Chemická termodynamická rovnováha

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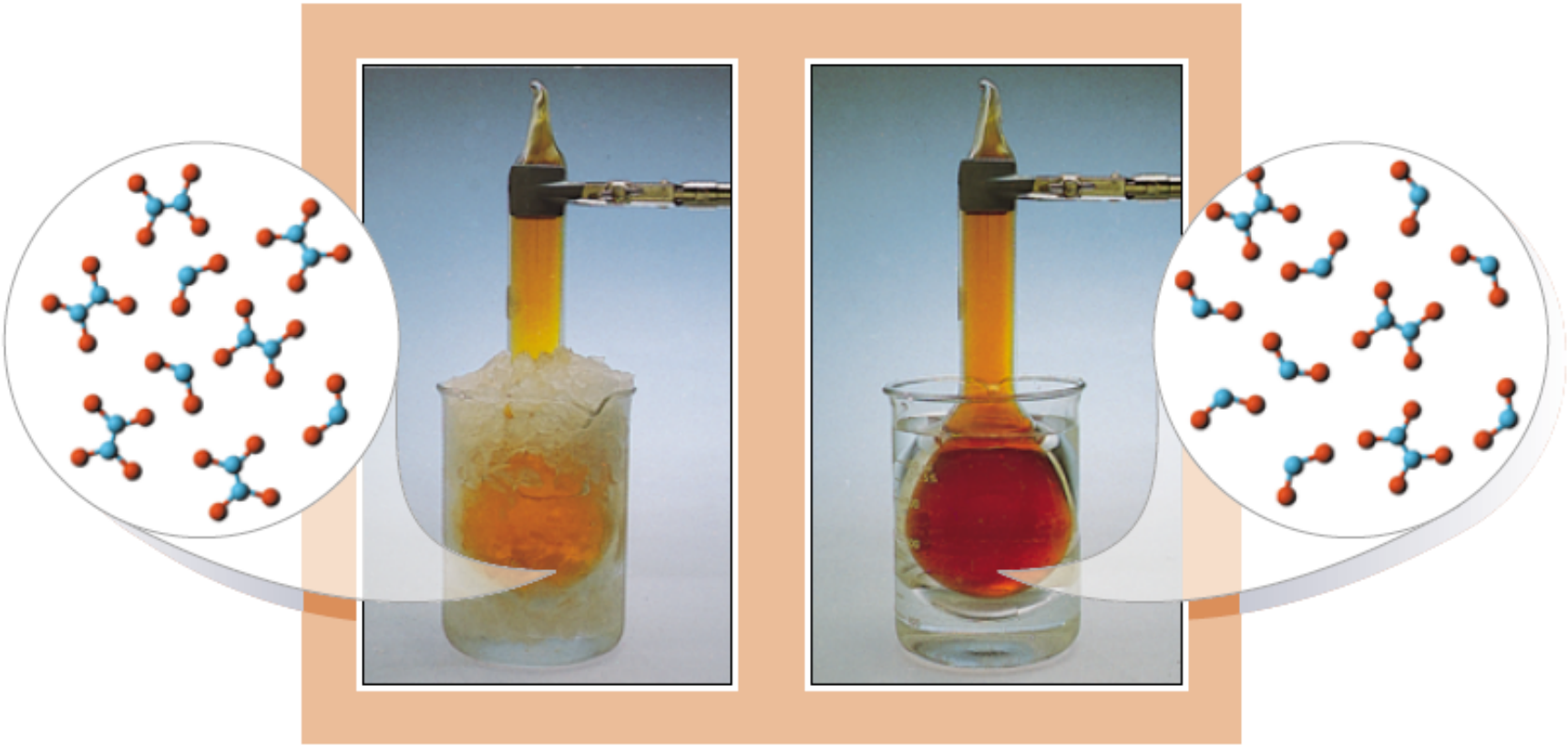
C3420 Fyzikální chemie

Obsah

NO_2

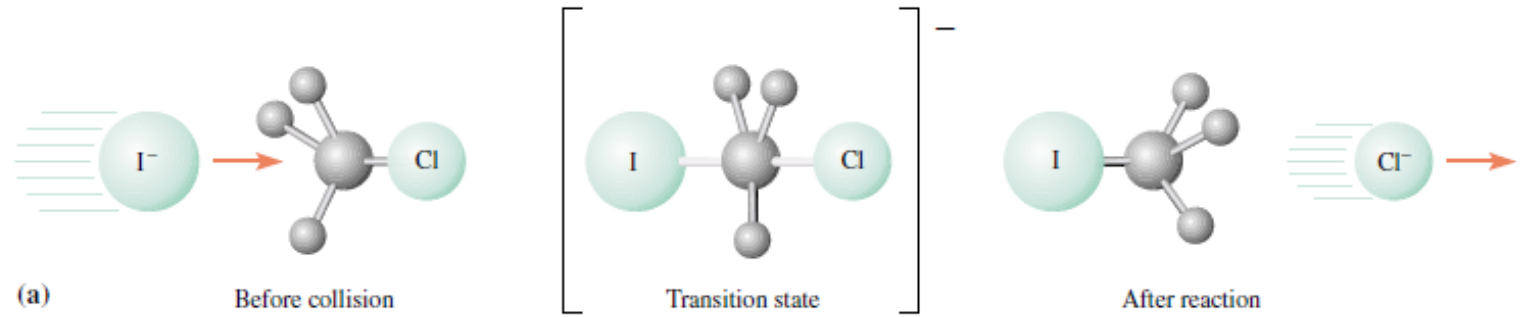


The gas-phase equilibrium for the *exothermic* reaction

$$2NO_2(g) \rightleftharpoons N_2O_4(g) \qquad \Delta H^0_{rxn} = -57.2 \text{ kJ/mol rxn}$$

The two flasks contain the same *total* amounts of gas. NO_2 is brown, whereas N_2O_4 is colorless. The higher temperature (50°C) of the flask on the right favors the reverse reaction; this mixture is more highly colored because it contains more NO_2. The flask on the left, at the temperature of ice water, contains less brown NO_2 gas.

S_N1



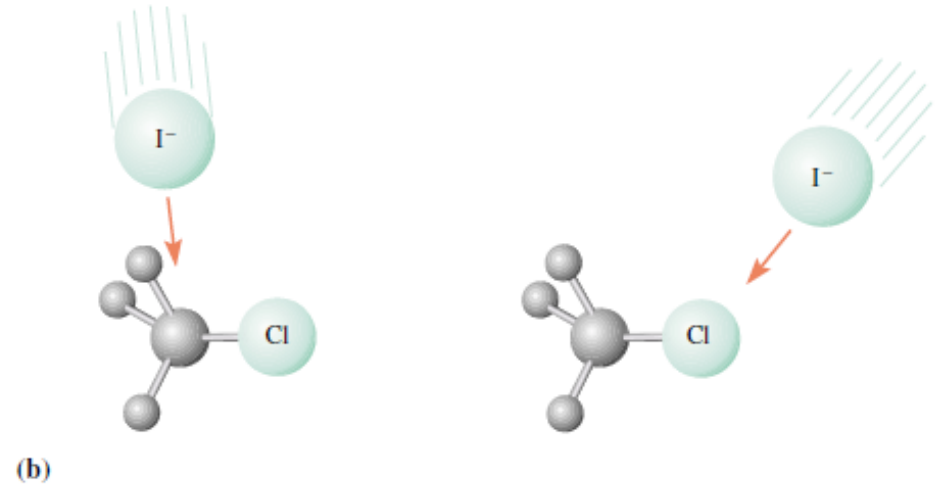
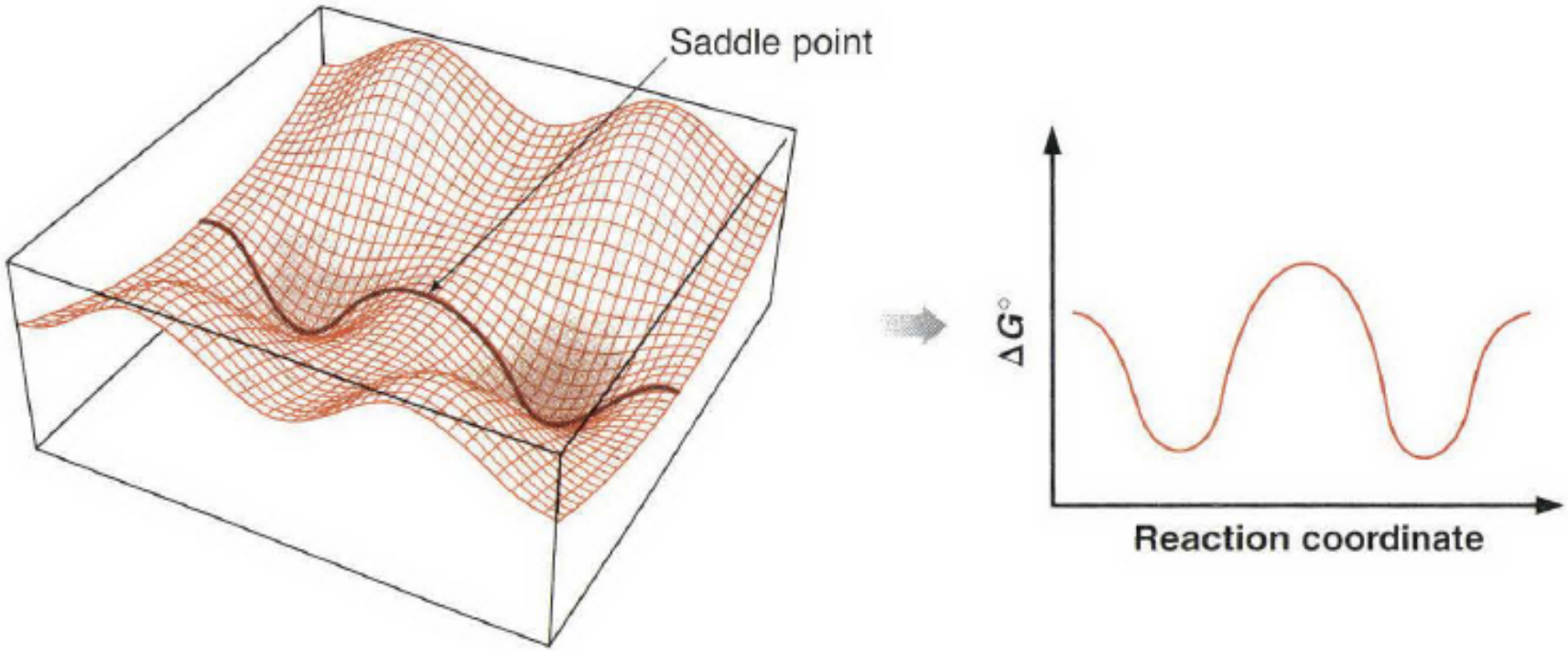
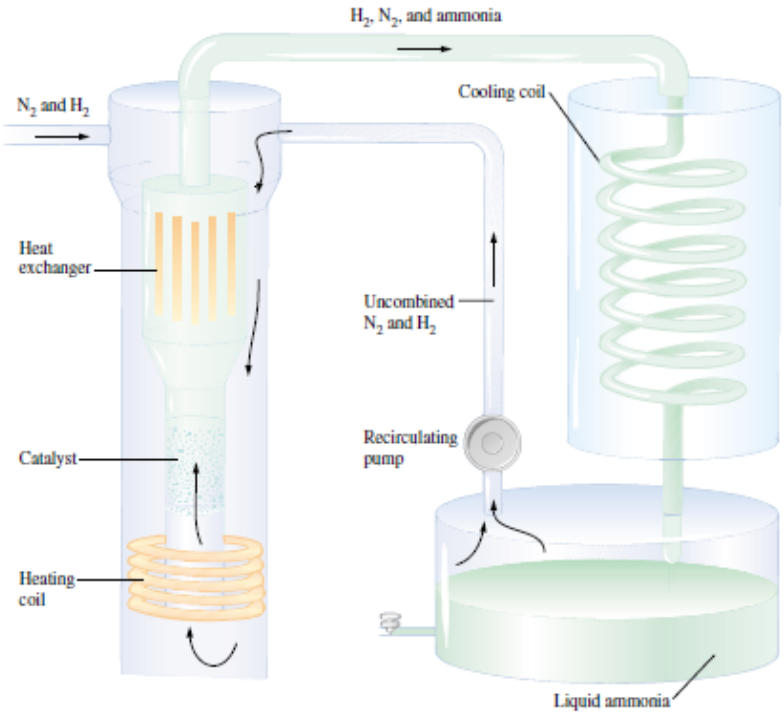


Figure 16-11 (a) A collision that could lead to reaction of I^- + CH_3Cl to give $CH_3I + Cl^-$. The I^- must approach along the "back side" of the C—Cl bond. (b) Two collisions that are not in the "correct" orientation to cause a reaction.

Plochy potnciálních energií - PES

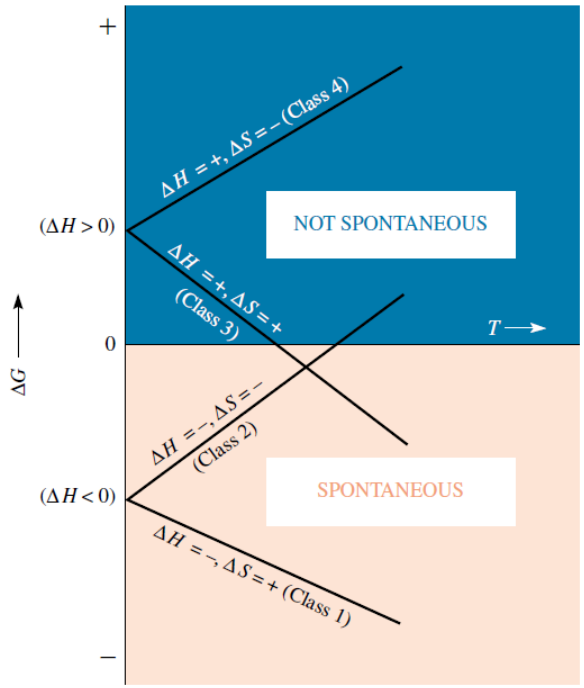


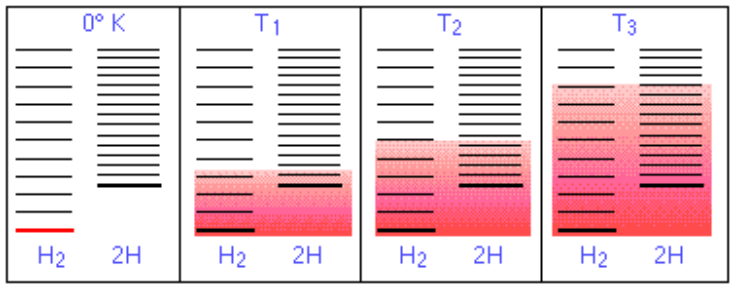
Haber-Boshova syntéza amoniaku



Spontálnost chemických reakcí

http://chemwiki.ucdavis.edu/Textbook Maps 23.2 Entropy Rules





[t]

TABLE 15-7 *Thermodynamic Classes of Reactions*

Class	Examples	ΔH (kJ/mol)	ΔS (J/mol·K)	Temperature Range of Spontaneity
1	$2H_2O_2(\ell) \longrightarrow 2H_2O(\ell) + O_2(g)$	−196	+126	All temperatures
	$H_2(g) + Br_2(\ell) \longrightarrow 2HBr(g)$	−72.8	+114	All temperatures
2	$NH_3(g) + HCl(g) \longrightarrow NH_4Cl(s)$	−176	−285	Lower temperatures (<619 K)
	$2H_2S(g) + SO_2(g) \longrightarrow 3S(s) + 2H_2O(\ell)$	−233	−424	Lower temperatures (<550 K)
3	$NH_4Cl(s) \longrightarrow NH_3(g) + HCl(g)$	+176	+285	Higher temperatures (>619 K)
	$CCl_4(\ell) \longrightarrow C(\text{graphite}) + 2Cl_2(g)$	+135	+235	Higher temperatures (>517 K)
4	$2H_2O(\ell) + O_2(g) \longrightarrow 2H_2O_2(\ell)$	+196	−126	Nonspontaneous, all temperatures
	$3O_2(g) \longrightarrow 2O_3(g)$	+285	−137	Nonspontaneous, all temperatures

Neideální chování

Table 8.1
Equilibrium Constants for the Reaction $\frac{1}{2}N_2(g) + \frac{3}{2}H_2(g) \rightleftharpoons NH_3(g)$ at 450°C[a]

Total pressure/bar	P_{NH_3}/bar	P_{N_2}/bar	P_{H_2}/bar	K_P	K_γ	$K_f(K_PK_\gamma)$
10.2	0.204	2.30	7.67	0.0064	0.994	0.0064
30.3	1.76	6.68	21.9	0.0066	0.975	0.0064
50.6	4.65	10.7	35.2	0.0068	0.95	0.0065
101.0	16.6	19.4	65.0	0.0072	0.89	0.0064
302.8	108	42.8	152	0.0088	0.70	0.0062
606	326	56.5	223	0.0130	0.50	0.0065

[a] Data from A. J. Larson, *J. Am. Chem. Soc.* **46**, 367 (1924).