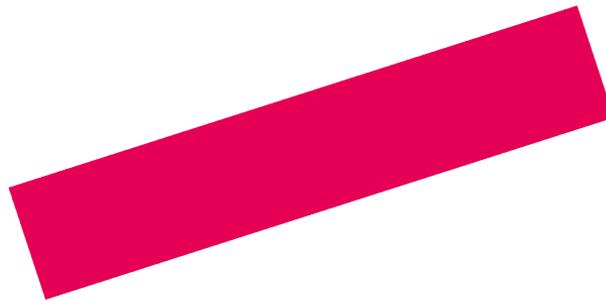


ITBC

Chemie Course 2



Hoofdstuk 7

Chemische reacties:

Energie

Snelheid

Evenwicht

Spontaniteit van reacties.

Entropie

Vrije energie

Waarom verloopt de ene reactie wel en de andere niet?

Komt er energie vrij of wordt er energie opgenomen?

Verloopt een reactie snel of langzaam?

Verloopt een reactie volledig (aflopend) of gedeeltelijk (evenwicht)?

Vandaag

Uitleg 7.1 t/m 7.3

- energie
- enthalpie
- exotherm / endotherm

Maken opdrachten

7.1 Energie en chemische binding

Twee soorten energie:

1. potentiële energie
2. kinetische energie

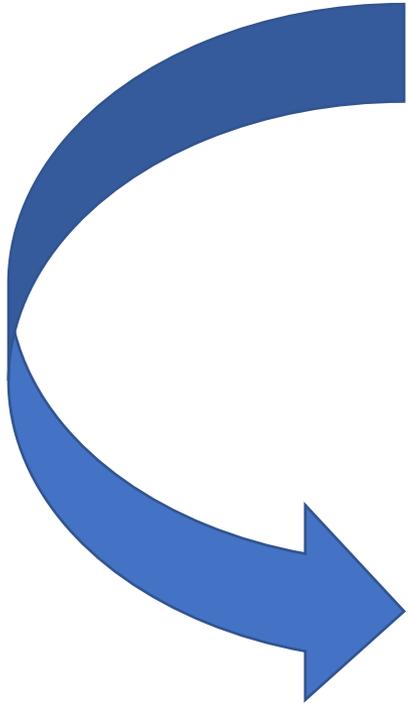


High potential energy,
zero kinetic energy



Decreasing potential energy,
increasing kinetic energy

Chemische verbindingen



Potentiële energie:

- aantrekkende krachten tussen ionen (ion binding) en atomen (covalente binding)

Kinetische energie:

- warmte-ontwikkeling (bewegende deeltjes)

7.2 Warmte-effect

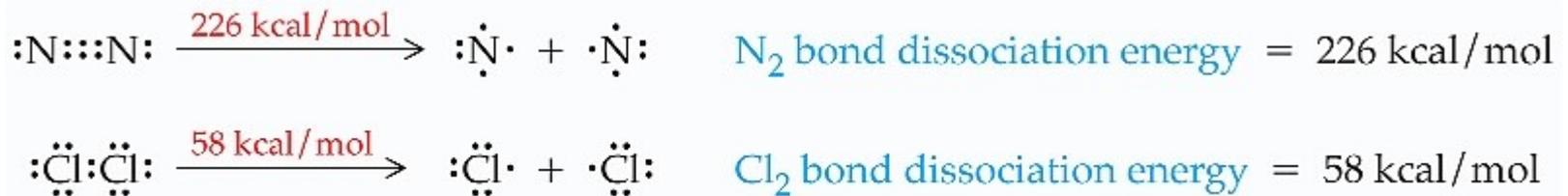
Het verbreken van een binding **KOST** energie.
De vorming van een binding **LEVERT** energie.

Wat kost meer energie? Het verbreken van:

N_2 of Cl_2

7.2 Warmte-effect

Het verbreken van een binding **KOST** energie.
De vorming van een binding **LEVERT** energie.



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7.3 Endotherm en exotherm

Endotherme reactie:

De reactie neemt warmte uit de omgeving op

- de omgeving raakt warmte kwijt
- het systeem neemt die warmte op (**positief**)

Exotherme reactie:

De reactie staat warmte aan de omgeving af

- de omgeving neemt die warmte op
- het systeem raakt die warmte kwijt (**negatief**)

Enthalpie-verandering

Het warmte-effect van een chemische verandering wordt weergegeven als een **enthalpie-verandering** (ΔH)

Endotherm: er wordt warmte opgenomen

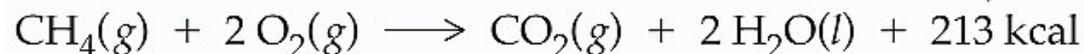
ΔH positief

Exotherm: er komt warmte vrij

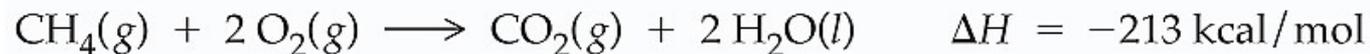
ΔH negatief

An exothermic reaction—negative ΔH

Heat is a product.



or



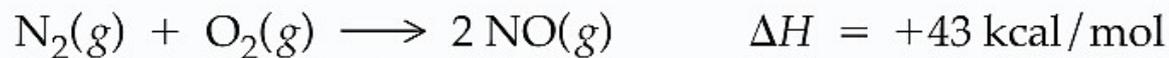
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An endothermic reaction—positive ΔH

Heat is a reactant.



or



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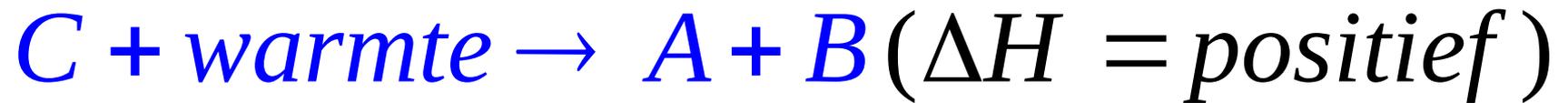


TABLE 7.1 Average Bond Dissociation Energies

Bond	Bond Dissociation Energy (kcal/mol, kJ/mol)	Bond	Bond Dissociation Energy (kcal/mol, kJ/mol)	Bond	Bond Dissociation Energy (kcal/mol, kJ/mol)
C—H	99, 413	N—H	93, 391	C=C	147, 614
C—C	83, 347	N—N	38, 160	C≡C	201, 839
C—N	73, 305	N—Cl	48, 200	C=O*	178, 745
C—O	86, 358	N—O	48, 201	O=O	119, 498
C—Cl	81, 339	H—H	103, 432	N=O	145, 607
Cl—Cl	58, 243	O—H	112, 467	C≡N	213, 891
H—Cl	102, 427	O—Cl	49, 203	N≡N	226, 946

*The C=O bond dissociation energies in CO₂ are 191 kcal/mol (799 kJ/mol).

Een voorbeeldje

Bereken de ΔH voor de reactie waarbij waterstof en zuurstof met elkaar reageren en water vormen.

Endotherm of exotherm?

Nog een voorbeeldje

Bereken de ΔH voor de reactie waarbij methaan wordt verbrand.

Endotherm of exotherm?

Vandaag

Stukje herhaling van vorige les

Spontaniteit van reacties

Entropie

7.4 Waarom verlopen reacties?

Verloopt een exotherme reactie altijd spontaan?

Verloopt een endotherme reactie nooit spontaan?

Sommige exotherme reacties verlopen **niet** spontaan!

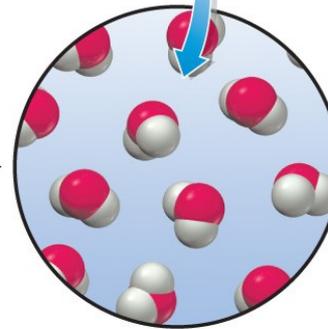
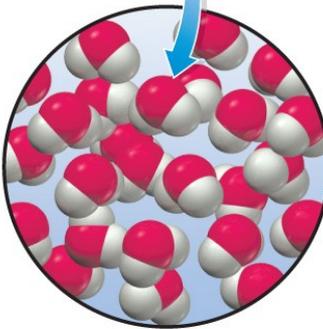
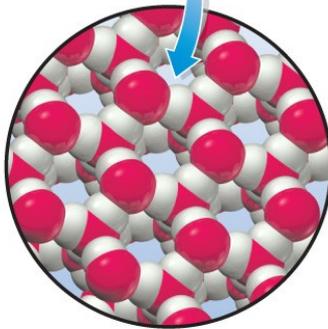
Sommige endotherme reacties verlopen **wel** spontaan!

Verklaring

Wat hebben spontane endotherme processen met elkaar gemeen?

- een toename in de wanorde !!!
- een maat voor de wanorde is de entropie (S)

$$S(\text{gas}) > S(\text{vloeistof}) > S(\text{vaste stof})$$



Liquids have more randomness and higher entropy than **solids**.

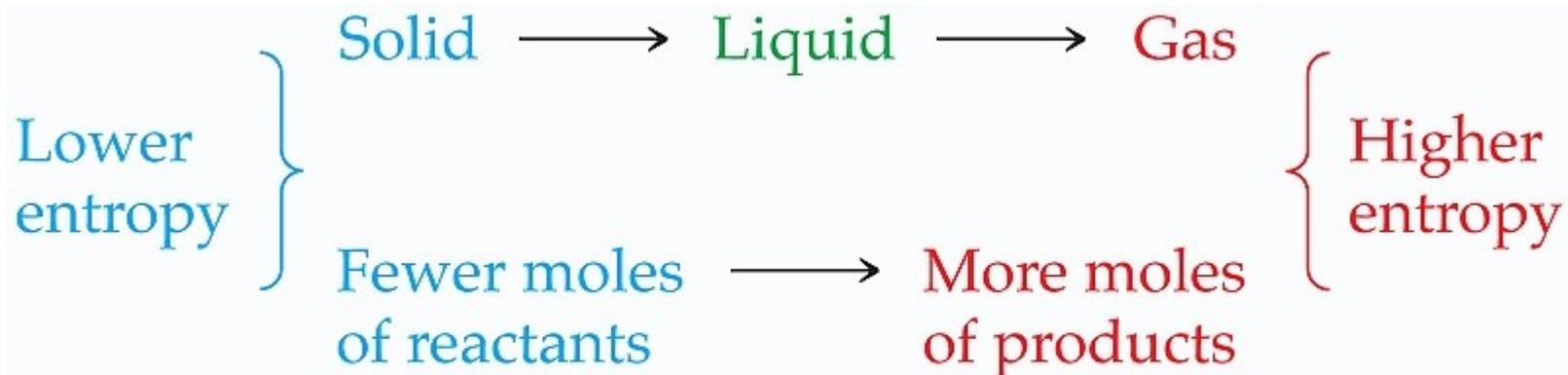
Gases have more randomness and higher entropy than **liquids**.

Less randomness,
lower entropy



More randomness,
higher entropy

Entropie



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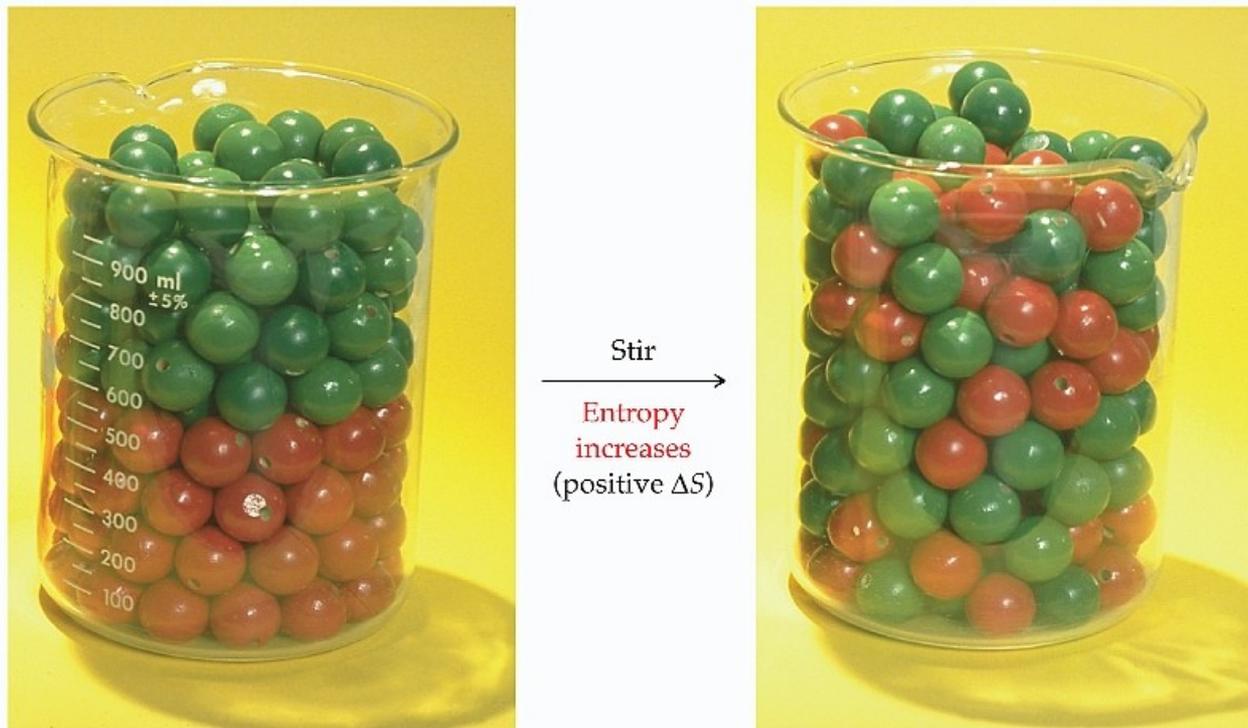
Entropie verandering (ΔS)

$$\Delta S = S_{\text{nieuw}} - S_{\text{oud}}$$

$\Delta S =$ positief: entropie is **toegenomen**

$\Delta S =$ negatief: entropie is **afgenomen**

ΔS



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Verhogen of verlagen van de entropie?

- De rook van een sigaret die zich door een ruimte verspreidt.
- Koken van water.
- De volgende chemische reactie:



Twee factoren

Het verloop van een spontane reactie is afhankelijk van twee factoren:

1. enthalpieverandering (ΔH)
2. entropieverandering (ΔS)

Spontaan: $\Delta H = \text{negatief}$, $\Delta S = \text{positief}$

Niet spontaan: $\Delta H = \text{positief}$, $\Delta S = \text{negatief}$

Wat als

$\Delta H = \text{negatief}$, $\Delta S = \text{negatief}$

$\Delta H = \text{positief}$, $\Delta S = \text{positief}$

Wat, als

$\Delta H = \text{negatief}$, $\Delta S = \text{negatief}$

$\Delta H = \text{positief}$, $\Delta S = \text{positief}$



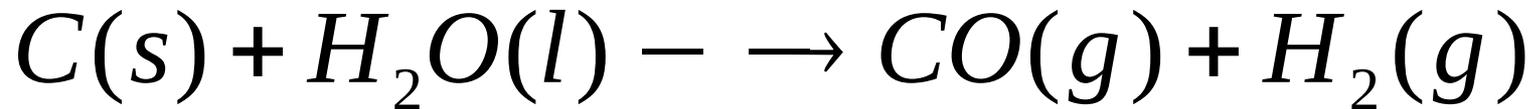
Vrije energie (G)

De **verandering** in vrije energie (ΔG) is bepalend voor het al dan niet spontaan verlopen van een reactie!

Free-energy change



Invloed T



$$\Delta H = +31300 \text{ cal/mol}$$

$$\Delta S = +32 \text{ cal/(mol}\cdot\text{K)}$$

25 °C (298 K): $\Delta H > T\Delta S$, $\Delta G = +$ dus NIET spontaan

700 °C (973 K): $T\Delta S > \Delta H$, $\Delta G = -$ dus WEL spontaan

Exergoon en endergoon

Exergoon: $\Delta G =$ negatief (spontaan)

Endergoon: $\Delta G =$ positief (niet spontaan)

TABLE 19.3 • How Signs of ΔH and ΔS Affect Reaction Spontaneity

ΔH	ΔS	$-T\Delta S$	$\Delta G = \Delta H - T\Delta S$	Reaction Characteristics	Example
-	+	-	-	Spontaneous at all temperatures	$2 \text{O}_3(g) \longrightarrow 3 \text{O}_2(g)$
+	-	+	+	Nonspontaneous at all temperatures	$3 \text{O}_2(g) \longrightarrow 2 \text{O}_3(g)$
-	-	+	+ or -	Spontaneous at low T ; nonspontaneous at high T	$\text{H}_2\text{O}(l) \longrightarrow \text{H}_2\text{O}(s)$
+	+	-	+ or -	Spontaneous at high T ; nonspontaneous at low T	$\text{H}_2\text{O}(s) \longrightarrow \text{H}_2\text{O}(l)$

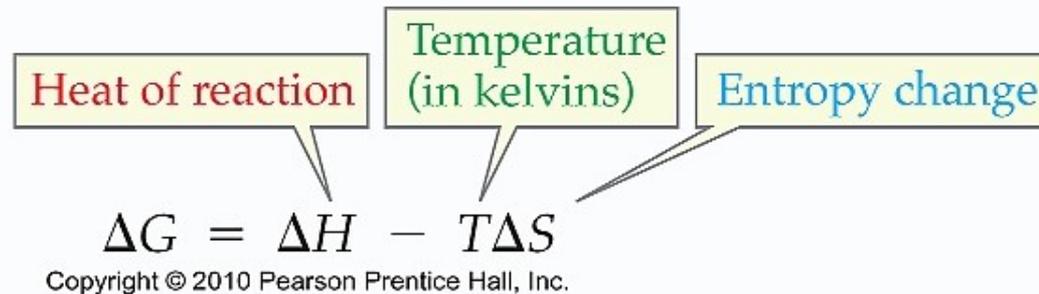
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Table 3-2 Variation of Reaction Spontaneity (Sign of ΔG) with the Signs of ΔH and ΔS

ΔH	ΔS	$\Delta G = \Delta H - T \Delta S$
-	+	The reaction is both enthalpically favored (exothermic) and entropically favored. It is spontaneous (exergonic) at all temperatures.
-	-	The reaction is enthalpically favored but entropically opposed. It is spontaneous only at temperatures <i>below</i> $T = \Delta H/\Delta S$.
+	+	The reaction is enthalpically opposed (endothermic) but entropically favored. It is spontaneous only at temperatures <i>above</i> $T = \Delta H/\Delta S$.
+	-	The reaction is both enthalpically and entropically opposed. It is <i>unspontaneous</i> (endergonic) at all temperatures.

Samenvattend

Free-energy change



ΔH negatief → exotherm

ΔH positief → endotherm

ΔS negatief → Verlaging van de entropie

ΔS positief → Verhoging van de entropie

ΔG negatief → Exergoon (spontaan)

ΔG positief → Endergoon (spontaan)

Nu

Maken opdrachtenblad tot en met 8

Daarna nabespreken.

Eerder klaar? Bereken bij 7.6 bij welke temperatuur de reactie wel spontaan verloopt.

Vandaag

Reactiesnelheid

Evenwichten

Principe van le Chatelier

7.5 Reactiesnelheid

Reactiesnelheid

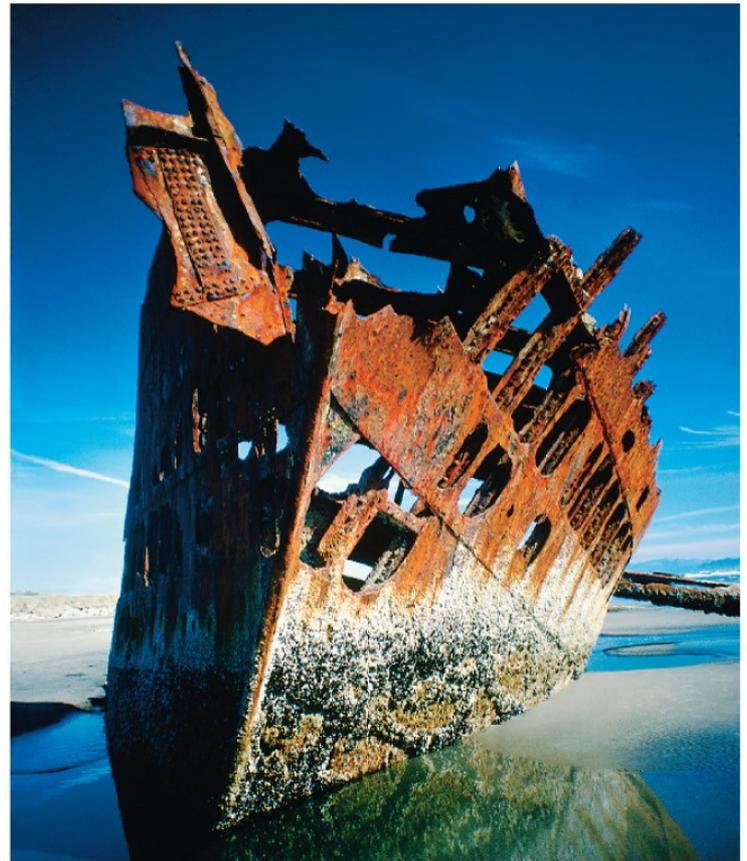
= aantal mol product gevormd in één liter per tijdseenheid

= aantal mol reactant verbruikt in één liter per tijdseenheid



The reaction between sodium
and bromine

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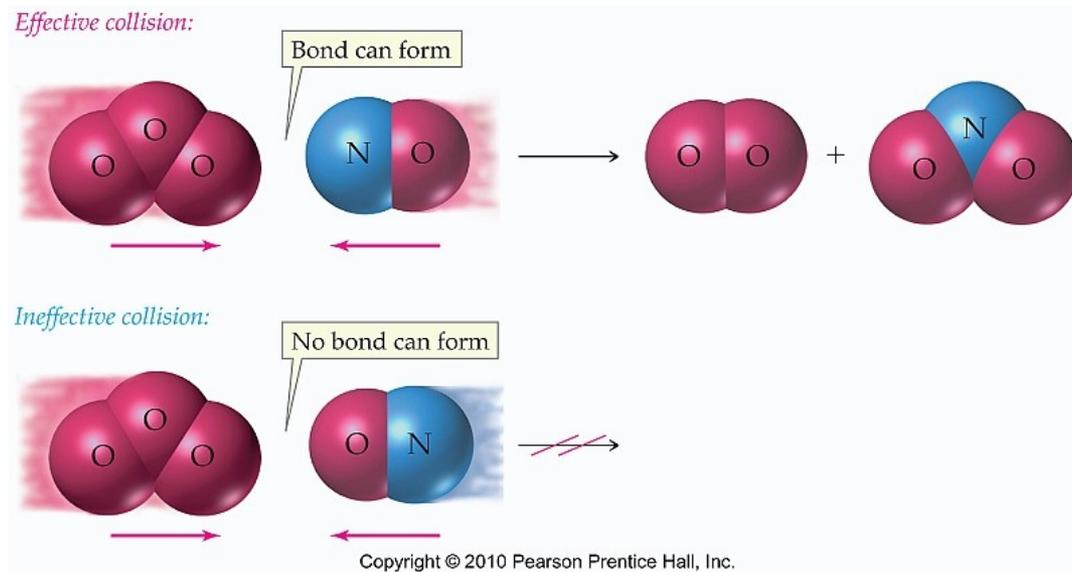
or

The rusting of iron?

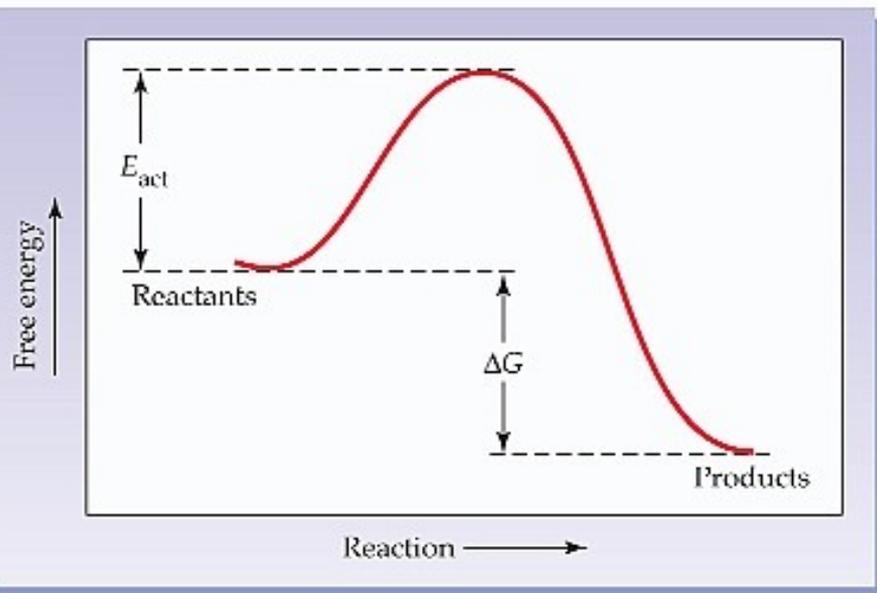
Wanneer verloopt er een reactie?

Effectieve botsing

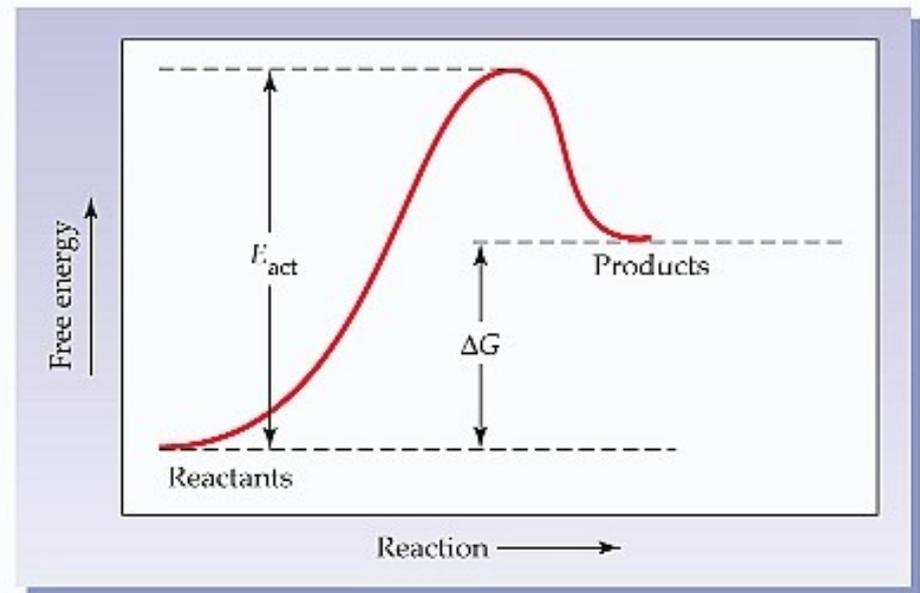
- voldoende krachtig
- goed georiënteerd



Verandering in vrije energie



(a) An exergonic reaction



(b) An endergonic reaction

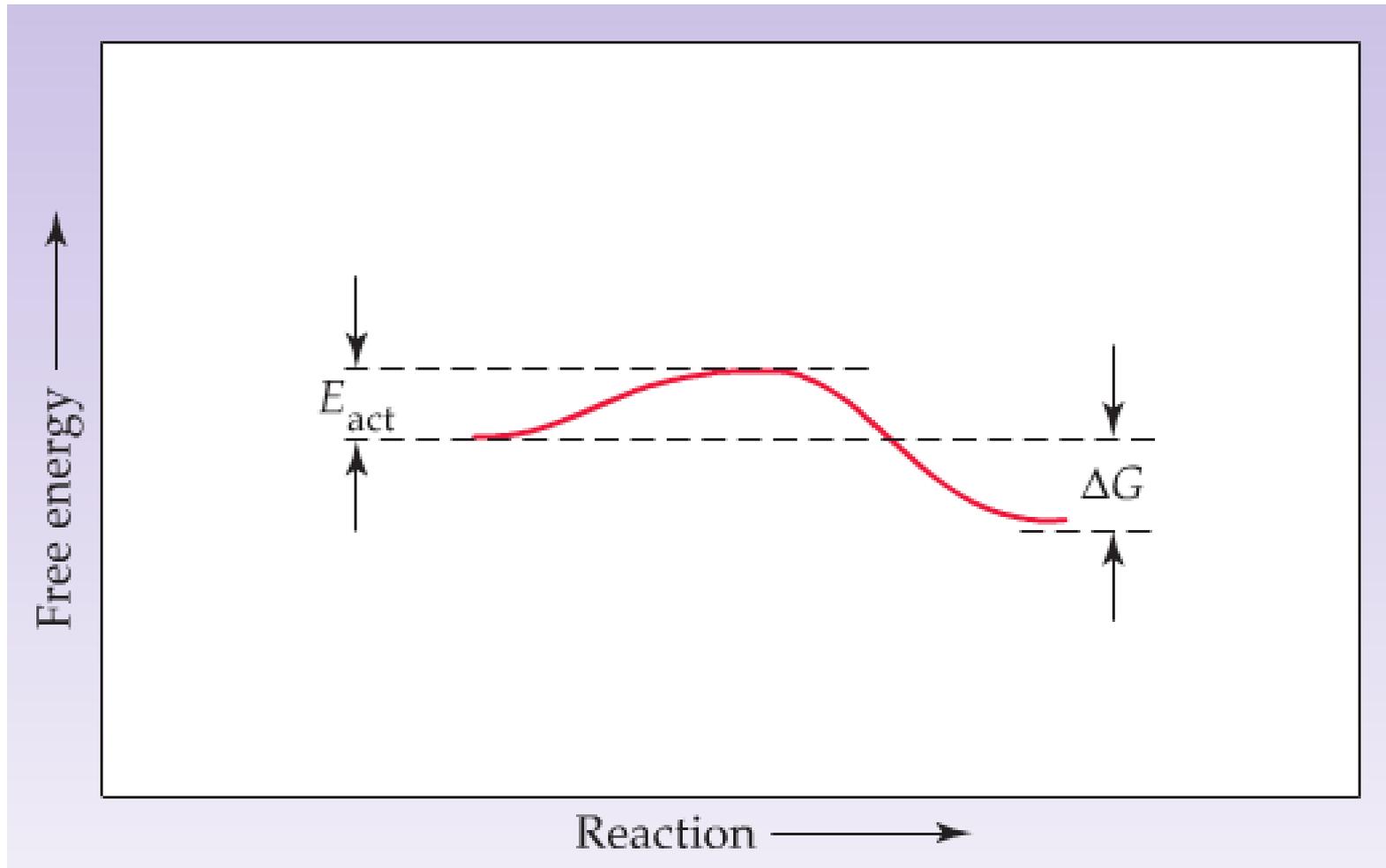
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Activeringsenergie

Activeringsenergie:
energie die nodig is om de reactie te starten

De grootte van de activeringsenergie bepaalt de snelheid van de reactie

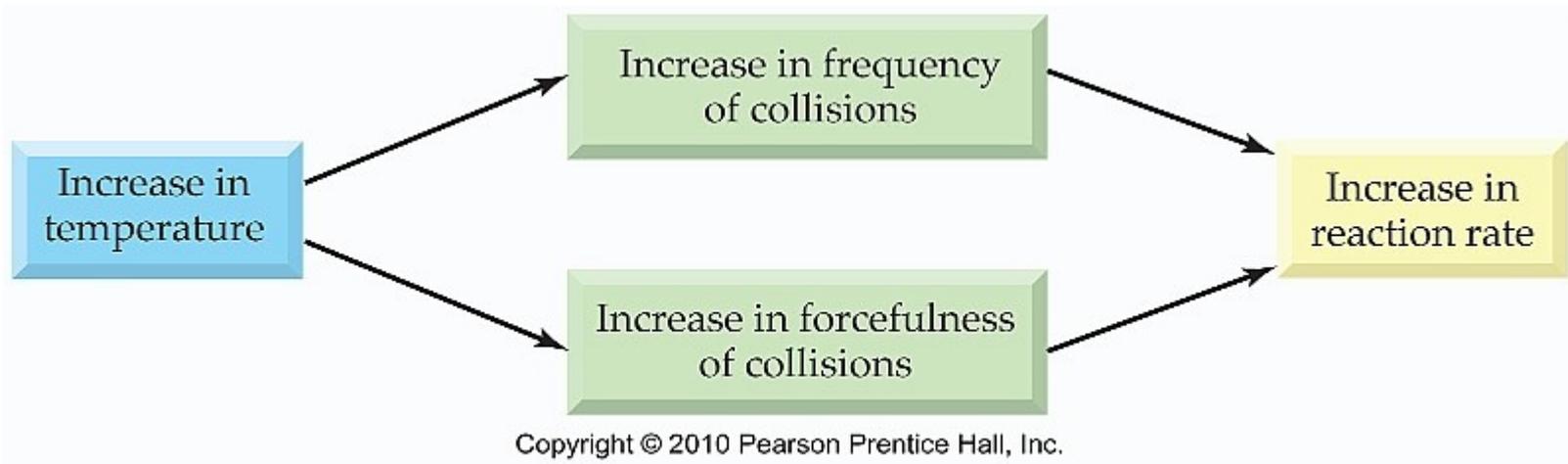
Snel of langzaam?



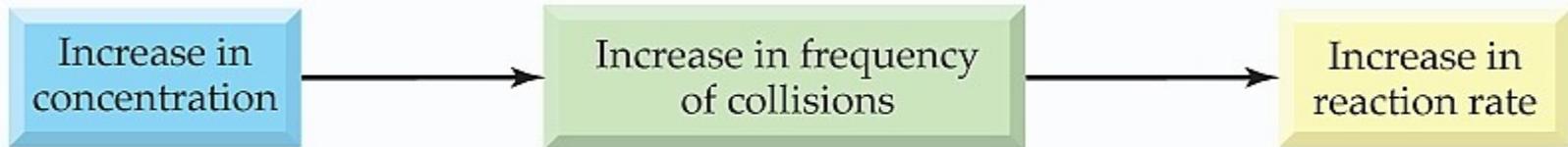
Hoe kunnen we reactiesnelheden beïnvloeden?

7.6 Invloed temperatuur, concentratie en katalysator

Temperatuur

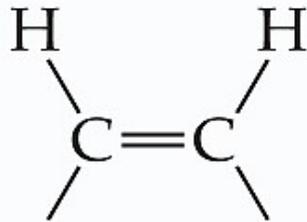
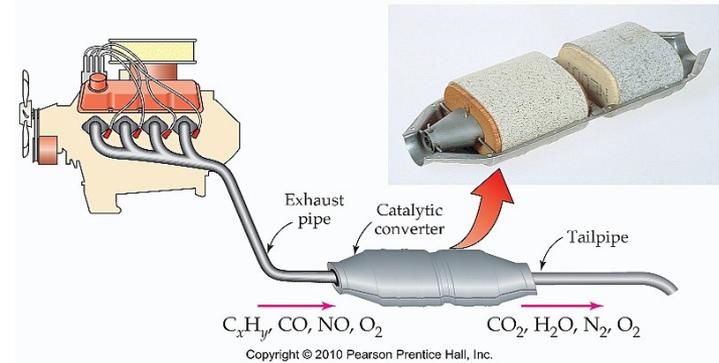


Concentration



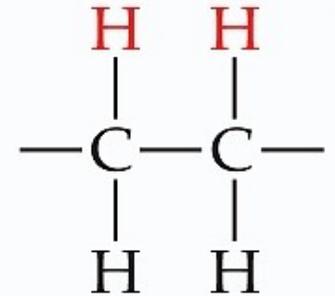
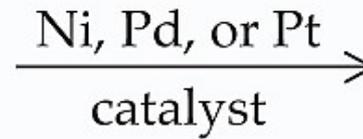
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Katalysator



A double bond in
vegetable oil

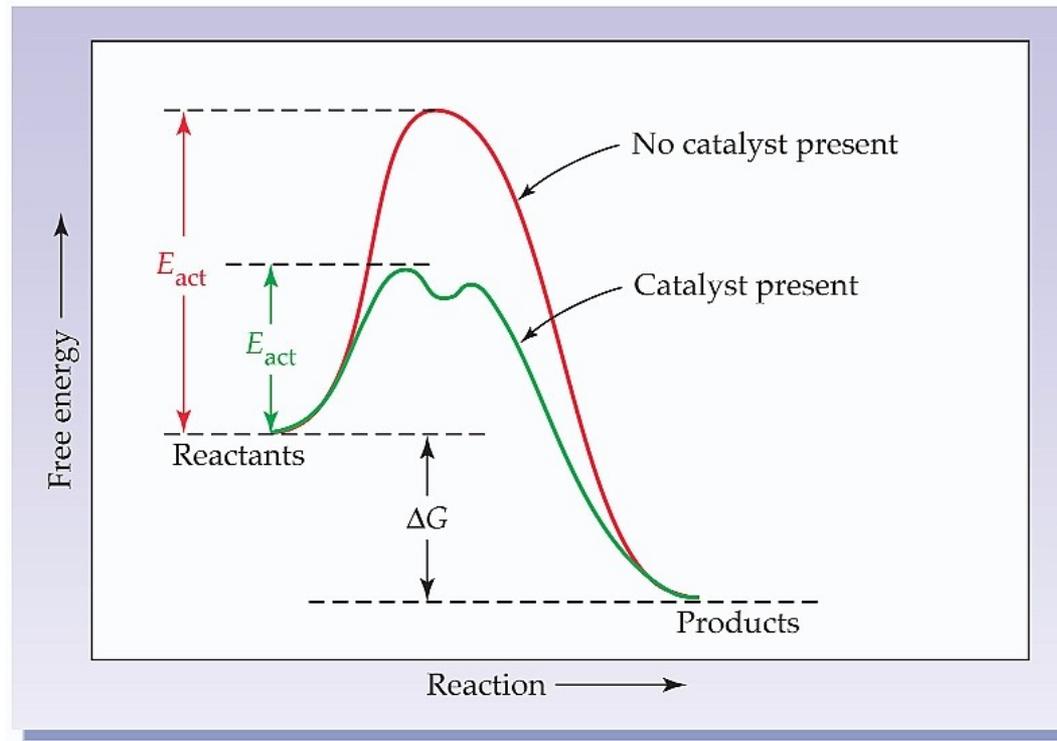
+



A single bond
in margarine

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Wat doet een katalysator?



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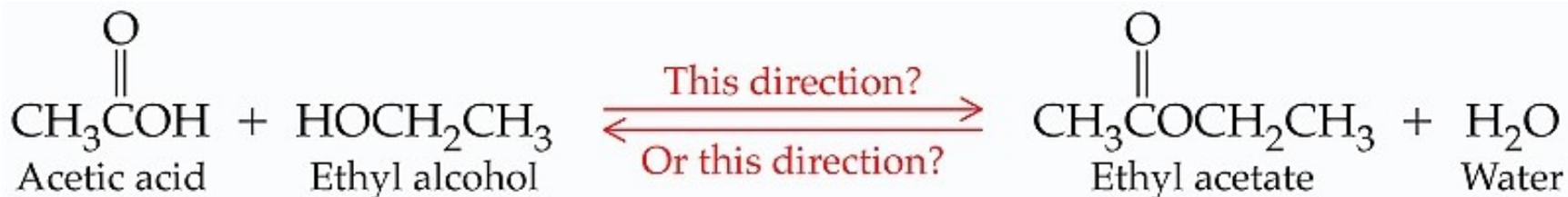
TABLE 7.2 Effects of Changes in Reaction Conditions on Reaction Rate

CHANGE	EFFECT
Concentration	Increase in reactant concentration increases rate. Decrease in reactant concentration decreases rate.
Temperature	Increase in temperature increases rate. Decrease in temperature decreases rate.
Catalyst added	Increases reaction rate.

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7.7 Chemisch evenwicht

Veel reacties zijn omkeerbaar!



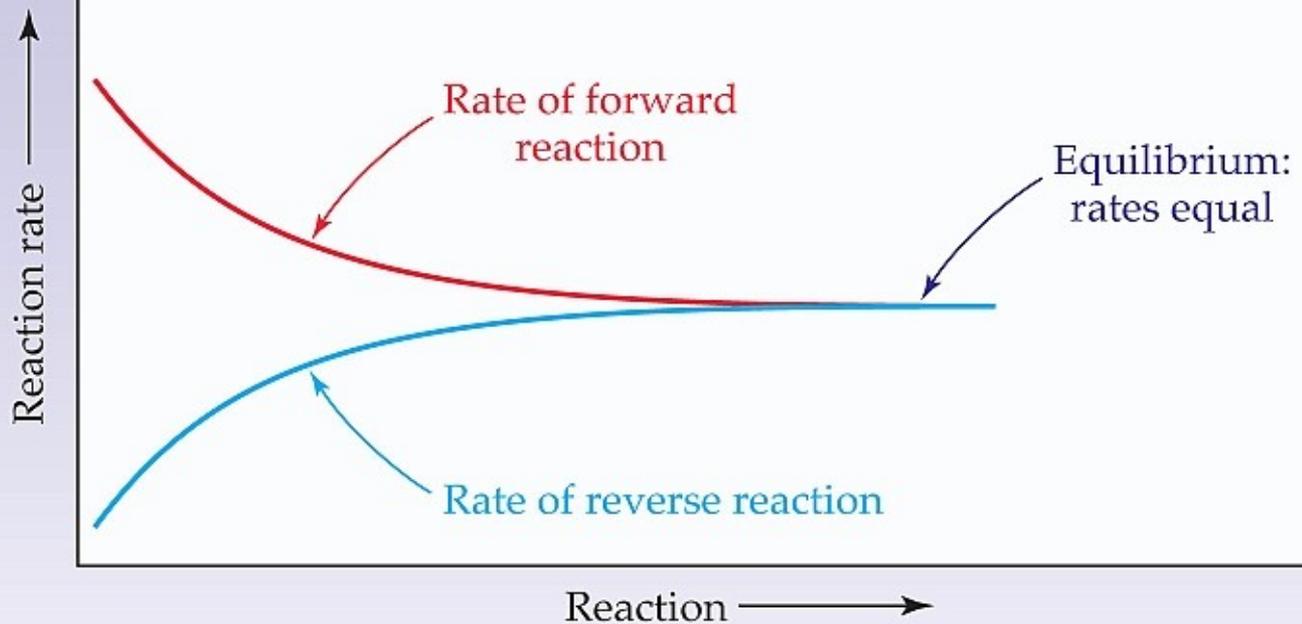
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Chemisch evenwicht

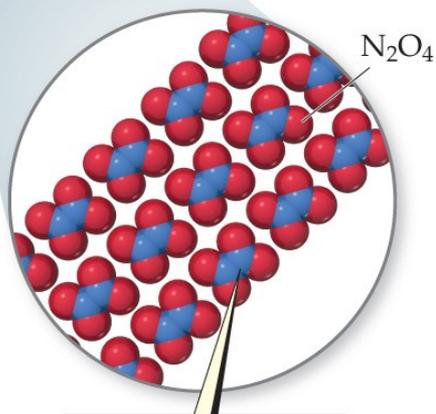
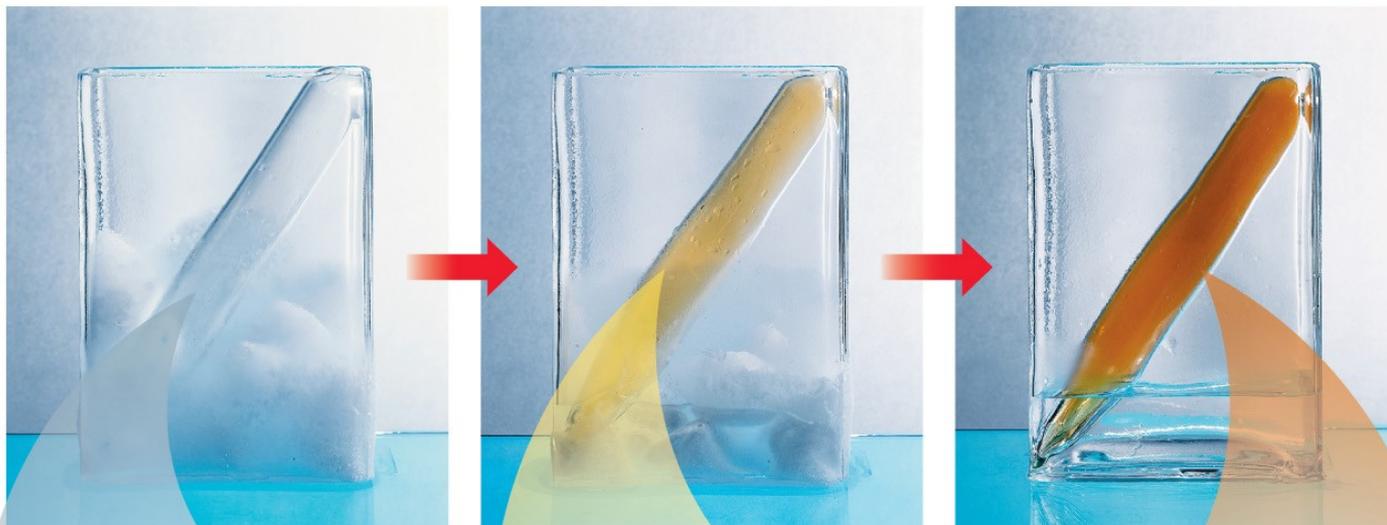
dynamisch

- continu een reactie maar géén concentratie veranderingen waarneembaar

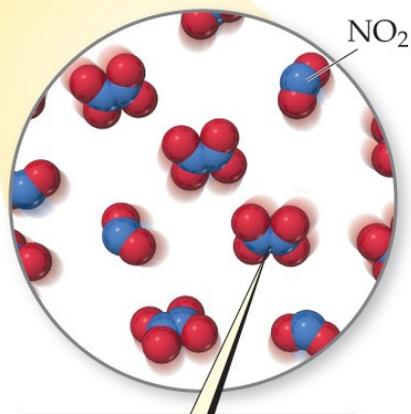
snelheid reactie naar rechts = snelheid reactie naar links



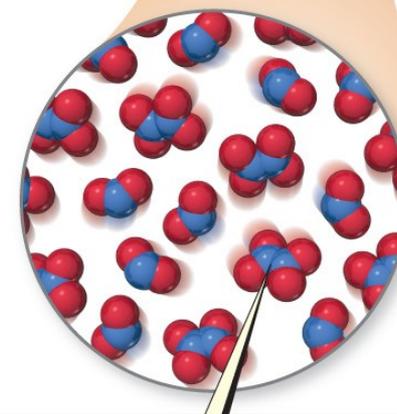
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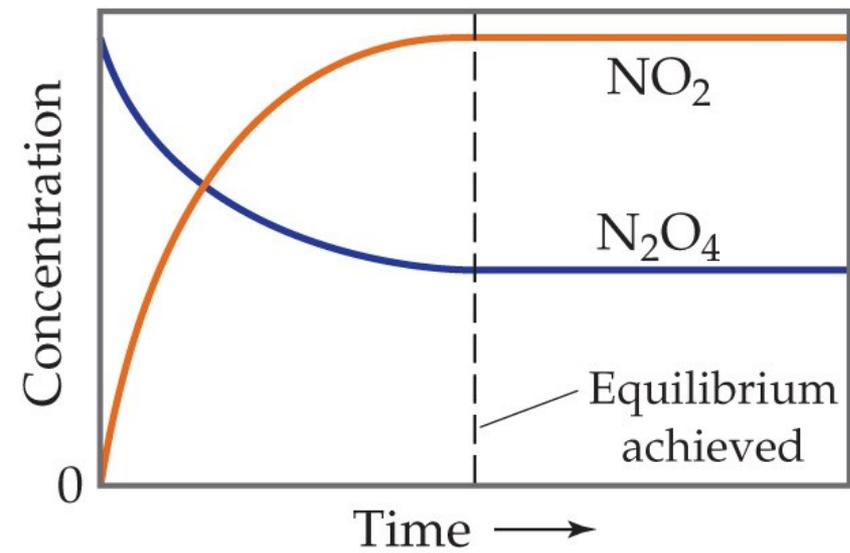


Frozen N_2O_4 sample is nearly colorless

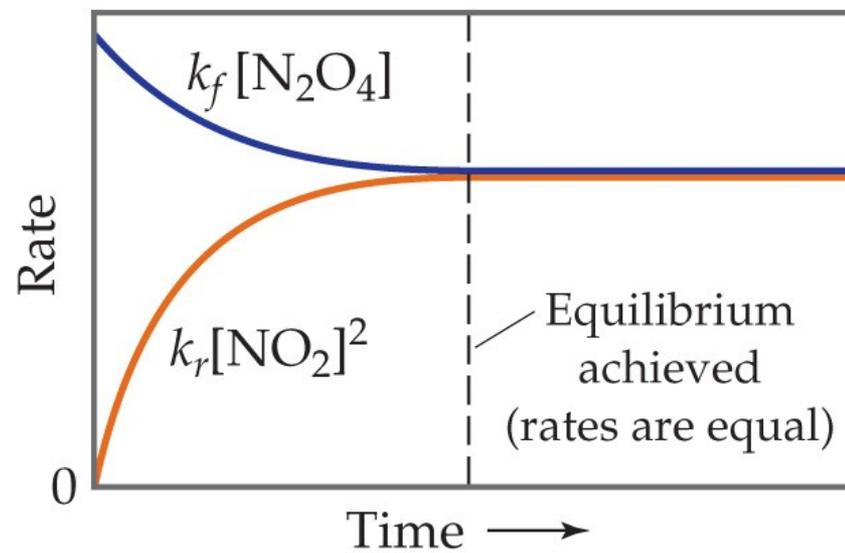


Warmed N_2O_4 dissociates to brown $\text{NO}_2(\text{g})$

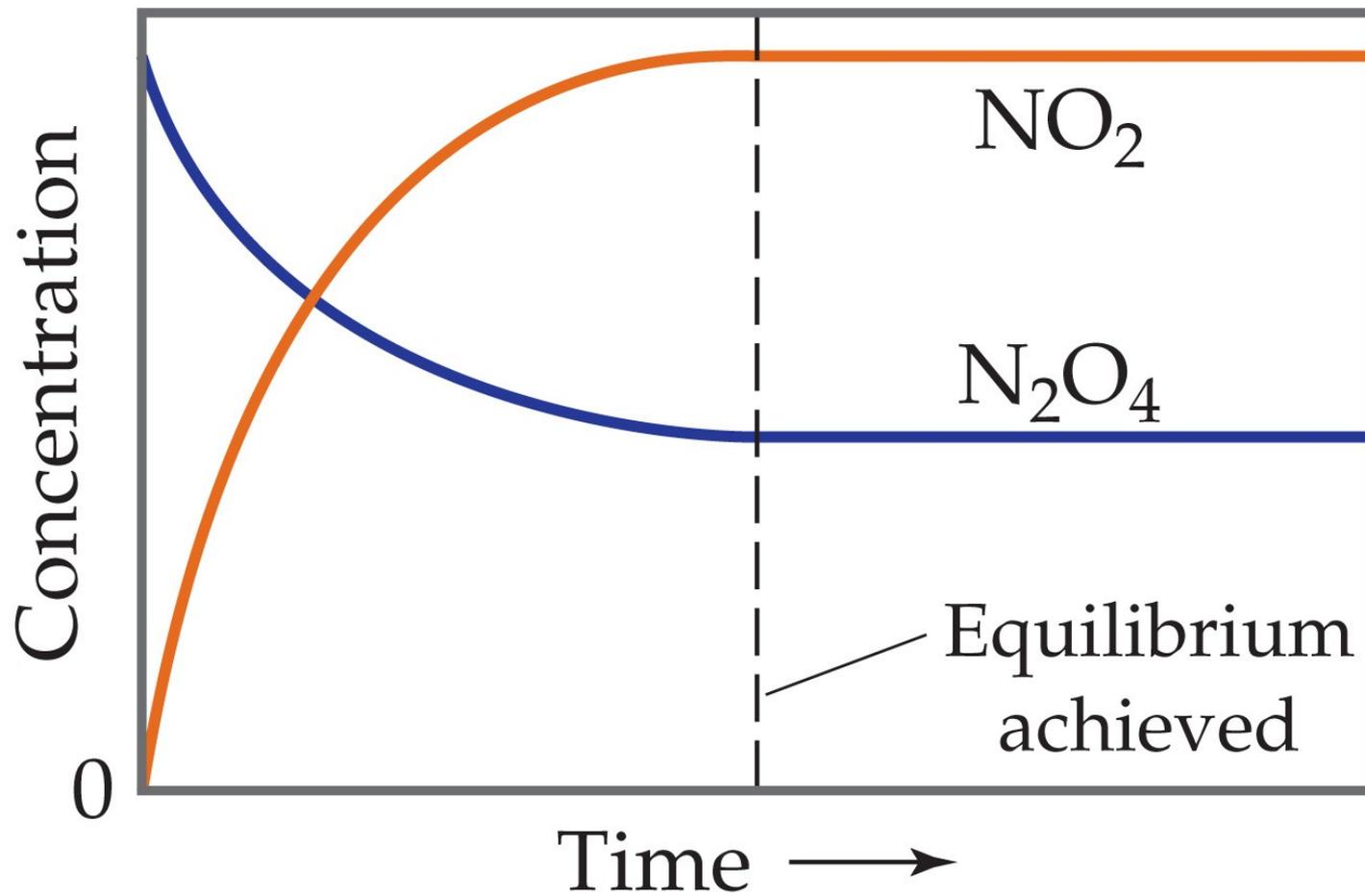




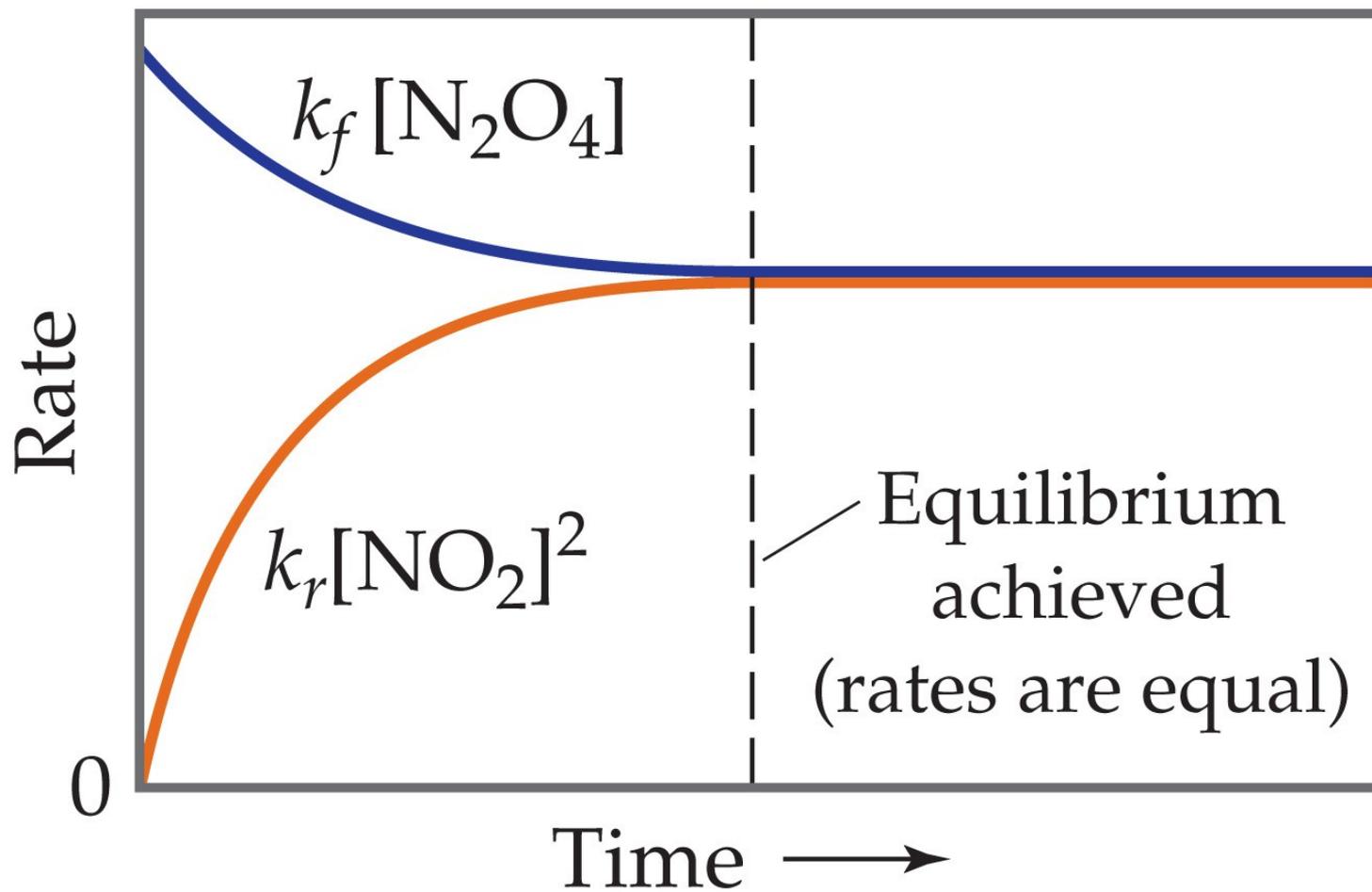
(a)



(b)

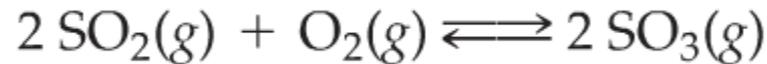


(a)



(b)

7.8 Evenwichtsvoorwaarde



$$\text{Experiment 1.} \quad \frac{[\text{SO}_3]^2}{[\text{SO}_2]^2[\text{O}_2]} = \frac{(0.938 \text{ mol/L})^2}{(0.0620 \text{ mol/L})^2(0.538 \text{ mol/L})} = 425$$

$$\text{Experiment 2.} \quad \frac{[\text{SO}_3]^2}{[\text{SO}_2]^2[\text{O}_2]} = \frac{(0.850 \text{ mol/L})^2}{(0.150 \text{ mol/L})^2(0.0751 \text{ mol/L})} = 428$$

$$\frac{[\text{SO}_3]^2}{[\text{SO}_2]^2[\text{O}_2]} = 429$$

Algemeen



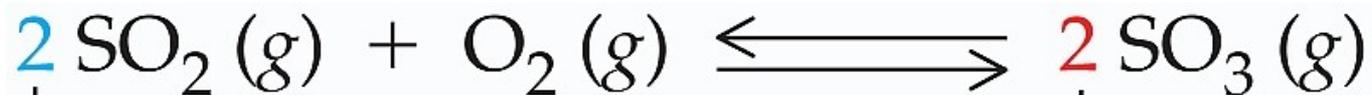
Equilibrium equation

Equilibrium constant

$$K = \frac{[M]^m [N]^n \dots}{[A]^a [B]^b \dots}$$

Product concentrations

Reactant concentrations



$$K = \frac{[\text{SO}_3]^2}{[\text{SO}_2]^2 [\text{O}_2]}$$

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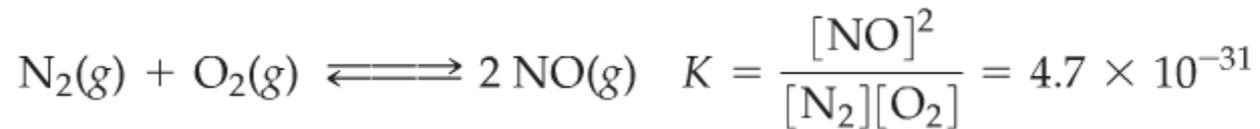
Evenwichtsvoorwaarde

De coëfficiënten uit de reactievergelijking worden exponenten in de evenwichtsvoorwaarde!!!

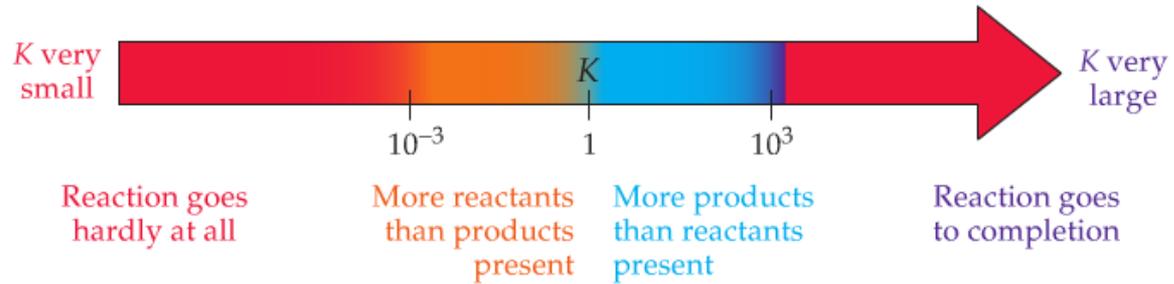
Niet in evenwichtsvoorwaarde:

- vaste stoffen
- zuiver vloeistoffen

Voorbeelden



$$K = \frac{[\text{CH}_3\text{CO}_2\text{CH}_2\text{CH}_3][\text{H}_2\text{O}]}{[\text{CH}_3\text{CO}_2\text{H}][\text{CH}_3\text{CH}_2\text{OH}]} = 3.4$$



- K much smaller than 0.001** Only reactants are present at equilibrium; essentially no reaction occurs.
- K between 0.001 and 1** More reactants than products are present at equilibrium.
- K between 1 and 1000** More products than reactants are present at equilibrium.
- K much larger than 1000** Only products are present at equilibrium; reaction goes essentially to completion.

Nu

Maken opdrachten 11 t/m 15

7.9 Principe van Le Chatelier

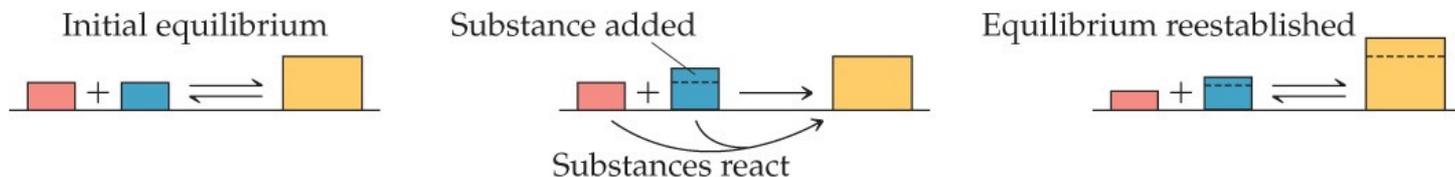
Le Châtelier's principle When a stress is applied to a system at equilibrium, the equilibrium shifts to relieve the stress.

Le Chatelier's Principle

If a system at equilibrium is disturbed by a change in **concentration, pressure, or temperature**, the system will shift its equilibrium position so as to counter the effect of the disturbance.

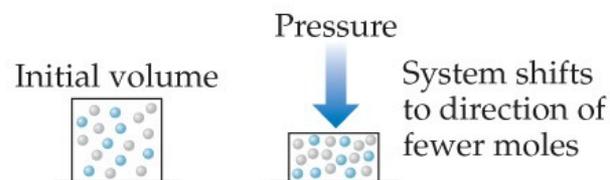
Concentration: adding or removing a reactant or product

If a substance is added to a system at equilibrium, the system reacts to consume some of the substance. If a substance is removed from a system, the system reacts to produce more of substance.



Pressure: changing the pressure by changing the volume

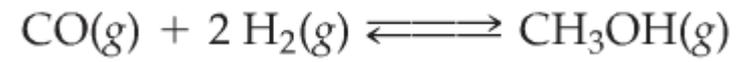
At constant temperature, reducing the volume of a gaseous equilibrium mixture causes the system to shift in the direction that reduces the number of moles of gas.

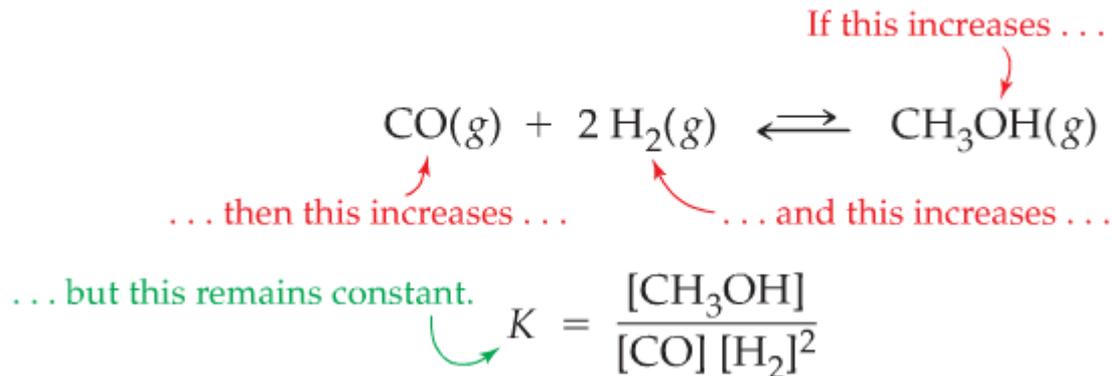
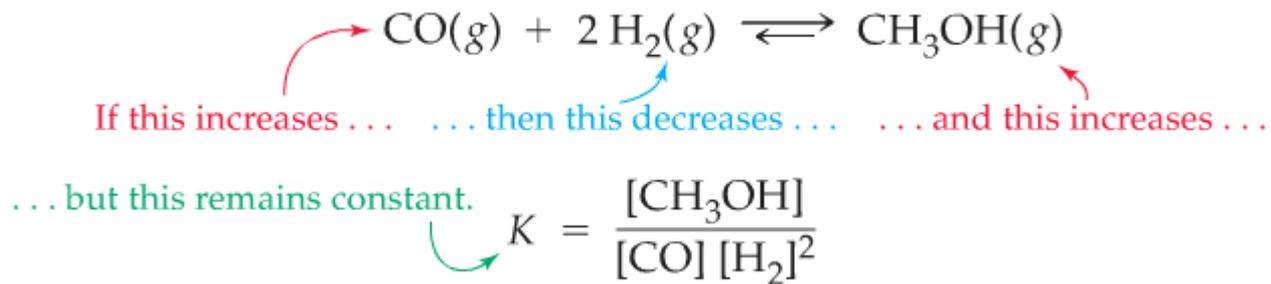
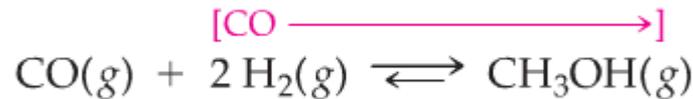
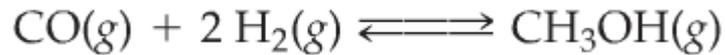


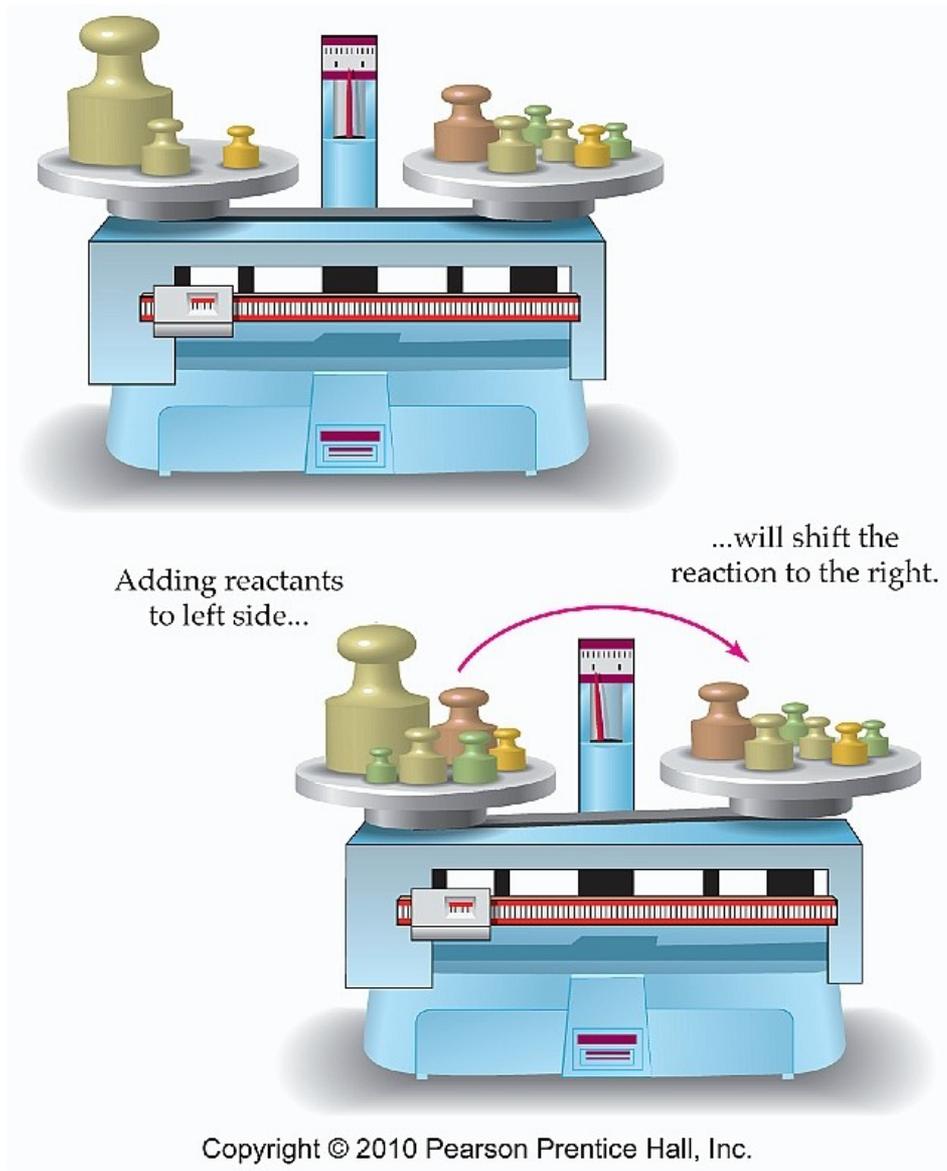
Temperature:

If the temperature of a system at equilibrium is increased, the system reacts as if we added a reactant to an endothermic reaction or a product to an exothermic reaction. The equilibrium shifts in the direction that consumes the "excess reactant," namely heat.



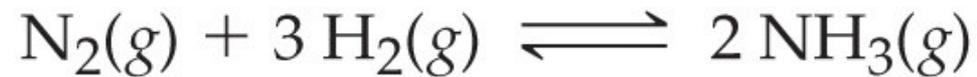


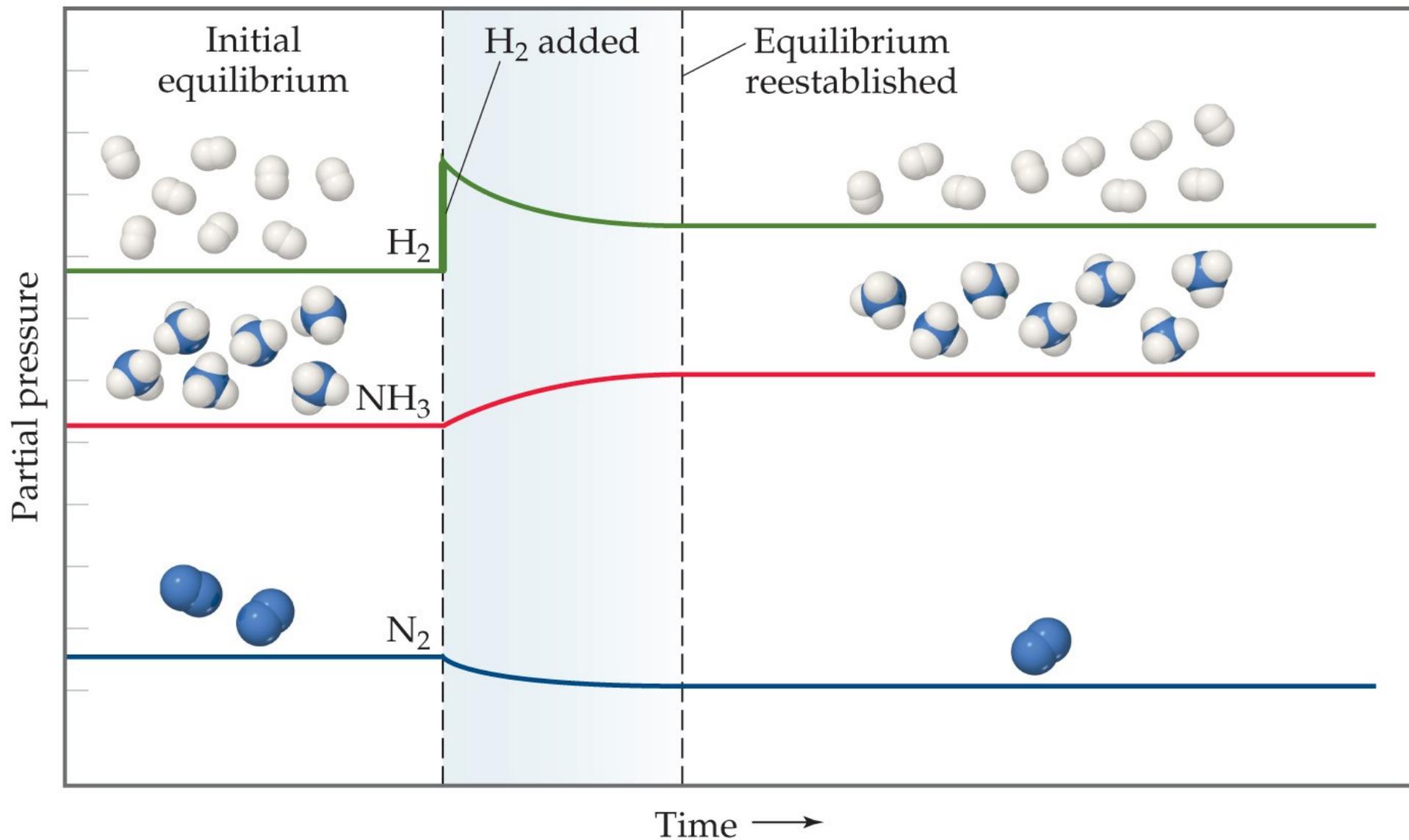
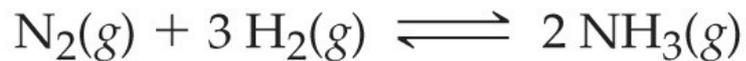


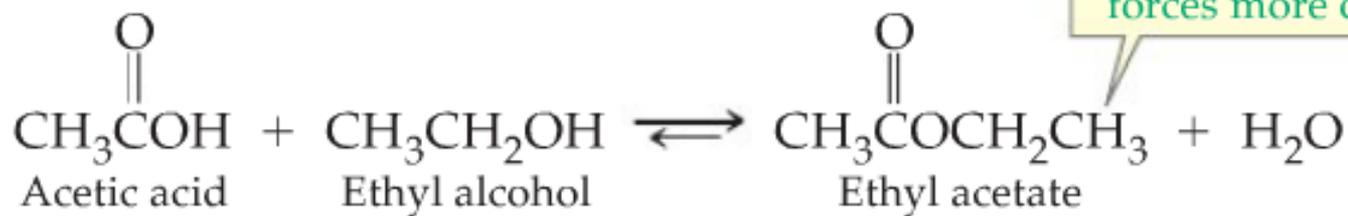


Een voorbeeldje

Wat gebeurt er als we H₂ toevoegen aan de volgende reactie:

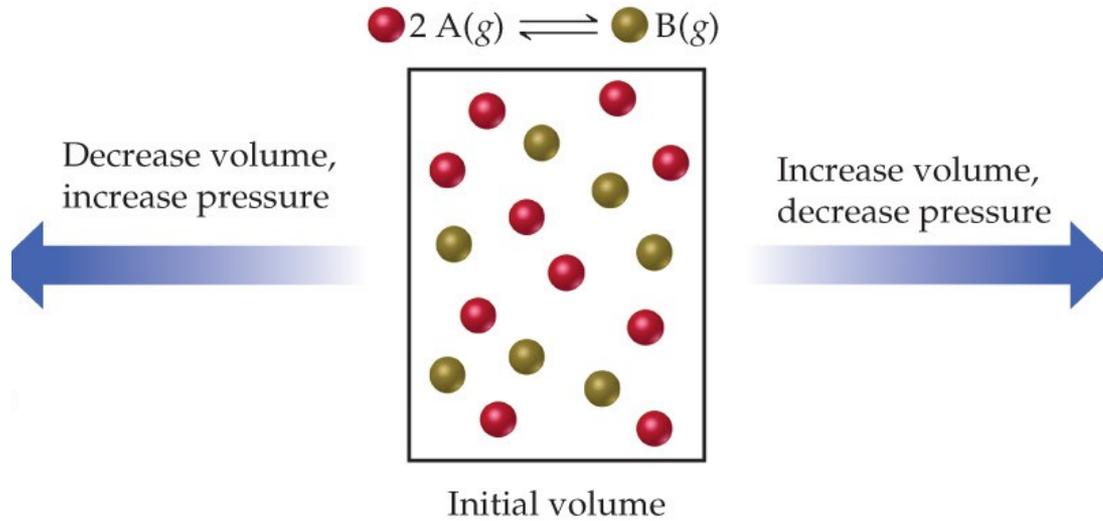




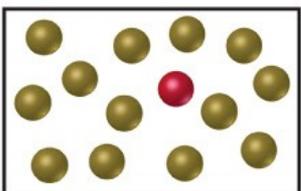


Continuously removing this product from the reaction forces more of it to be produced.

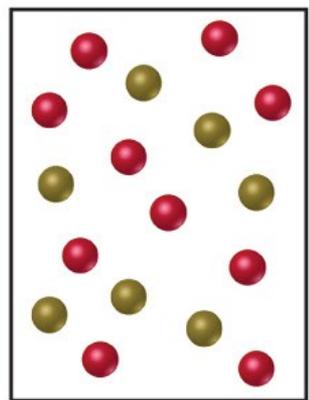
Volume



Volume

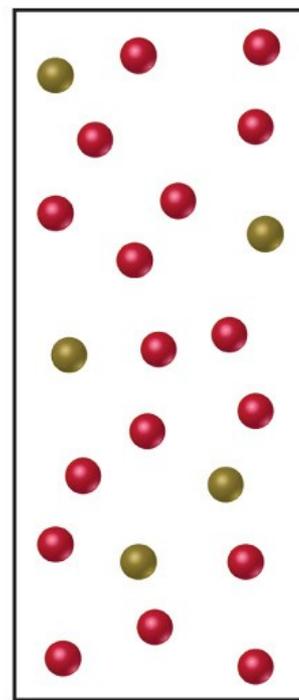


Decrease volume,
increase pressure



Initial volume

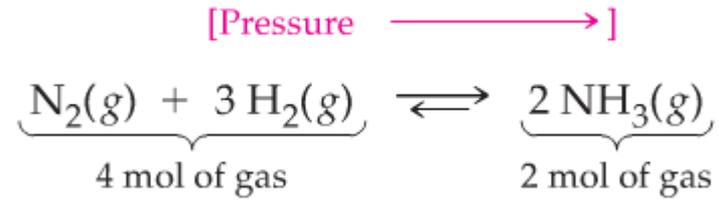
Increase volume,
decrease pressure



New equilibrium favors
reactants to increase total
moles of gas

New equilibrium favors
products to reduce total
moles of gas

Volume



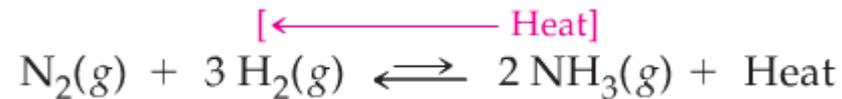
Temperatuur

Endothermic reaction
(Heat is absorbed)

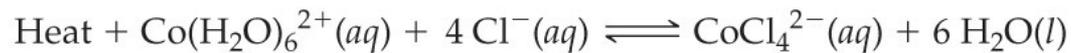
Favored by increase in temperature

Exothermic reaction
(Heat is released)

Favored by decrease in temperature

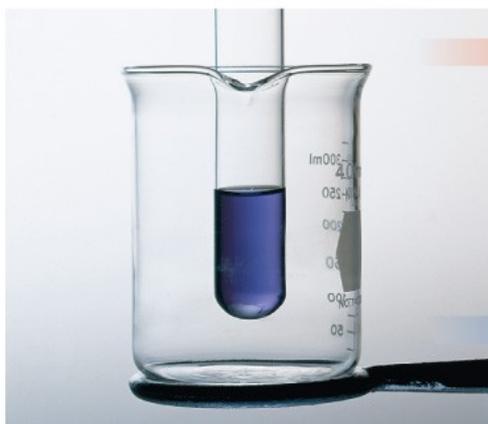


$\Delta H > 0$, endothermic reaction

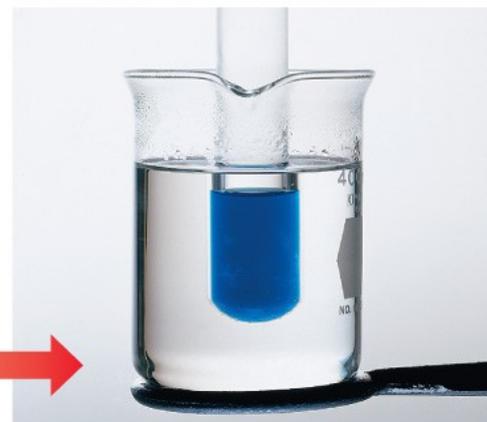


Pink

Blue

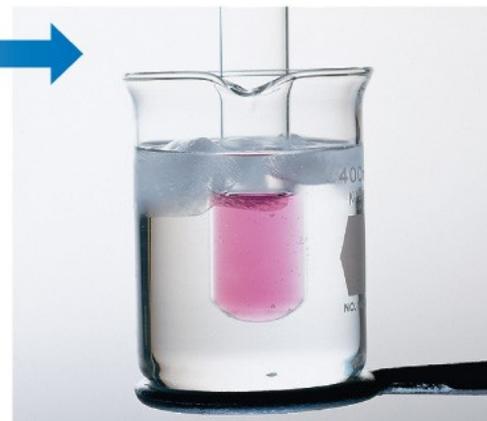


Heat



Add heat: reaction shifts right to increase blue CoCl_4^{2-} concentration and decrease pink $\text{Co}(\text{H}_2\text{O})_6^{2+}$ concentration

Cool



Remove heat: reaction shifts left to decrease blue CoCl_4^{2-} concentration and increase pink $\text{Co}(\text{H}_2\text{O})_6^{2+}$ concentration

At equilibrium, significant amounts of both pink $\text{Co}(\text{H}_2\text{O})_6^{2+}$ and blue CoCl_4^{2-} are present; solution appears violet

TABLE 7.3 Effects of Changes in Reaction Conditions on Equilibria

CHANGE	EFFECT
Concentration	Increase in reactant concentration or decrease in product concentration favors forward reaction.
	Increase in product concentration or decrease in reactant concentration favors reverse reaction.
Temperature	Increase in temperature favors endothermic reaction.
	Decrease in temperature favors exothermic reaction.
Pressure	Increase in pressure favors side with fewer moles of gas.
	Decrease in pressure favors side with more moles of gas.
Catalyst added	Equilibrium reached more quickly; value of K unchanged.

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Nu

Maken opdrachten 17 t/m 19

Wat moet je doen?

Bestudeer:

- De tekst in het boek
- Alle Worked Examples

Maak:

- Problems: 7.1, 7.4, 7.6, 7.10, 7.11, 7.12, 7.13, 7.15, 7.16
- Additional problems: 7.31, 7.38, 7.43, 7.44, 7.48, 7.54, 7.56, 7.58, 7.60, 7.62, 7.64, 7.66, 7.68,

Bronnen

Afbeeldingen afkomstig van:

- McMurry - Fundamentals of general, organic, and biological chemistry. 7th edition, uitgever: Pearson.
 - Veplicht boek boekenlijst opleiding