

Geschwindigkeit

$$v_c = \frac{1}{r_i} \frac{dc_i}{dt} \quad \text{edukate negativ}$$

$$= \pi c_i^{m_i}$$

Stoss

Bei Molekül Reombi hilfreich
 $0 = d:u = 0 - u$

Quasistationär & Vorgelagertes GGW

QS: $\frac{dc_i}{dt} = \dots \stackrel{!}{=} 0$ Vor GGW $A \xrightleftharpoons[u_n]{u_1} B$ $A \cdot u_1 = B \cdot u_n$ ist da
 GGW Δ ist da
 hin gleich Rück $\Delta = \frac{1}{r_i} (c_i - c_i^{eq}) \Rightarrow 2B \Delta + c_i^q = c_i$
 $-\Delta + c_i^{eq} = c_i$

Freiheitsgrad

| N/Atom | F _{rot} | F _{vib} | F _{trans} | F _{tot} |
|-----------|------------------|------------------|--------------------|---|
| lin | 2 | 3N-5 | 3 | 3N |
| non-lin | 3 | 3N-6 | 3 | 3N |
| <u>u2</u> | 2 3 | 3N-5-1 3N-6-1 | 3 | 3N-1 \rightarrow rxn koordinat \rightarrow Streckerschwingung |

lin, nonlin $\bar{u}2$

Vibration

$$E_{vib,n} = h\nu \left(n + \frac{1}{2}\right) = hc \tilde{\nu} \left(n + \frac{1}{2}\right)$$

ν (1/s) $\tilde{\nu}$ (1/cm)

$q_{vib} \sim \frac{1}{1 - e^{-hc\tilde{\nu}/kT}}$ \rightarrow Temp q_{vib}

$q_{vib} \sim \frac{1}{1 - e^{-hc\tilde{\nu}/kT}}$ \leftarrow Featon

$$\tilde{\nu} = \frac{1}{2\pi c} \cdot \sqrt{\frac{k}{\mu}} \quad \begin{matrix} \rightarrow \text{starr} \\ \rightarrow \text{rel mass} \end{matrix}$$

μ bei isotopen gleich

$$\tilde{\nu}_1 = \tilde{\nu}_2 \sqrt{\frac{\mu_2}{\mu_1}}$$

Rotation

$$q_{rot,lin}(T, b) \quad q_{rot}(T, a, b, c)$$

$\frac{dk}{l} \quad \frac{1}{m}$

$$B_{r2} \stackrel{\mu}{\approx} 2B_r$$

Trans

$$V \cdot \left(\frac{2\pi mkBT}{h^2} \right)^{3/2}$$

EI

$q_{el} \approx 1$ ausre anders gegeben

$$\frac{d(B_{r2})}{dT} = -\ln[B_{r2}] + \frac{1}{T} [B_{r2}]^2$$

$$\frac{d[B_r]}{dT} = 2 \ln[B_{r2}] - 2 \frac{1}{T} [B_r]^2$$

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Handwritten mathematical equations, possibly involving fractions or algebraic expressions.

Handwritten text in the middle right section.

Handwritten mathematical equations, possibly involving variables and constants.

Handwritten text in the middle left section.

Large handwritten text block in the middle section, possibly a paragraph or a detailed explanation.

A table with multiple columns and rows, containing handwritten data or calculations.

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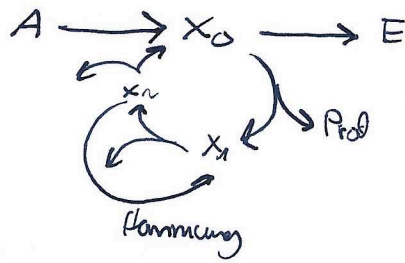
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Kettenreaktion

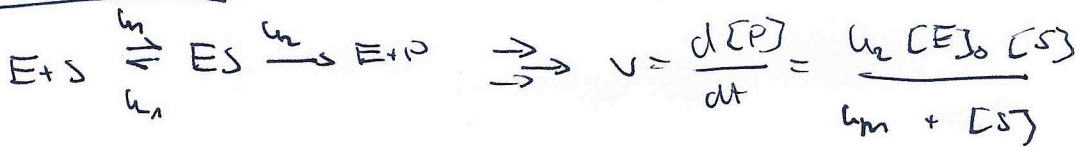
Kettenstart, Ketenträger, Inhibierung / Hemmung
 Kettenverzweigung, Kettenabbruch

-> Stabilitätsanalyse siehe Notizen



Kinetische Matrix -> siehe Notizen

Enzymkinetik

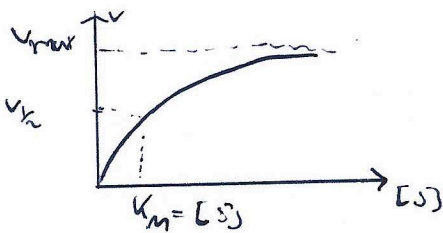


$$K_m = \frac{k_{-1} + k_2}{k_1}$$

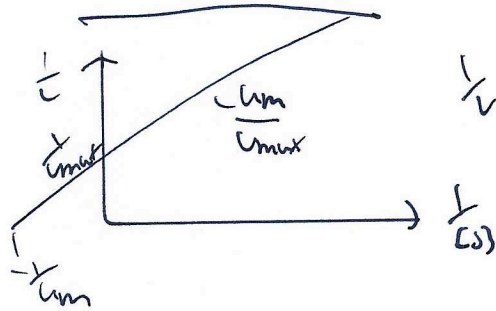
Oder mit Vorzeichen $v = \frac{k_2 [E]_0 [S]}{K_s + [S]}$ $K_s = \frac{k_{-1}}{k_1}$

Plots

normal



Lineweaver - Burk



$$\frac{1}{v} = \frac{k_m}{v_{max}} \cdot \frac{1}{[S]} + \frac{1}{v_{max}}$$

$$v_{max} = k_2 [E]_0 \quad [S] \gg K_m: v = k_2 [E]_0$$

$$[S] = k_m: v = \frac{1}{2} v_{max}$$

$$[S] \ll \frac{k_2}{k_1} [E]_0 [S]$$

die anderen in Notizen

Kompetitive Hemmung

$$v = \frac{d[P]}{dt} = \frac{k_2 [E]_0 [S]}{K_m + \frac{k_m}{k_I} [I] + [S]}$$

$$K_I = \frac{k_{-3}}{k_3} \quad \alpha = 1 + \frac{[I]}{k_I}$$

unkompetitiv

$$v_P = \frac{v_{max} [S]}{k_m + [S]}$$

$$v_{max} = \frac{k_2 [E]_0}{1 + \frac{[I]}{k_I}} \quad K_m = \frac{k_m}{1 + \frac{[I]}{k_I}}$$

nicht kompetitiv

$$v = \frac{v_{max} [S]}{k_m + \alpha [S]} \quad \alpha = 1 + \frac{[I]}{k_I}$$

Lineareierung in Notizen



1) $\sin(\alpha + \beta) = \sin\alpha \cos\beta + \cos\alpha \sin\beta$
 2) $\sin(\alpha - \beta) = \sin\alpha \cos\beta - \cos\alpha \sin\beta$
 3) $\cos(\alpha + \beta) = \cos\alpha \cos\beta - \sin\alpha \sin\beta$
 4) $\cos(\alpha - \beta) = \cos\alpha \cos\beta + \sin\alpha \sin\beta$

$$\sin(\alpha + \beta) = \sin\alpha \cos\beta + \cos\alpha \sin\beta$$

$$\sin(\alpha - \beta) = \sin\alpha \cos\beta - \cos\alpha \sin\beta$$

$$\cos(\alpha + \beta) = \cos\alpha \cos\beta - \sin\alpha \sin\beta$$

$$\cos(\alpha - \beta) = \cos\alpha \cos\beta + \sin\alpha \sin\beta$$



$y = mx + c$
 $m = \frac{y}{x}$
 $c = y - mx$



1) $y = \sqrt{x}$
 2) $y = x^2$
 3) $y = \frac{1}{x}$
 4) $y = \ln(x)$

$$\frac{d}{dx} x^n = nx^{n-1}$$

$$\frac{d}{dx} \ln(x) = \frac{1}{x}$$

$$\frac{d}{dx} e^x = e^x$$

$$\frac{d}{dx} \sin(x) = \cos(x)$$

$$\frac{d}{dx} \cos(x) = -\sin(x)$$

$$\frac{d}{dx} \sin(x) = \cos(x)$$

$$\frac{d}{dx} \cos(x) = -\sin(x)$$

$$\frac{d}{dx} e^x = e^x$$

$$\frac{d}{dx} \ln(x) = \frac{1}{x}$$

1) $\sin(x)$
 2) $\cos(x)$
 3) e^x
 4) $\ln(x)$

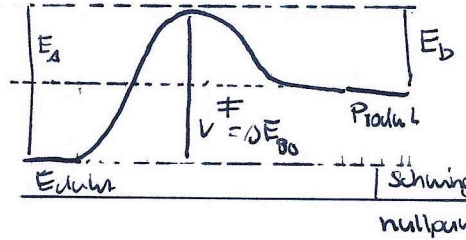
U2

$$q = q_{\text{trans}} \cdot q_{\text{rot}} \cdot q_{\text{vib}} \cdot q_{\text{el}} \cdot q_{\text{elektron}}$$

$$k_{\text{uni}} = \frac{k_B T}{h} \cdot \frac{q^\ddagger}{q_{\text{ Edukt}}} \cdot e^{-\frac{\Delta E}{k_B T}}$$

$$k_{\text{bi}} = \frac{k_B T}{h} \cdot \frac{q^\ddagger}{q_{\text{ Edukt}}} \cdot e^{-\frac{\Delta E}{k_B T}}$$

$$E_b = E_a - \Delta E_{ab}$$



$$m^\ddagger = m_E \Rightarrow \frac{q_{\text{trans}}^\ddagger}{q_{\text{trans}}^\ddagger} = 1$$

$$\frac{q_{\text{ Edukt}} \cdot q_{\text{ Edukt}}}{\pi^2 \nu^2 (v_{\text{vib}})}$$

$$\left(\frac{h^2}{8\pi^2 \mu k_B T} \right) \cdot \frac{q_{\text{vib}}^\ddagger}{q_{\text{vib}}^\ddagger \cdot q_{\text{vib}}^\ddagger} \cdot e^{-\frac{E_0}{k_B T}}$$

Stoßtheorie

$$k = \langle v_{\text{rel}} \rangle \cdot \langle \sigma \rangle \quad [k] = \frac{\text{m}^3}{\text{s}} = \frac{1}{\text{m}^3 \cdot \text{s}}$$

$$\langle v_{\text{rel}} \rangle = \sqrt{\frac{8k_B T}{\pi \mu}} \quad \text{oder} \quad k(E) = \langle \sigma \rangle \cdot \sqrt{\frac{2E}{\mu}}$$

harte Kugel

$$\sigma_0 = \pi (r_1 + r_2)^2 = \langle \sigma_R \rangle$$

mit Schwellen \$E_0\$

$$\langle \sigma \rangle = \sigma_0 \cdot \left(1 + \frac{E_0}{k_B T} \right) e^{-\frac{E_0}{k_B T}}$$

$$E_0 = \frac{1}{2} \mu v^2 \quad v = \sqrt{\frac{2E_0}{\mu}}$$

Schwelle & Langsam

$$\langle \sigma \rangle = \sigma_0 \cdot e^{-\frac{E_0}{k_B T}}$$

$$\langle \sigma \rangle = \int_0^\infty \frac{E}{k_B T} \sigma(E) e^{-\frac{E}{k_B T}} \frac{dE}{k_B T}$$

Arrhenius

$$k(T) = A \cdot e^{-\frac{E_a}{k_B T}}$$

linear: $\ln(k(T)) = \ln(A) - \frac{E_0}{k_B} \cdot \frac{1}{T}$

$$E_a = RT^2 \cdot \frac{d \ln(k(T))}{dT}$$

\$\rightarrow\$ setz \$k(T)\$ ein und leite \$\rightarrow\$ ab

Linienverbreiterung

\$\rightarrow\$ siehe Notizen

Diffusion \$A+B \rightarrow\$ Produkt

$$R_{AB} = R_A + R_B \quad D_{AB} = D_A + D_B$$

ohne: $v = k_{AB} \cdot c_A \cdot c_B$

mit: $v = k_{\text{eff}} \cdot c_A \cdot c_B$

$$k_{\text{eff}} = \frac{4\pi R_{AB} \cdot D_{AB}}{1 + 4\pi R_{AB} \cdot D_{AB}}$$

-Vereinfachung: **welcher Fall tritt ein?**

$$k_{AB} \ll 4\pi R_{AB} \cdot D_{AB}$$

$$k_{AB} \gg 4\pi R_{AB} \cdot D_{AB}$$

$$\frac{1}{k_{\text{eff}}} = \frac{1}{4\pi R_{AB} \cdot D_{AB}} + \frac{1}{k_{AB}}$$

$$k_{AB} = k_{\text{uni}}$$

$$k_{\text{eff}} \approx \frac{1}{k_{AB}} \Rightarrow k_{\text{eff}} = k_{AB}$$

$$k_{\text{eff}} \approx 4\pi R_{AB} \cdot D_{AB}$$

$$k_{\text{eff}} = 4\pi R_{AB} \cdot D_{AB} \left(1 - \frac{4\pi R_{AB} \cdot D_{AB}}{k_{AB}} \right)$$

1. Fall $\frac{1D}{dt} = -D \nabla^2 c$

2. Fall $1D: \frac{\partial c}{\partial t} = D \nabla^2 \frac{\partial c^2}{\partial x^2}$

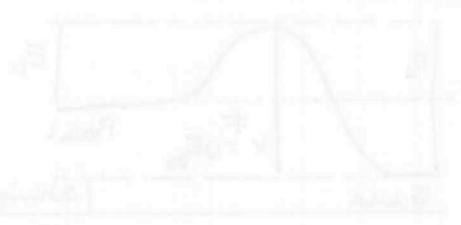
Spezielle Lösung \$\rightarrow\$ für mehr siehe Leit. Sich
w. Diff 1D

3D $\vec{j} = -D \vec{\nabla} c$

3D: $\frac{\partial c}{\partial t} = \vec{\nabla} \cdot (D \vec{\nabla} c)$

$$c(r) = c_0 + \frac{c_1 - c_0}{r} \cdot r$$

Q: How do we find the area under the curve?



Area under the curve

Approximation



$\Delta x = \frac{b-a}{n}$
 $x_i = a + (i-1)\Delta x$
 $x_{i+1} = a + i\Delta x$
 $\Delta x = \frac{b-a}{n}$
 $x_i = a + (i-1)\Delta x$
 $x_{i+1} = a + i\Delta x$



$$\begin{aligned}
 \Delta x &= \frac{b-a}{n} \\
 x_i &= a + (i-1)\Delta x \\
 x_{i+1} &= a + i\Delta x \\
 \Delta x &= \frac{b-a}{n} \\
 x_i &= a + (i-1)\Delta x \\
 x_{i+1} &= a + i\Delta x
 \end{aligned}$$

Approximation
 $\Delta x = \frac{b-a}{n}$
 $x_i = a + (i-1)\Delta x$
 $x_{i+1} = a + i\Delta x$

$$\Delta x = \frac{b-a}{n}$$

The area under the curve is approximated by the sum of the areas of the rectangles.

Approximation
 $\Delta x = \frac{b-a}{n}$
 $x_i = a + (i-1)\Delta x$
 $x_{i+1} = a + i\Delta x$

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Lambert-Beer

$$dI = \sigma \cdot I \cdot c \cdot dx \quad \rightarrow \quad \ln\left(\frac{I_0}{I}\right) = \sigma \cdot c \cdot l = A \quad \rightarrow \text{Länge}$$

+ Querschnitt $\xrightarrow{I_0} \text{KXN} \xrightarrow{I}$ $pV = nRT \quad \frac{n}{V} = c = \frac{P}{RT}$

wenn $\ln\left(\frac{I_0}{I}\right) = \sigma \cdot c \cdot l$ ist σ nicht σ_R sondern $\sigma_{\text{tot}} = \sigma_R + \sigma_A$ Steuerung \uparrow

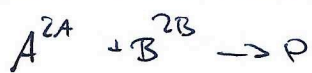
Formeln

$\langle E \rangle = \frac{3}{2} k_B T$ mittlere Translationsenergie

$v_{\text{rms}} = \sqrt{\frac{2k_B T}{m}}$ wurmscheinlichste Geschwindigkeit

$Z_{AB}^V = \langle \sigma \rangle \cdot (v_{\text{rms}}) \cdot c_A \cdot c_B$ # Stöße pro Volumen pro Zeit

Geladene Teilchen



$h = \frac{k_B T}{h} \cdot \frac{z_A \cdot z_B}{\gamma^{\ddagger}} \cdot e^{-\frac{\Delta^\ddagger G^0}{RT}} \cdot (c^\ddagger)^{\ddagger} [A^{z_A}][B^{z_B}]$ $\frac{1}{h}$ für Einheit

$\log(h) = \log(h') + \log\left(\frac{z_A \cdot z_B}{\gamma^{\ddagger}}\right)$ \hookrightarrow Aktivität

$h' = \frac{k_B T}{h} \cdot e^{-\frac{\Delta^\ddagger G^0}{RT}} \cdot (c^\ddagger)^{\ddagger}$

Wahre Konstante

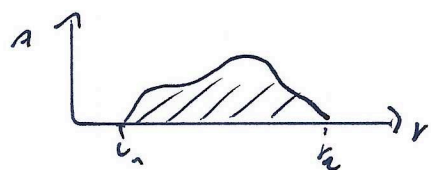
$\log(\delta_i) = -\beta \cdot z_i^2 \cdot \sqrt{\frac{I}{m \cdot 10^{-3}}}$ β gegeben $I = \frac{1}{2} \sum_i z_i^2 \cdot m_i \cdot c_i$ molalität $\frac{\text{mol}}{\text{kg}}$

in Brönstedgleichung

$\log_{10}(h) = \log_{10}(h') + 2\beta z_A z_B \cdot \sqrt{\frac{I}{m \cdot 10^{-3}}}$ \rightarrow gram grad \rightarrow normieren in Notizen

Absorption

$A = \ln\left(\frac{I_0}{I}\right) = \sigma(v) \cdot c \cdot l \Rightarrow c(\lambda) = \frac{A(\lambda)}{\sigma(v) \cdot l}$



$\int_{\lambda_1}^{\lambda_2} \ln\left(\frac{I_0}{I}\right) d\lambda = c \cdot l \cdot \int_{\lambda_1}^{\lambda_2} \sigma(v) d\lambda$

gibt 2 Fälle \rightarrow Notizen

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

$$\frac{1}{\sigma\sqrt{2\pi}} = \frac{1}{\sqrt{2\pi}} \cdot \frac{1}{\sigma}$$

The standard deviation σ is a measure of the spread of the data.

Substituting $\mu = 0$ and $\sigma = 1$

$$f(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}$$

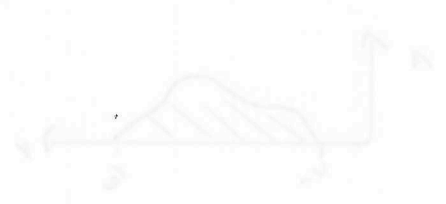
The area under the curve is given by the integral:

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2} dx$$

This integral is equal to 1, representing the total probability.

$$\int_{-\infty}^{\infty} f(x) dx = 1$$

$$\int_{-\infty}^{\infty} x f(x) dx = \mu$$



$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

$$\int_{-\infty}^{\infty} f(x) dx = 1$$

Mathematische Methoden

Integrationsmethoden

1. $\frac{dc}{dt} = -kc$

$\rightarrow \ln(c(t)) = \ln(c_0) - kt$

\rightarrow auftragen

Rechenfinden ob 1. oder 2. Ordnung?

2. $\frac{dc}{dt} = -kc^2$

$\rightarrow \frac{1}{c} = \frac{1}{c_0} - kt$

\rightarrow auftragen

höherer, besserer $R^2 \rightarrow$ besserer fit

Halbwertszeit

$t_{1/2}$ vs c_0 auftragen mit $t_{1/2}(c) = a \cdot c_0^{1-m}$

$\ln(t_{1/2}) = \ln(a) + (1-m) \ln(c_0)$ $a = \frac{2^{m-1}}{\ln(2)}$

\hookrightarrow auch \ln berechenbar

wenn Gesetz $\frac{dc}{dt} = -kc^m$

isolations

cell außer 1 im Überschuss, dann integration über $\frac{1}{c}$

Aufangsgeschwindigkeit

$v_c = \frac{1}{v_1} \frac{dc_1}{dt} = k c_1^m$

am Anfang

$v_c^0 \approx \frac{1}{v_1} \frac{dc_1}{dt} = k_{eff} \cdot c_1^m$ $\ln(v_c^0) = \ln(k_{eff}) + m \ln(c_1)$

frage $\ln(v_c^0)$ vs $\ln(c_1)$ auf

Diff quotient

$-\frac{dc}{dt} = k(c)^m$

$\ln\left(-\frac{\Delta c}{\Delta t}\right) = \ln(k) + m \ln(c)$

$\Rightarrow k = -\frac{1}{(c)^m} \cdot \frac{\Delta c}{\Delta t}$

| | | | | |
|-----|-------|---------------|---------------|---------------|
| | $t=0$ | $t=20$ | $t=40$ | $t=60$ |
| c | 20 | 15 | 12 | 6 |
| | | $\Delta c=5$ | $\Delta c=3$ | $\Delta c=6$ |
| | | $\Delta t=20$ | $\Delta t=20$ | $\Delta t=20$ |
| | | $c=17.5$ | $c=13.5$ | $c=9$ |

Mathematical Induction

Principle of Mathematical Induction

Let $P(n)$ be a statement involving n . If $P(1)$ is true and $P(k) \Rightarrow P(k+1)$ is true for all $k \in \mathbb{N}$, then $P(n)$ is true for all $n \in \mathbb{N}$.

Method of Mathematical Induction

Step 1: Base Case: Verify $P(1)$ is true.
Step 2: Inductive Step: Assume $P(k)$ is true, prove $P(k+1)$ is true.

Example: Prove that $1 + 2 + 3 + \dots + n = \frac{n(n+1)}{2}$ for all $n \in \mathbb{N}$.

$$\left. \begin{aligned} P(1) &= 1 = \frac{1(1+1)}{2} \\ P(k) &= 1 + 2 + \dots + k = \frac{k(k+1)}{2} \end{aligned} \right\} \text{Assume true}$$

$$P(k+1) = 1 + 2 + \dots + k + (k+1) = \frac{k(k+1)}{2} + (k+1)$$

Step 1

Step 2: Assume $P(k)$ is true, prove $P(k+1)$ is true.

$$= \frac{k(k+1) + 2(k+1)}{2} = \frac{(k+1)(k+2)}{2} = P(k+1)$$

∴ $P(n)$ is true for all $n \in \mathbb{N}$.

Example

Prove that $1^2 + 3^2 + 5^2 + \dots + (2n-1)^2 = \frac{n(8n^2-1)}{3}$ for all $n \in \mathbb{N}$.

Proof

$$P(1) = 1^2 = \frac{1(8 \cdot 1^2 - 1)}{3} = 1$$

Assume

$$P(k) = 1^2 + 3^2 + \dots + (2k-1)^2 = \frac{k(8k^2-1)}{3}$$

Prove $P(k+1)$ is true.

Prove

$$P(k+1) = 1^2 + 3^2 + \dots + (2k-1)^2 + (2k+1)^2$$

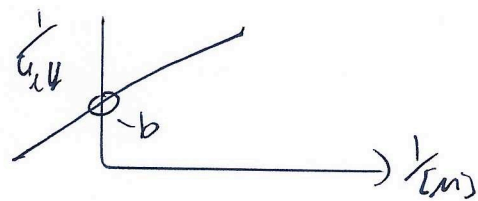
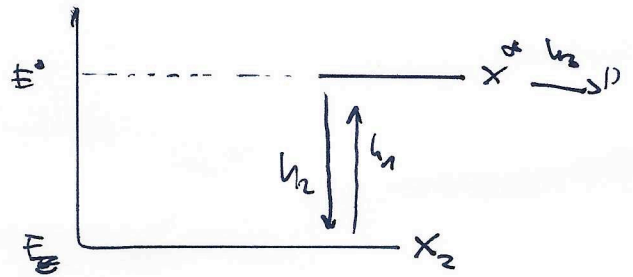
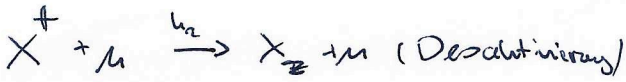
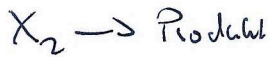
$$= \frac{k(8k^2-1)}{3} + (2k+1)^2 = \frac{k(8k^2-1) + 3(2k+1)^2}{3}$$

Periodische Störung → Notizen und Methoden

Umsatzgeschwindigkeit, allgemein kinetik, Transport → Notizen
 Besetzungswahrscheinlichkeit und -dichte, Strahl experiment

Lindemann-Mechanismen

Bei Zersetz (Unimolekular)



$$k_{eff} = \frac{k_3 \cdot k_1}{k_2 + \frac{k_3}{[M]}} \quad \left| \quad \frac{1}{k_{eff}} = \frac{k_2}{k_1 \cdot k_3} + \frac{1}{k_1} \cdot \frac{1}{[M]} \right.$$

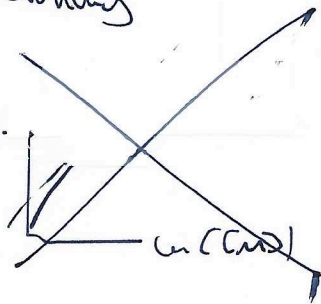
$k_{ca} = k_1 \quad k_{cd} = k_2$

niederdruck

$k_{eff} = k_1 [M]$

→ aktivierung ist v bestimmend

2. Ordnung

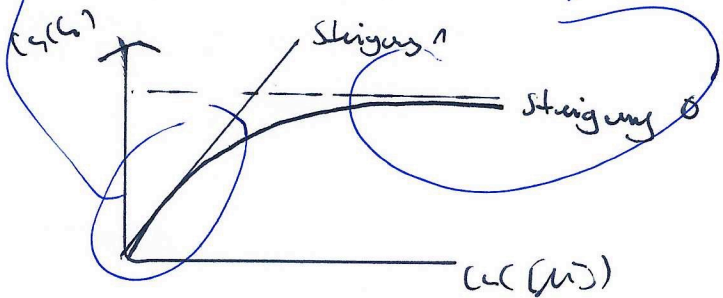


Hochdruck

$k_{eff} = \frac{k_3 \cdot k_1}{k_2}$

→ Rxn ist v bestimmend

1. Ordnung



Partial Derivatives - Hk 1 und Hk 2

Wichtigste Eigenschaft: $\frac{\partial}{\partial x} \frac{\partial f}{\partial y} = \frac{\partial}{\partial y} \frac{\partial f}{\partial x}$ (Symmetrie)
Zweiter Hauptsatz: $\frac{\partial}{\partial x} \frac{\partial f}{\partial x} = \frac{\partial^2 f}{\partial x^2}$

Wichtige Formeln

$\frac{\partial}{\partial x} (x^a) = a \cdot x^{a-1}$

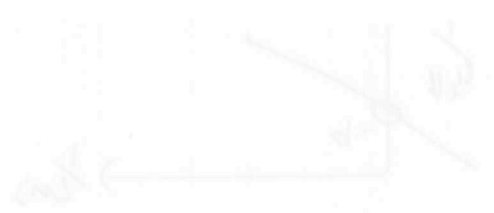
$\frac{\partial}{\partial x} (x^a \cdot y^b) = a \cdot x^{a-1} \cdot y^b + b \cdot x^a \cdot y^{b-1} \cdot \frac{\partial y}{\partial x}$



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Wichtige Formeln

$\frac{\partial}{\partial x} (x^a \cdot y^b) = a \cdot x^{a-1} \cdot y^b + b \cdot x^a \cdot y^{b-1} \cdot \frac{\partial y}{\partial x}$

$\frac{\partial}{\partial x} (x^a \cdot y^b) = a \cdot x^{a-1} \cdot y^b + b \cdot x^a \cdot y^{b-1} \cdot \frac{\partial y}{\partial x}$



Langewir-Moder

ω + nicht geladen Teilchen

$$\sigma(E) = \sqrt{\frac{G}{E_c}}$$

$$G = \frac{d^2 z^2}{8 \epsilon_0^2}$$

d = Polaritabilität

$$h = \sigma(E) \cdot \sqrt{\frac{2Eh}{N}} = \sqrt{\frac{2G}{N}}$$

~~hängt~~ G hängt nicht von Teil E_{ph}

Potentialfunktion zu $\sigma_p \rightarrow$ Notin

Handwritten text at the top of the page, possibly a title or header.

$$\frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \right)$$

Handwritten text below the first equation, possibly a derivation or explanation.

$$\frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \right)$$

Handwritten text at the bottom of the page, possibly a conclusion or final note.

Matrix Bsp

$$A_1 \begin{matrix} u_{21} \\ -u_{12} \end{matrix} B \quad -u_{21} = 2 \quad -u_{12} = 0$$

$$\underline{K} = \begin{bmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{bmatrix} \text{ exist } \sum_i m_{ij} = 0$$

$$\Rightarrow u_{11} = -u_{21}$$

$$\underline{K} = \begin{bmatrix} 2 & 0 \\ -2 & 0 \end{bmatrix} = \begin{bmatrix} -u_{21} & u_{12} \\ u_{21} & -u_{12} \end{bmatrix} \quad u_{11} = 2 \quad u_{21} = -2 \\ u_{22} = 0 \quad u_{12} = 0$$

$$\det(\underline{K} - A \underline{I}) \stackrel{!}{=} 0$$

$$(2-\lambda)(-\lambda) - 0 = 0$$

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$-2\lambda \quad \lambda^2 = 0 \Rightarrow \lambda_1 = 0 \quad \lambda_2 = +2$$

$$\underline{C} \underline{W} = \underline{X} \begin{pmatrix} e^{-\lambda_1 t} & 0 \\ 0 & e^{\lambda_2 t} \end{pmatrix} \underline{X}^{-1} \underline{C}_0$$

$$\underline{X} = \begin{bmatrix} 0 & 1 \\ 1 & -1 \end{bmatrix}$$

$$\underline{X}^{-1} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & e^{-2t} \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} \cdot \underline{C}_0$$

$$= \begin{bmatrix} 0 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ e^{-2t} & 0 \end{bmatrix} = \begin{bmatrix} e^{-2t} & 0 \\ 1 - e^{-2t} & 1 \end{bmatrix} \cdot \underline{C}_0$$

$$-k_{21} = 3$$

$$k_{12} = 2$$

$$\underline{\underline{K}} = \begin{bmatrix} 3 & -2 \\ -3 & 2 \end{bmatrix}$$

$$\det(\underline{\underline{K}} - a \underline{\underline{1}}) = (3-a)(2-a) - 6$$

$$= a^2 - 5a + 6 - 6$$

$$= a(a-5)$$

$$a_1 = 0 \quad a_2 = 5$$

$$\underline{\underline{C}}(t) = \underline{\underline{u}} \quad (24)$$

$$\underline{\underline{C}} = \begin{pmatrix} 1M \\ 0 \end{pmatrix}$$

$$\underline{\underline{C}}(t) = \underline{\underline{X}} \begin{bmatrix} e^{0t} & 0 \\ 0 & e^{-5t} \end{bmatrix} \underline{\underline{X}}^{-1} \cdot \underline{\underline{C}} = \underline{\underline{X}} \begin{bmatrix} 2 & 1 \\ 3 & -1 \end{bmatrix}$$

$$= \begin{bmatrix} 2 & 1 \\ 3 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & e^{-5t} \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 3 & -2 \end{bmatrix} \cdot \frac{1}{5} \cdot \underline{\underline{C}}$$

$$\underline{\underline{X}} = \begin{bmatrix} 2 & 1 \\ 3 & -1 \end{bmatrix}$$

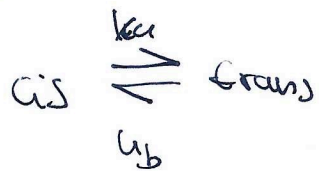
$$\underline{\underline{X}}^{-1} = \frac{1}{5} \begin{bmatrix} 1 & 1 \\ 3 & -2 \end{bmatrix}$$

$$= \begin{bmatrix} 2 & 1 \\ 3 & -1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 3e^{-5t} & -2e^{-5t} \end{bmatrix} \cdot \frac{1}{5} \cdot \underline{\underline{C}}$$

$$= \begin{bmatrix} 2 + 3e^{-5t} & 2 - 2e^{-5t} \\ 3 - 3e^{-5t} & 3 + 2e^{-5t} \end{bmatrix} \cdot \frac{1}{5} \begin{pmatrix} 1M \\ 0 \end{pmatrix}$$

$$= \frac{1}{5} \begin{pmatrix} 2 + 3e^{-5t} \\ 3 - 3e^{-5t} \end{pmatrix}$$

Relaxationszeit



da Betrachtung für Annäherung an Gleich
→ Gleich angenommen $\Rightarrow \rightarrow = \leftarrow$

$$\frac{d[\text{cis}]}{dt} = -k_a [\text{cis}] + k_b [\text{trans}]$$

$$\frac{d[\text{trans}]}{dt} = -k_b [\text{trans}] + k_a [\text{cis}]$$

setze Umsetzvariable fest

$$\Delta = \frac{1}{V_i} (c_i - c_i^{\text{eq}}) \Rightarrow \Delta = \frac{1}{V_i} ([\text{cis}] - [\text{cis}]^{\text{eq}})$$

$$\Delta = [\text{cis}] - [\text{cis}]^{\text{eq}}$$

$$\left. \begin{aligned} \Rightarrow [\text{cis}] &= \Delta + [\text{cis}]^{\text{eq}} \\ [\text{trans}] &= -\Delta + [\text{trans}]^{\text{eq}} \end{aligned} \right\} \text{ in } \underline{I}$$

$$\frac{d[\Delta - [\text{cis}]^{\text{eq}}]}{dt} = \cancel{-k_a [\Delta]} - k_a (\Delta + [\text{cis}]^{\text{eq}}) + k_b (\Delta + [\text{trans}]^{\text{eq}})$$

$$\frac{d\Delta}{dt} = -k_a \Delta - \cancel{k_a [\text{cis}]^{\text{eq}}} - \cancel{k_b \Delta} + k_b [\text{trans}]^{\text{eq}}$$

da Gleich

$$= -k_a \Delta - k_b \Delta$$

$$= -\Delta (k_a + k_b) \Rightarrow \tau = \frac{1}{k_a + k_b} = \frac{1}{k_a + k_b}$$

Freiheitsgrade

| N Atome | Frot | Fuib | F _{trans} | Frot |
|-------------|---------------|-------------------------|--------------------|------------------------------------|
| linear | 2 | 3N-5 | 3 | 3N |
| nonlin | 3 | 3N-6 | 3 | 3N |
| \bar{u}_2 | $\frac{2}{3}$ | $\frac{3N-5-1}{3N-6-1}$ | 3 | $3N-1 \rightarrow$ Rot. Koordinate |

\swarrow lin
 \searrow nonlin

$\lambda_{\text{rot}} \text{ rot} = 3 \cdot 10$

Arrhenius

$\ln(\tau) = A \cdot e^{-\frac{E_A}{k_B T}} \rightarrow$ linearisieren

alle auf Einheiten

$\ln(\tau) = \ln(A) - \frac{E_A}{k_B T}$

$\ln(\tau) = \ln(A) - \frac{E_A}{k_B} \cdot \frac{1}{T} \quad \frac{1}{T} \vee \ln(\tau)$

$m = -20,145 \text{ eV} \quad b = 20,87$

$m = -\frac{E_A}{k_B} \quad \ln(\tau) = b$

$E_A = m \cdot k_B$
 $= 2,78 \cdot 10^{-19} \text{ J}$
 $A = e^b$