Struktur und Simulation
Übung 02

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Aufgabe 1

$$p_i = \frac{1}{N} \qquad S = -k \sum_i^N p_i \log p_i$$

$$\begin{aligned} S &= -k \sum_i^N \frac{1}{N} \log \frac{1}{N} \\ &= -k \sum_i^N \frac{1}{N} (\log 1 - \log N) \\ &= -k \sum_i^N -\frac{\log N}{N} \\ &= -k \cdot N \cdot \frac{-\log N}{N} \\ &= k \log N \end{aligned}$$

Aufgabe 2

Die Entropie des Dimer-Systems ist gleich der doppelten Entropie des einzelnen Monomers, wenn keine Wechselwirkungen einberechnet werden.

0.1 Mono:

$T = 3K$:

state	E[kJ/mol]	$e^{-\frac{E}{RT}}$	p	$p \log p$
1	0	1.000000e+00	1.505166e-35	-1.206866e-33
2	-1	2.577554e+17	3.879647e-18	-1.555381e-16
3	-2	6.643785e+34	1.000000e+00	0.000000e+00
		Z= 6.643785e+34		S = 1.555381e-16

T = 300K :

state	E[kJ/mol]	$e^{-\frac{E}{RT}}$	p	$p \log p$
1	0	1.000000e+00	2.117404e-01	-3.287046e-01
2	-1	1.493180e+00	3.161664e-01	-3.640614e-01
3	-2	2.229586e+00	4.720932e-01	-3.543432e-01
		Z = 4.722765e+00		S = 1.047109e+00

T = 300000K :

state	E[kJ/mol]	$e^{-\frac{E}{RT}}$	p	$p \log p$
1	0	1.000000e+00	3.331997e-01	-3.661909e-01
2	-1	1.000401e+00	3.333333e-01	-3.662041e-01
3	-2	1.000802e+00	3.334670e-01	-3.662172e-01
		Z = 3.001203e+00		S = 1.098612e+00

0.2 Dimere:

0.2.1 Ohne Wechselwirkung:

T = 3K :

state	E[kJ/mol]	$e^{-\frac{E}{RT}}$	p	$p \log p$
(1,1)	0	1.000000e+00	2.265525e-70	-3.633067e-68
(1,2)	-1	2.577554e+17	5.839513e-53	-7.023320e-51
(1,3)	-2	6.643785e+34	1.505166e-35	-1.206866e-33
(2,1)	-1	2.577554e+17	5.839513e-53	-7.023320e-51
(2,2)	-2	6.643785e+34	1.505166e-35	-1.206866e-33
(2,3)	-3	1.712472e+52	3.879647e-18	-1.555381e-16
(3,1)	-2	6.643785e+34	1.505166e-35	-1.206866e-33
(3,2)	-3	1.712472e+52	3.879647e-18	-1.555381e-16
(3,3)	-4	4.413988e+69	1.000000e+00	0.000000e+00
		Z = 4.413988e+69		S = 3.110762e-16

T = 300K :

state	E[kJ/mol]	$e^{-\frac{E}{RT}}$	p	$p \log p$
(1,1)	0	1.000000e+00	4.483398e-02	-1.392000e-01
(1,2)	-1	1.493180e+00	6.694518e-02	-1.810118e-01
(1,3)	-2	2.229586e+00	9.996119e-02	-2.302080e-01
(2,1)	-1	1.493180e+00	6.694518e-02	-1.810118e-01
(2,2)	-2	2.229586e+00	9.996119e-02	-2.302080e-01
(2,3)	-3	3.329172e+00	1.492600e-01	-2.839023e-01
(3,1)	-2	2.229586e+00	9.996119e-02	-2.302080e-01
(3,2)	-3	3.329172e+00	1.492600e-01	-2.839023e-01
(3,3)	-4	4.971052e+00	2.228720e-01	-3.345660e-01
		Z = 2.230451e+01		S = 2.094218e+00

T = 300.000K :

state	E[kJ/mol]	$e^{-\frac{E}{RT}}$	p	$p \log p$
(1,1)	0	1.000000e+00	1.110220e-01	-2.440294e-01
(1,2)	-1	1.000401e+00	1.110666e-01	-2.440827e-01
(1,3)	-2	1.000802e+00	1.111111e-01	-2.441360e-01
(2,1)	-1	1.000401e+00	1.110666e-01	-2.440827e-01
(2,2)	-2	1.000802e+00	1.111111e-01	-2.441360e-01
(2,3)	-3	1.001203e+00	1.111557e-01	-2.441894e-01
(3,1)	-2	1.000802e+00	1.111111e-01	-2.441360e-01
(3,2)	-3	1.001203e+00	1.111557e-01	-2.441894e-01
(3,3)	-4	1.001605e+00	1.112002e-01	-2.442427e-01
		Z = 9.007220e+00		S = 2.197224e+00

0.2.2 mit Wechselwirkung:

$T = 3K$:

state	E[kJ/mol]	$e^{-\frac{E}{RT}}$	p	$p \log p$
(1,1)	-5	1.137729e+87	1.505166e-35	-1.206866e-33
(1,2)	-1	2.577554e+17	3.409991e-105	-8.202554e-103
(1,3)	0	0.000000e+00	1.322956e-122	-3.712685e-120
(2,1)	-1	2.577554e+17	3.409991e-105	-8.202554e-103
(2,2)	-7	7.558829e+121	1.000000e+00	0.000000e+00
(2,3)	0	0.000000e+00	1.322956e-122	-3.712685e-120
(3,1)	0	0.000000e+00	1.322956e-122	-3.712685e-120
(3,2)	0	0.000000e+00	1.322956e-122	-3.712685e-120
(3,3)	0	0.000000e+00	1.322956e-122	-3.712685e-120
		Z = 7.558829e+121		S = 1.206866e-33

$T = 300K$:

state	E[kJ/mol]	$e^{-\frac{E}{RT}}$	p	$p \log p$
(1,1)	-5	7.422674e+00	2.753368e-01	-3.551185e-01
(1,2)	-1	1.493180e+00	5.538804e-02	-1.602593e-01
(1,3)	0	0.000000e+00	3.709402e-02	-1.221988e-01
(2,1)	-1	1.493180e+00	5.538804e-02	-1.602593e-01
(2,2)	-7	1.654949e+01	6.138871e-01	-2.995427e-01
(2,3)	0	0.000000e+00	3.709402e-02	-1.221988e-01
(3,1)	0	0.000000e+00	3.709402e-02	-1.221988e-01
(3,2)	0	0.000000e+00	3.709402e-02	-1.221988e-01
(3,3)	0	0.000000e+00	3.709402e-02	-1.221988e-01
		Z = 2.695852e+01		S = 1.586174e+00

$T = 300.000K$:

state	E[kJ/mol]	$e^{-\frac{E}{RT}}$	p	$p \log p$
(1,1)	-5	1.002007e+00	2.501502e-01	-3.466316e-01
(1,2)	-1	1.000401e+00	2.497494e-01	-3.464767e-01
(1,3)	0	0.000000e+00	2.496493e-01	-3.464379e-01
(2,1)	-1	1.000401e+00	2.497494e-01	-3.464767e-01
(2,2)	-7	1.002810e+00	2.503509e-01	-3.467089e-01
(2,3)	0	0.000000e+00	2.496493e-01	-3.464379e-01
(3,1)	0	0.000000e+00	2.496493e-01	-3.464379e-01
(3,2)	0	0.000000e+00	2.496493e-01	-3.464379e-01
(3,3)	0	0.000000e+00	2.496493e-01	-3.464379e-01
		Z = 4.005619e+00		S = 3.118483e+00

Aufgabe 3

$$
\begin{aligned}
-kT \log Z &= G \\
&= U - TS \\
&= \sum_i p_i E_i - T \cdot -k \sum_i p_i \log p_i \\
&= \sum_i p_i E_i - T \cdot \left(-k \sum_i p_i \log \frac{e^{-E_i/kT}}{Z} \right) \\
&= \sum_i p_i E_i - T \cdot \left(-k \sum_i p_i \log e^{-E_i/kT} - p_i \log Z \right) \\
&= \sum_i p_i E_i - T \cdot \left(-k \sum_i p_i \left(\frac{E_i}{kT} \right) - p_i \log Z \right) \\
&= \sum_i p_i E_i - \sum_i p_i E_i + T \cdot \left(-k \sum_i p_i \log Z \right) \\
&= T \cdot \left(-k \sum_i p_i \log Z \right) \\
&= -kT \cdot \log Z
\end{aligned}
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