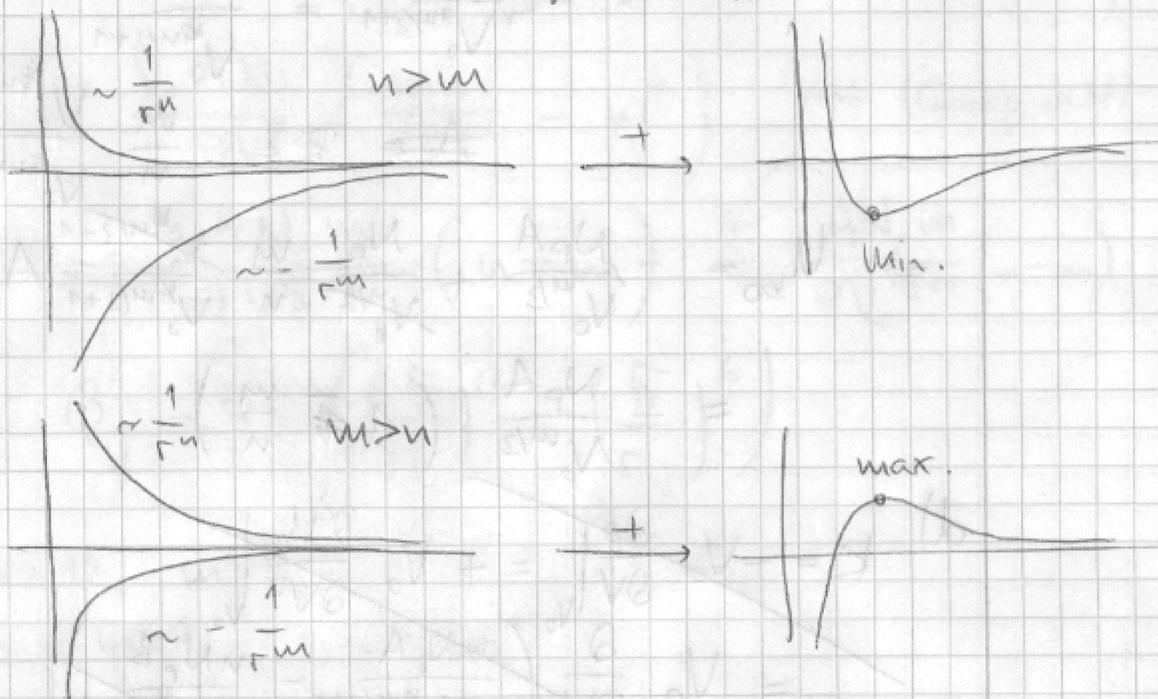
A1

B1

a) anziehend: - Van-der-Waals: Dipol-Dipol-WW (Fluktuationsbindung)
- Coulomb-WW (Ionenbindung)
- kovalente Bindung

abstoßend: - Auswirkung des Pauli-Prinzips (e^- müsste angeregt werden, kostet Energie → repulsive Kraft)

b)



c) $$\varphi_{ij} = -\frac{a}{r_{ij}^m} + \frac{b}{r_{ij}^n}$$

$$= -\frac{a}{p_{ij}^m r_0^m} + \frac{b}{p_{ij}^n r_0^n} \quad , \quad r_0^m = \left(r_0^3\right)^{m/3} = \left(\frac{V}{N}\right)^{m/3}$$

$$= -\frac{a}{p_{ij}^m}\left(\frac{V}{N}\right)^{-m/3} + \frac{b}{p_{ij}^n}\left(\frac{V}{N}\right)^{-n/3}$$

$$= -\frac{aN^{m/3}}{p_{ij}^m V^{m/3}} + \frac{bN^{n/3}}{p_{ij}^n V^{n/3}}$$

$$U_b \cancel{= \frac{1}{2}\sum_{j\neq i} \varphi_{ij}} = \frac{1}{2}\sum_{ij}\varphi_{ij}$$

$$= \frac{N}{2}\sum_{j\neq i}\varphi_{ij} = N_P \sum_{j\neq i} -\frac{aN^{m/3}}{p_{ij}^m V^{m/3}} + \frac{bN^{n/3}}{p_{ij}^n V^{n/3}}$$

mit $A = \sum_{j\neq i} \frac{aN^{m/3}}{p_{ij}^m}$, $B = \sum_{j\neq i}\frac{bN^{n/3}}{p_{ij}^n}$

$$\rightarrow U_b = -\frac{N_p A}{V^{m/3}} + \frac{N_p B}{V^{n/3}}$$

Gleichgewicht $\rightarrow \frac{\partial U_b}{\partial V}\Big|_{V_0} = 0$

$$\rightarrow \frac{\partial U_b}{\partial V}\Big|_{V_0} = \frac{m}{3}\frac{N_p A}{V_0^{m/3+1}} - \frac{n}{3}\frac{N_p B}{V_0^{n/3+1}} \overset{!}{=} 0$$

$$\frac{Am}{V_0^{m/3+1}} = \frac{Bn}{V_0^{n/3+1}}$$

$$B = \frac{m}{n}\frac{V_0^{n/3+1}}{V_0^{m/3+1}} A$$

$$\Rightarrow U_{b0} = -\frac{N_pA}{V_0^{m/3}} + \frac{N_p}{\cancel{V_0^{n/3}}}\frac{m}{n}\frac{\cancel{V_0^{n/3+1}}}{V_0^{m/3+1}}A$$

$$= -\frac{N_pA}{V_0^{m/3}}\left(1 - \frac{m}{n}\right)$$

d)

$$K = -V_0 \frac{\partial p}{\partial V}\Big|_{V_0} = +V_0 \frac{\partial^2 U_b}{\partial V^2}\Big|_{V_0}$$

$$= V_0 \frac{\partial}{\partial V}\left(\frac{mN_pA}{3V^{m/3+1}} - \frac{nN_pB}{3V^{n/3+1}}\right)\Big|_{V_0}$$

$$= V_0\left(-\left(\frac{m}{3}+1\right)\frac{mN_pA}{3V^{m/3+2}} + \left(\frac{n}{3}+1\right)\frac{nN_pB}{3V^{n/3+2}}\right)\Big|_{V_0}$$

$$= -\frac{m^2N_pA}{9V_0^{m/3+1}} + \frac{n^2N_pB}{9V_0^{n/3+1}} - \frac{mN_pA}{3V_0^{m/3+2}} + \frac{nN_pB}{3V_0^{n/3+2}}$$

$$= -\frac{1}{9}AN_p\left(\frac{m^2}{V_0^{m/3+1}} - \frac{n^2}{V_0^{n/3+1}}\frac{m}{n}\frac{V_0^{n/3+1}}{V_0^{m/3+1}}\right)$$

$$= -\frac{4}{9}AN_p\frac{1}{V_0^{m/3+1}}\left(m^2 - mn\right)$$

$$= -\frac{4AN_pm}{9V_0^{m/3+1}}\left(m - n\right)$$

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d) $k = -V_0 \frac{\partial p}{\partial V} = V_0 \frac{\partial^2 U_b}{\partial V^2}$

B1 $$= V_0 \frac{\partial}{\partial V}\left(\frac{mAN_p}{3V^{m/3+1}} - \frac{nBN_p}{3V^{n/3+1}}\right)$$

$$= V_0\left(-\left(\frac{m}{3}+1\right)\frac{mAN_p}{3V^{m/3+2}} + \left(\frac{n}{3}+1\right)\frac{nBN_p}{3V^{n/3+2}}\right)$$

$$= \frac{V_0AN_p}{3}\left(\left(\frac{n}{3}\cancel{+1}\right)\frac{\cancel{n}}{\cancel{V^{n/3+2}}}\cdot\frac{m}{\cancel{n}}\frac{\cancel{V^{n/3+2}}}{V^{m/3+2}} - \left(\frac{m}{3}\cancel{+1}\right)\frac{m}{V^{m/3+2}}\right)$$

$$= \frac{V_0AN_p}{9V^{m/3+2}}\left(\frac{mn}{1} - m^2\right)$$

$V=V_0$ (Gleichgewicht)

$$= \frac{V_0AN_pm}{9V^{m/3+2}}(n-m) = \frac{AN_pm}{9V_0^{m/3+1}}(n-m)$$

A2 $$\varphi_{ij} = 4\varepsilon\left(\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^6\right)$$

a) $n=12,\ m=6$

$a = 4\varepsilon\sigma^6,\quad b = 4\varepsilon\sigma^{12}$

$$U_{b0}\ \cancel{U_b|_{V_0}} = -\frac{\cancel{N_pA}}{\cancel{V_0^{m/3}}} + \frac{\cancel{N_p}A}{V_0^{m/3}}\cdot\frac{m}{n} = -\frac{\cancel{N_pA}}{\cancel{V_0^{m/3}}} + \frac{N_pB}{V_0^{n/3}} = U_b\big|_{V_0}$$

$$\Rightarrow \frac{Am}{nV_0^{m/3}} = +\frac{B}{V_0^{n/3}}$$

$$\rightarrow \frac{\cancel{6}A}{2\,\cancel{12}\,\cancel{V_0^2}} = \frac{B}{\cancel{V_0^4}V_0^2} \rightarrow V_0 = \sqrt{\frac{2B}{A}}$$

$$V_0 = Nr_0^3 = \sqrt{\frac{2\sum b\frac{N^{n/3}}{p_{ij}^n}}{\sum a\frac{N^{m/3}}{p_{ij}^m}}}$$

$$= \sqrt{\frac{2\cdot \cancel{4\varepsilon}\sigma^{\cancel{12}6} N^{\cancel{4}2}}{\cancel{4\varepsilon\sigma^6}\cancel{N^2}}}\cdot\sqrt{\frac{12{,}13}{14{,}45}} = \sqrt{\frac{2\cancel{\varepsilon}\sigma^6N^2}{14{,}45}\cdot 12{,}13}$$

$$\Rightarrow r_0^3 = \sqrt{\frac{2\cancel{8}\cdot 12{,}13}{14{,}45}}\, \sigma^3$$

$$\Rightarrow \sigma = \left(\frac{14{,}45}{2\cancel{8}\cdot 12{,}13}\right)^{1/6} \cdot r_0$$

	σ [nm]
Ne	0,287
Ar	0,344
Kr	0,369
Xe	0,399

b) $$K = \frac{V_0 A N_p m}{9V^{m/3+2}}(n-m)$$

$$= \frac{2V_0 A N_p \cdot \cancel{6}\,2}{\cancel{3}V^{m/3+2}} = \frac{4V_0 A N_p}{V_0^4}$$

$$= \frac{4AN_p}{V_0^3} = \frac{4N_p}{V_0^3}\sum a \frac{N^2}{p_{ij}^6}$$

$$= \frac{4N_p a N^2}{V_0^3}\cdot 14{,}45 = \frac{16\sigma^6 \varepsilon \overset{N/2}{N_p} N^2}{V_0^3}\cdot 14{,}45$$

$$= 8\sigma^6\varepsilon \frac{N^3}{V_0^3}\cdot 14{,}45$$

$$= 8\varepsilon\sigma^6 \frac{14{,}45}{r_0^9}$$

$$\Rightarrow \varepsilon = \frac{K r_0^9}{8\sigma^6\cdot 14{,}45} = 14{,}6\ \text{meV}$$

c) $$U_{B0} = -\frac{N_p A}{V_0^{m/3}}\left(1-\frac{m}{n}\right)$$

$$= -\frac{N_p A}{V_0^2}\left(1-\frac{1}{2}\right) = -\frac{N_p a N^2\cdot 14{,}45}{2V_0^2}$$

$$= -\frac{N_p}{2}\frac{4\varepsilon\sigma^6}{r_0^6}\cdot 14{,}45 = -28{,}9\, N_p\,\varepsilon\left(\frac{\sigma}{r_0}\right)^6$$

$$= -14{,}45\, N\,\varepsilon\left(\frac{\sigma}{r_0}\right)^6 = 11{,}14\ \frac{\text{kJ}}{\text{mol}}$$

$$\uparrow$$

$N = 1\,\text{mol} = N_A$

~~A3~~ zu A1 b)

~~d~~ a)

1d)

$$\varphi_{ij}(r) = -\frac{a}{r^m} + \frac{b}{r^n}$$

$$\frac{\partial \varphi_{ij}}{\partial r} = \frac{am}{r^{m+1}} - \frac{bn}{r^{n+1}} \overset{!}{=} 0 \rightarrow \tilde{r} = \left(\frac{nb}{am}\right)^{\frac{1}{n-m}}$$

B1

$$\frac{\partial^2 \varphi}{\partial r^2}(\tilde{r}) > 0 \Leftrightarrow nb(n+1)\left(\frac{am}{nb}\right)^{\frac{n+2}{n-m}} > am(m+1)\left(\frac{am}{nb}\right)^{\frac{m+2}{n-m}}$$

$$\Leftrightarrow \cancel{(nb)^{n-m}}(n+1)^{n-m}\cancel{(am)^{n+2}} > \cancel{(am)^{n-m}}(m+1)^{n-m}\cancel{(am)^{m+2}}\cancel{(nb)^{n-m}}$$

$$\Rightarrow n > m$$

A3

a) $$E_{Coulomb} = -\frac{\alpha_M Z_1 Z_2 e^2}{4\pi\varepsilon_0 r_0}\left(1 - \cancel{\frac{1}{n}}^{\,0}\right)$$

Ba^+O^-: $E = -5{,}21\,eV \cdot \alpha_M = -9{,}1\,eV$

$Ba^{2+}O^{2-}$: $E = -20{,}85\,eV \cdot \alpha_M = -36{,}4\,eV$

~~b) Gitterenergie~~

b) 1. Atome ionisieren
2. e^- hinzufügen } Energie bilanzieren

Ba^+O^-: $E^{+-} = (5{,}19 - 1{,}5)\,eV = 3{,}7\,eV$

$Ba^{2+}O^{2-}$: $E^{2+2-} = (5{,}19 + 9{,}96 - 1{,}5 + 9)\,eV = 22{,}7\,eV$

Gesamtbilanz: (3. zusammenbauen zum Molekül)

Ba^+O^-: $E_{ges}^{+-} = 3{,}7\,eV - 9{,}1\,eV = -5{,}4\,eV$

$Ba^{2+}O^{2-}$: $E_{ges}^{2+2-} = (22{,}7 - 36{,}4)\,eV = -13{,}7\,eV$ stabiler