Reaction quotient

$$Q = \prod_{\mathrm{J}} a_{\mathrm{J}}^{\nu_{\mathrm{J}}}$$

$$Q = \frac{\text{activities of products}}{\text{activities of reactants}}$$

At equilibrium,

$$K = \left(\prod_{\mathrm{J}} a_{\mathrm{J}}^{\nu_{\mathrm{J}}} \right)_{\text{equilibrium}}$$

thermodynamic equilibrium constant

$$\Delta_{\mathrm{r}} G = \Delta_{\mathrm{r}} G^{\ominus} + RT \ln Q$$

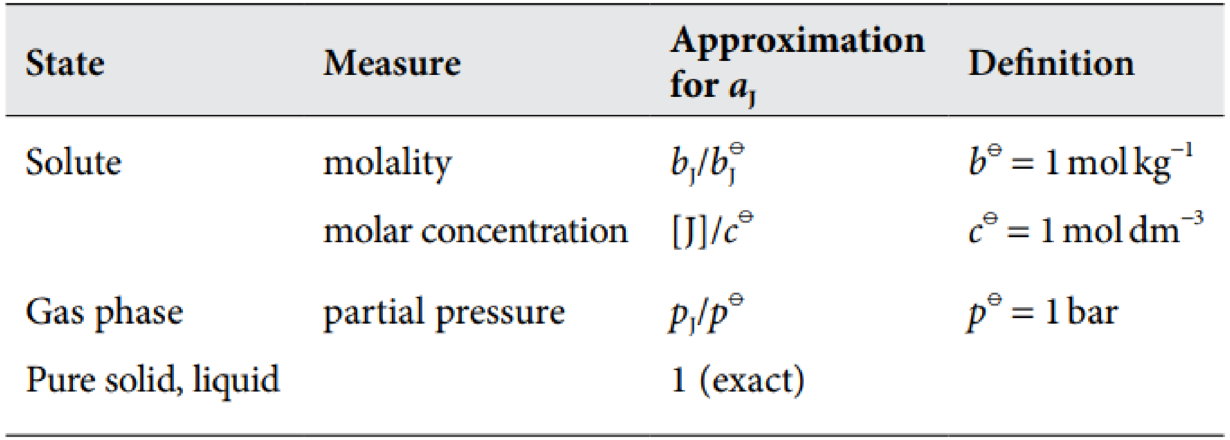
$$\Delta_{\mathrm{r}} G^{\ominus} = \sum_{\text{Products}} \nu \Delta_{\mathrm{f}} G^{\ominus} - \sum_{\text{Reactants}} \nu \Delta_{\mathrm{f}} G^{\ominus}$$

Activities

$$Q = \prod_{J} a_J^{\nu_J}$$

$$K = \left(\prod_{J} a_J^{\nu_J} \right)_{\text{equilibrium}}$$

Approximating Activity:



State	**Measure**	**Approximation for a_J**	**Definition**
Solute	molality	$b_J/b_J^{\ominus}$	$b^{\ominus} = 1\,\mathrm{mol\,kg^{-1}}$
	molar concentration	$[J]/c^{\ominus}$	$c^{\ominus} = 1\,\mathrm{mol\,dm^{-3}}$
Gas phase	partial pressure	$p_J/p^{\ominus}$	$p^{\ominus} = 1\,\mathrm{bar}$
Pure solid, liquid		1 (exact)	

Activities

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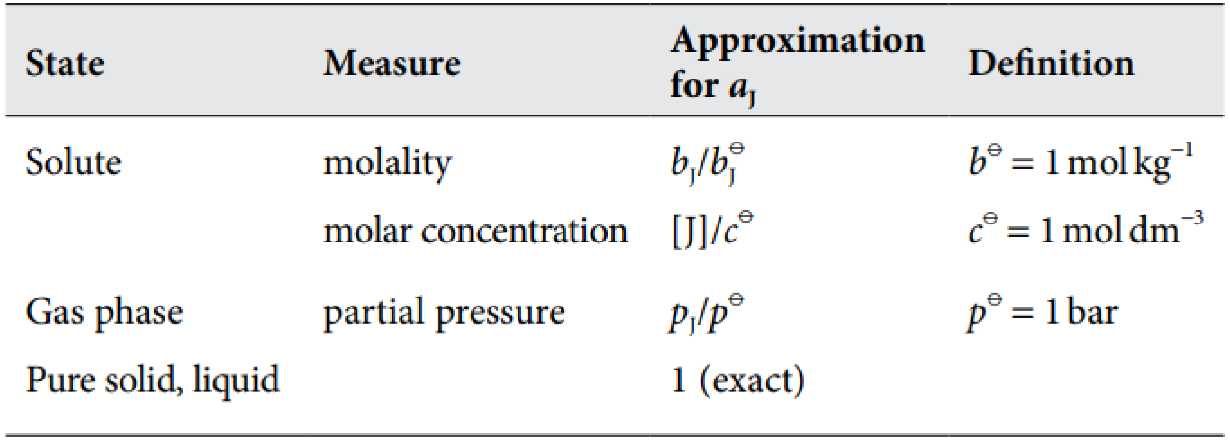

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The equilibrium constant for the heterogeneous equilibrium $CaCO_3(s) \rightleftharpoons CaO(s) + CO_2(g)$ is

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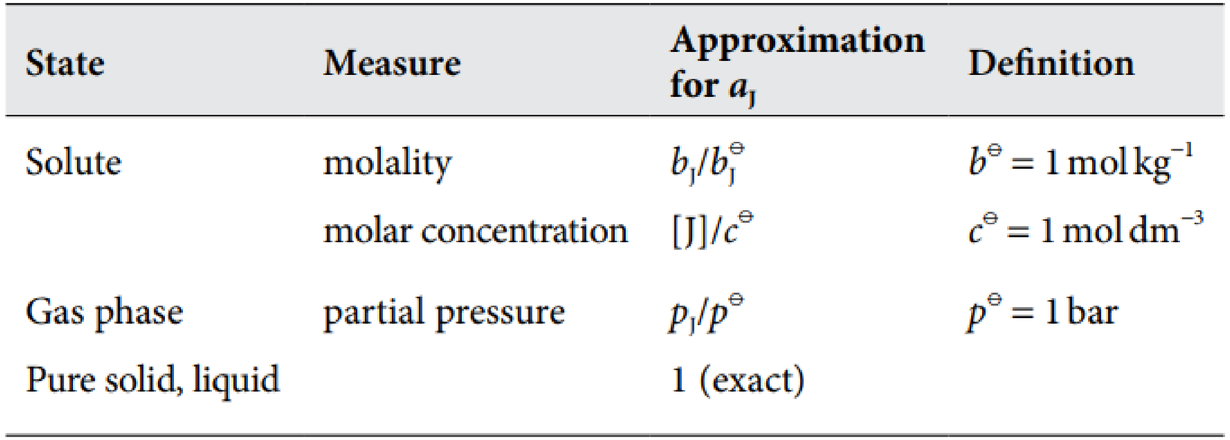

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Activities

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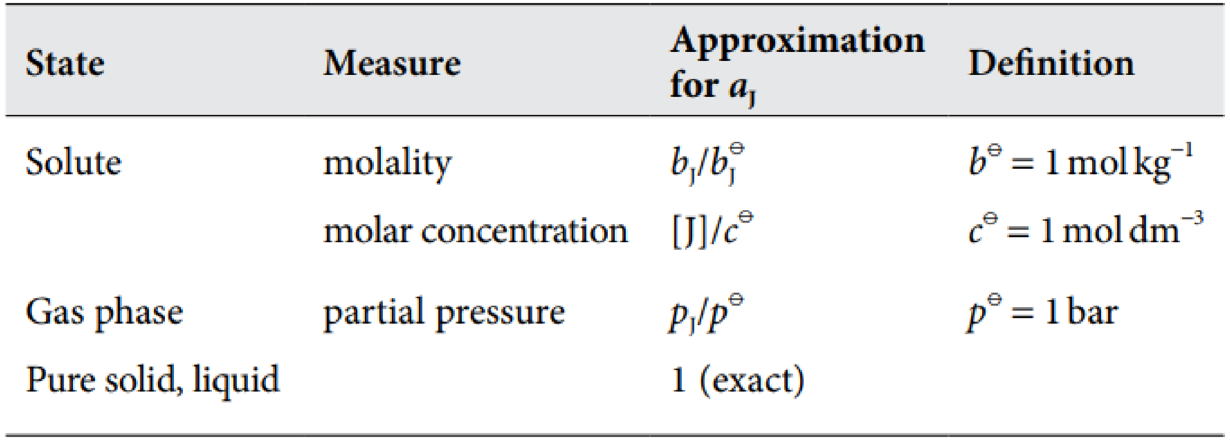

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Extent of dissociation

$$\alpha = (n - n_{\mathrm{eq}})$$

The amount of reactant that has decomposed

Extent of dissociation

$\alpha = (n - n_{\mathrm{eq}})$	The amount of reactant that has decomposed
$\alpha = (n - n_{\mathrm{eq}})/n.$	The fraction of reactant that has decomposed

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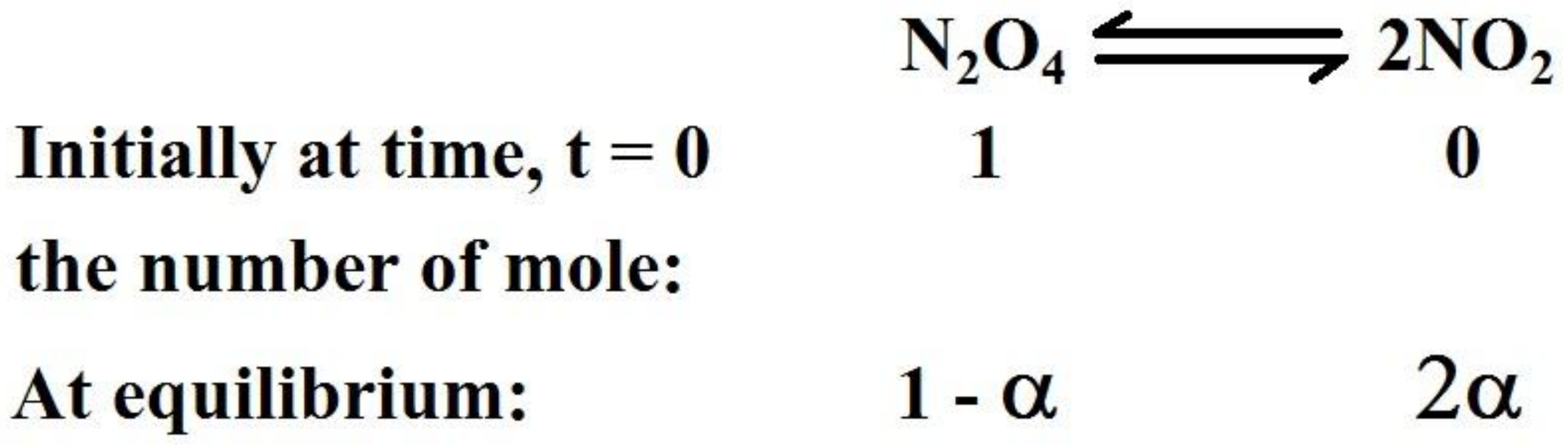

	N_2O_4	$\rightleftharpoons$	$2NO_2$
Initially at time, t = 0	**1**		**0**
the number of mole:			
At equilibrium:	$1 - \alpha$		2α

Extent of dissociation

$$\alpha = (n - n_{\text{eq}})/n.$$

The standard reaction Gibbs energy for the decomposition $H_2O(g) \rightarrow H_2(g) + \frac{1}{2} O_2(g)$ is $+118.08\,\text{kJ mol}^{-1}$ at 2300 K. What is the degree of dissociation of H_2O at 2300 K when the reaction is allowed to come to equilibrium at a total pressure of 1.00 bar?

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	$H_2O \rightarrow$	H_2	+	$\frac{1}{2}O_2$
Initial amount	n	0		0
Amount reacted	$-\alpha n$			

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	$H_2O \rightarrow$	H_2	$+$	$\frac{1}{2}O_2$
Initial amount	n	0		0
Amount reacted/produced (moles)	$-\alpha n$	$+\alpha n$		$+\frac{1}{2}\alpha n$

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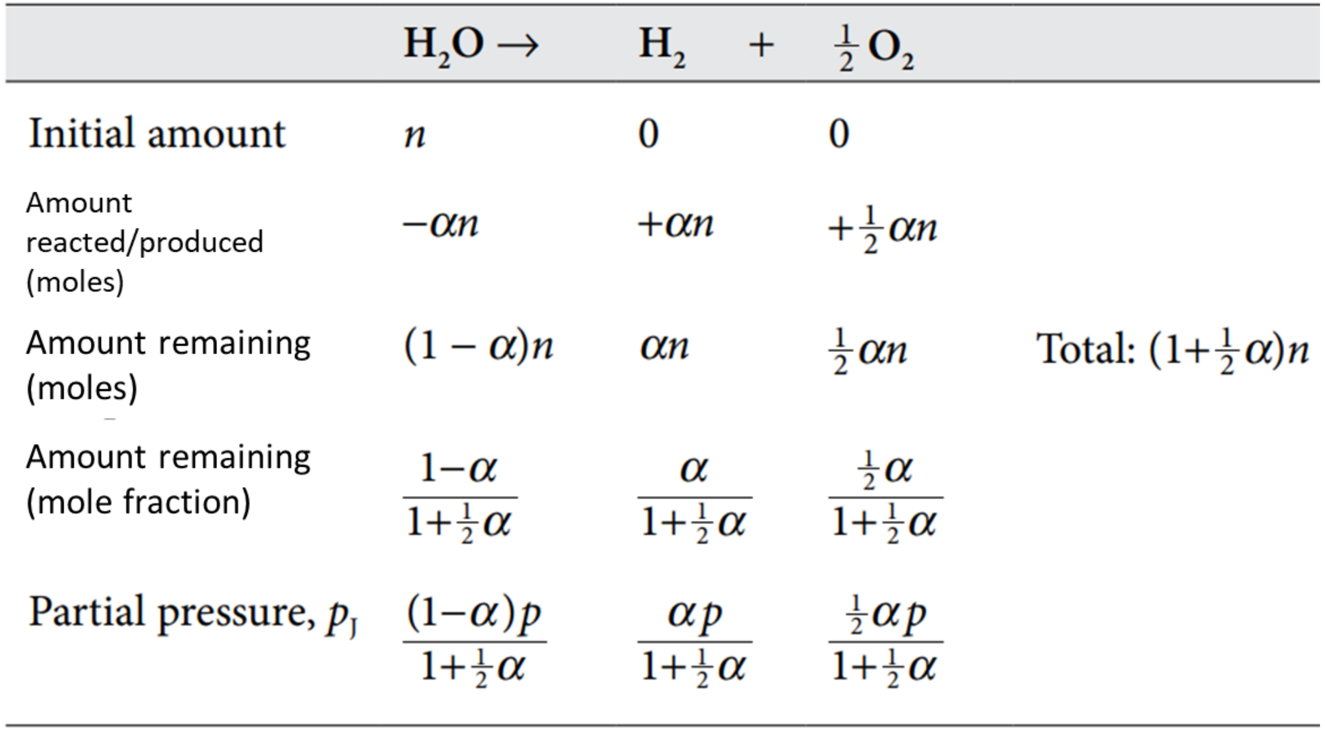
Partial pressure, p_J	$\frac{(1-\alpha)p}{1+\frac{1}{2}\alpha}$	$\frac{\alpha p}{1+\frac{1}{2}\alpha}$		$\frac{\frac{1}{2}\alpha p}{1+\frac{1}{2}\alpha}$	

Extent of dissociation

$$K = \frac{p_{H_2} p_{O_2}^{1/2}}{p_{H_2O}}$$



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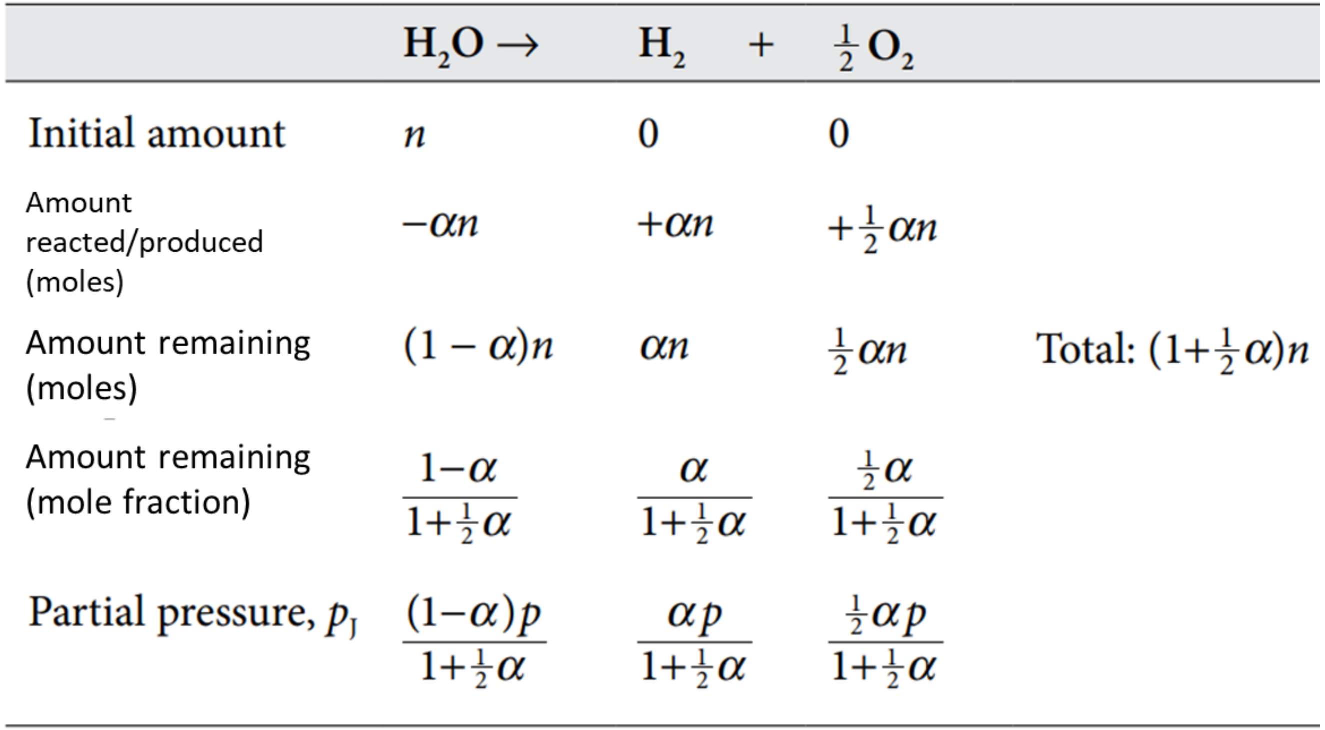

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Initial amount	n	0	0	
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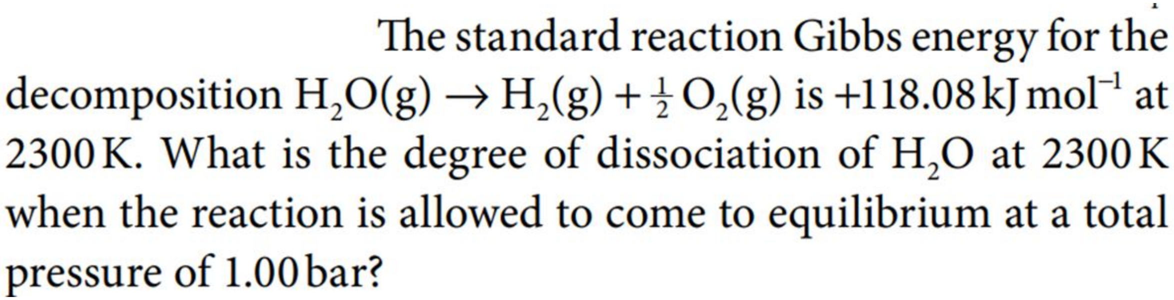

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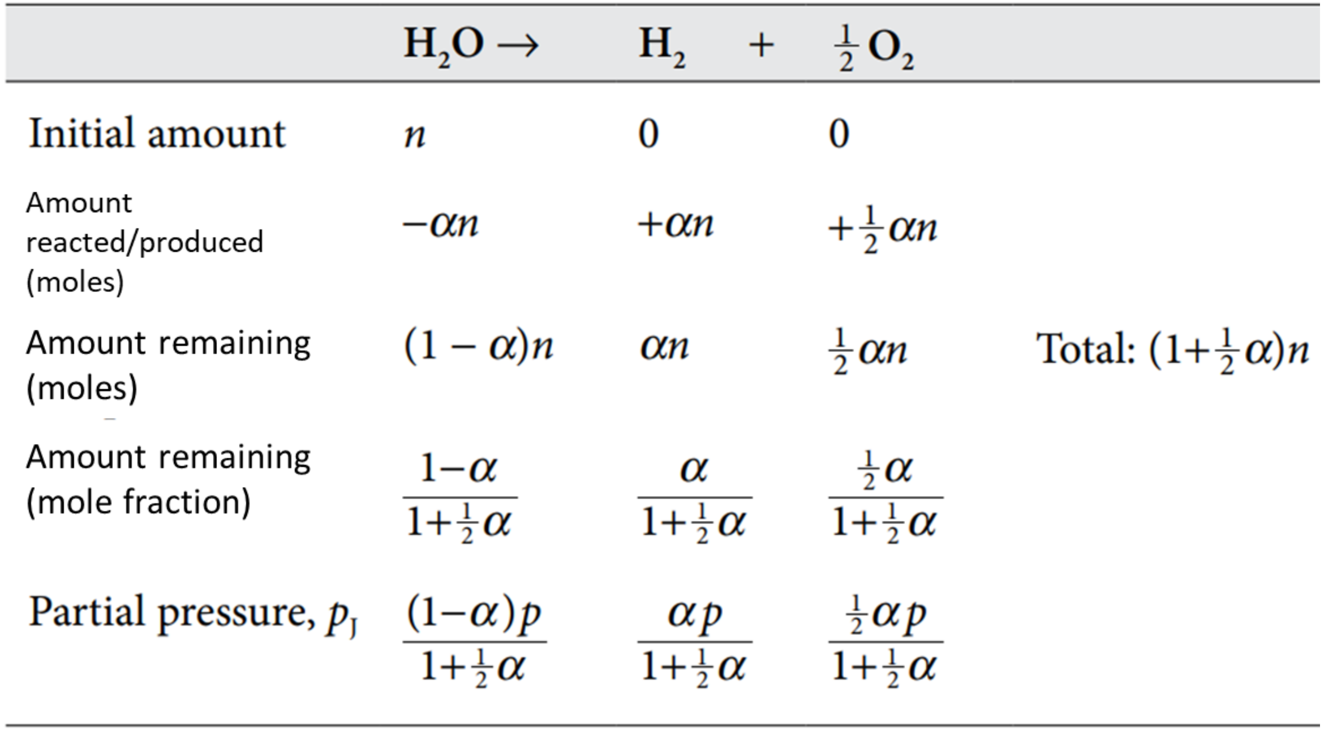

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$$\alpha \approx (2^{1/2} K)^{2/3}$$

$$\ln K = -\frac{\Delta_r G^{\ominus}}{RT} = -\frac{1.1808\times10^{5}\,\text{J}\,\text{mol}^{-1}}{(8.3145\,\text{J}\,\text{K}^{-1}\,\text{mol}^{-1})\times(2300\,\text{K})}$$

$$= -\frac{1.1808\times10^{5}}{8.3145\times2300} = -6.17\ldots$$

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$$K = 2.08 \times 10^{-3}$$

Extent of dissociation

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$$K = 2.08 \times 10^{-3}$$

$$\alpha \approx (2^{1/2} K)^{2/3} = 0.0205$$

Pressure dependence

$$\Delta_r G^{\ominus} = -RT \ln K$$

Pressure dependence

$$\Delta_r G^{\ominus} = -RT \ln K$$

Defined at a single, STD pressure (1 bar)

Does not change with the Pressure

Pressure dependence

$$\Delta_r G^{\ominus} = -RT \ln K$$

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However, the composition of the reaction mixture could change!

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Le Chatelier's principle

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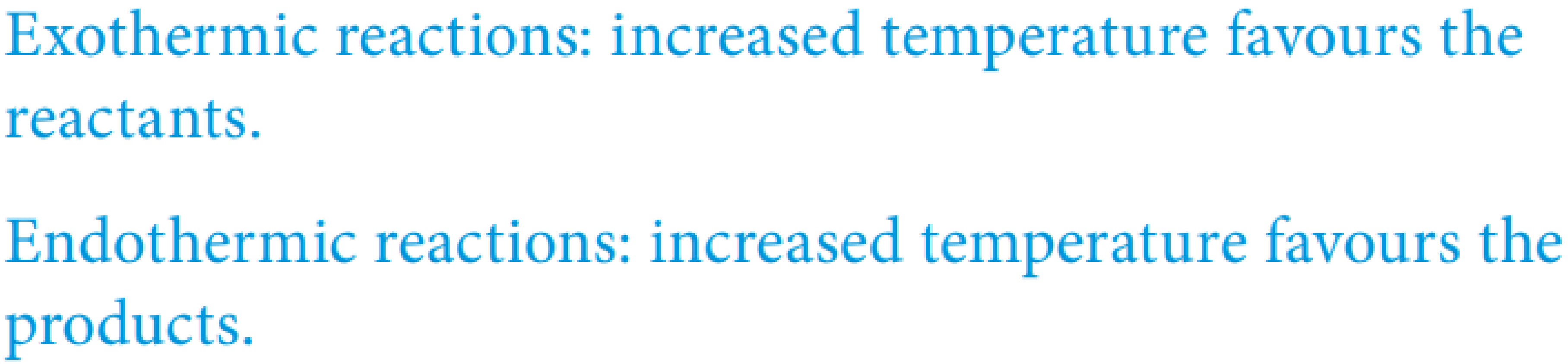
K is independent of pressure. But the amounts of A and B do depend on the pressure

Response to temperature



Exothermic reactions: increased temperature favours the reactants.

Endothermic reactions: increased temperature favours the products.

van 't Hoff equation

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Gibbs–Helmholtz equation:

$$\mathrm{d}(G/T)/\mathrm{d}T = -H/T^2$$

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$\Delta_r H^O$ is the standard reaction enthalpy at the temperature T

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Value of K at different T

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$$\ln K_2 - \ln K_1 = \frac{\Delta_r H^\ominus}{R}\int_{T_1}^{T_2} \frac{1}{T^2}\mathrm{d}T$$

Focus 6: **Chemical equilibrium**

- **The equilibrium constant**
- **The response of equilibria to the conditions**
- Electrochemical cells
- Electrode potentials