechanism,

if the RDS is: **mX + nY** $\rightarrow$ products

Then the
rate law expression
(for the whole reaction) is: $r = k\,[X]^m\,[Y]^n$

The exponents come from the coefficients in the RDS!!

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step 1	HBr	+	O_2	$\rightarrow$	HOOBr	(slow)	**RDS**
step 2	HOOBr	+	HBr	$\rightarrow$	2HOBr	(fast)	
step 3	2HOBr	+	2HBr	$\rightarrow$	H_2O + $2Br_2$	(fast)	

4 HBr + O_2 $\rightarrow$ 2 H_2O + 2 Br_2

$r = k\,[HBr]\,[O_2]$

Reaction mechanisms are best guesses

• we can't actually SEE these reactions happening

• there are **two requirements for a proposed reaction mechanism**:
1. the elementary steps add up to the overall reaction
2. the slowest step (RDS) is consistent with the experimentally-determined rate law

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Example 1

For the proposed reaction mechanism:

step 1	NO_2	+	F_2	$\rightarrow$	NO_2F + F	(slow)
step 2	NO_2	+	F	$\rightarrow$	NO_2F	(fast)
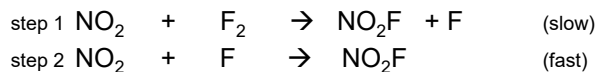
a) Write the overall equation
b) Identify any intermediates
c) Which step – 1 or 2 – is the RDS?
d) Use the RDS to write the rate law equation
e) Predict the effect on rate, if
   i) $[NO_2]$ is doubled
   ii) $[F_2]$ is halved

Homework

• P. 386 practice #1-3
• P. 387 #1-8 (skip 2, 4)