

$$1) C_V = T \left(\frac{\partial S}{\partial T} \right)_V \quad C_P = T \left(\frac{\partial S}{\partial T} \right)_P$$

$$= \left(\frac{\partial U}{\partial T} \right)_V \quad = \left(\frac{\partial H}{\partial T} \right)_P$$

$$\left(\frac{\partial C_V}{\partial T} \right)_P = \cancel{B} \left(T \frac{\partial S}{\partial T} \right)_P$$

$$\left(\frac{\partial S}{\partial V} \right)_T = - \left(\frac{\partial P}{\partial T} \right)_V$$

$$\left(\frac{\partial}{\partial V} \left(\frac{\partial S}{\partial T} \right)_V \right)_T = - \left(\frac{\partial^2 P}{\partial T^2} \right)_V$$

$$\left(\frac{\partial}{\partial V} \frac{C_V}{T} \right)_T = - \left(\frac{\partial^2 P}{\partial T^2} \right)_V$$

$$\left(\frac{\partial C_V}{\partial V} \right)_T = - T \left(\frac{\partial^2 P}{\partial T^2} \right)_V \quad P = \frac{NkT}{V} \stackrel{!}{=} - T \cdot (0) = 0$$

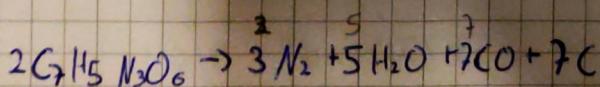
$$\left(\frac{\partial S}{\partial P} \right)_T = \left(\frac{\partial V}{\partial T} \right)_P$$

$$\left(\frac{\partial}{\partial P} \left(\frac{\partial S}{\partial T} \right)_P \right)_T = \left(\frac{\partial^2 V}{\partial T^2} \right)_P$$

$$\left(\frac{\partial}{\partial P} \frac{C_P}{T} \right)_T \cdot \left(\frac{\partial^2 V}{\partial T^2} \right)_P$$

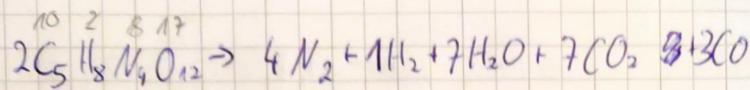
$$\left(\frac{\partial C_P}{\partial P} \right)_T = T \left(\frac{\partial^2 V}{\partial T^2} \right)_P = \frac{V \cdot NkT}{P} = T \cdot 0 = 0$$

2)



$$\begin{aligned} \Delta H &= -80.2 \rightarrow 30 \rightarrow 241.8 \rightarrow 1107 \rightarrow 216.7 \\ \text{kJ/mol} &\Rightarrow -160 \rightarrow 3037.9 - 1982.5 \Rightarrow \underline{\underline{\Delta H = -1822.5}} \end{aligned}$$

$$1 \text{L H}_2\text{O}(l) \Rightarrow \Delta H = \underline{\underline{-2042.5}}$$



$$-540.2 \rightarrow 0 \quad 0 \quad -7241.8 \rightarrow 3935 -110.5 \cdot 3$$

$$\Rightarrow \Delta H = -3698.6$$

$$H_2O(l) \quad \Delta H = -4006.6$$

In[14]:= mTNT := trinitrotoluene [molar mass]

$$\Delta H := -1822. \text{ kJ/mol} \quad \checkmark$$

UnitConvert [$\Delta H / mTNT * \text{kg}$, "kJ"]

Out[16]= -8021.77 kJ

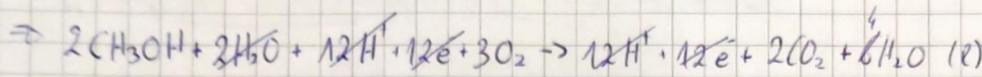
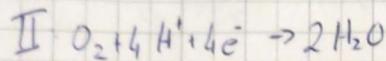
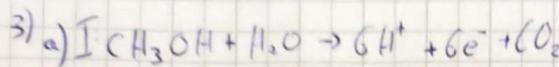
+ In[24]:= mNitro := barbitrate [molar mass]

$$\Delta H := -3698.6 \text{ kJ/mol} \quad \checkmark$$

UnitConvert [$\Delta H / mTNT * \text{kg}$, "kJ"]

Out[26]= -16283.9 kJ

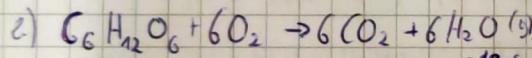
unit: kilograms



ΔH	-237.2	0	-393.5	-285.8	$\Rightarrow -1451.8 \frac{\text{kJ}}{\text{mol}}$
ΔS	209.2	205.2	213.8	70	$\approx -161.6 \frac{\text{J/K}}{\text{mol}}$
ΔG	-166.6	0	-394.4	-237.1	$\Rightarrow -1404 \frac{\text{kJ}}{\text{mol}}$

$$\varepsilon = \frac{\Delta G}{\Delta H} \approx 0.967 \dots$$

$$U = \underline{\Delta G}$$



ΔH	-1271	0	-293.5	-285.8 185.3	$\Rightarrow \Delta H = -2804.8 \frac{\text{kJ}}{\text{mol}}$ -293.5 -2551.6 $\frac{\text{kJ}}{\text{mol}}$
ΔS	209.2	205.3	213.8	70	$\Rightarrow \Delta S = -2724.8 \frac{\text{J/K}}{\text{mol}}$ 975.2 $\frac{\text{J/K}}{\text{mol}}$
ΔG	-910.56	0	-394.4	-237.1 285.6	$\Rightarrow \Delta G = -2878.44 \frac{\text{kJ}}{\text{mol}}$ -2829.6 $\frac{\text{kJ}}{\text{mol}}$

$$\Delta Q = \Delta H - \Delta G = \cancel{-277.04 \frac{\text{kJ}}{\text{mol}}} \quad \rightarrow \text{Wärme}$$

Freigesetzte, ΔQ wärmt Körper

```
In[35]:= mSugar :=  ChemicalFormula["C6H12O6"] ["MolarMass"] 
```

```
 $\Delta G :=$   -2829.  $\text{kJ/mol}$  
```

```
UnitConvert [ $\Delta G / \text{mSugar} * \text{100 g}$   ...,  , "kJ"]
```

```
Out[37]= -1570.31  $\text{kJ}$ 
```

$$4) H_{0,j} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j = -2J \sum_{\langle i,j \rangle} \sigma_i = -J \sum_i m_i$$

~~$$Z = \sum_{i=1}^N \exp(J \sum_{\langle i,j \rangle} \sigma_i \sigma_j) = \sum_{i=1}^N \exp(-J \sum_{\langle i,j \rangle} \sigma_i)$$~~

~~$$Z = \sum_{i=1}^N \exp(-\beta (-J \sum_{\langle i,j \rangle} \sigma_i)) = \sum_{i=1}^N \exp(\beta J \sum_{\langle i,j \rangle} \sigma_i)$$~~

$$Z = Z \sum_{\{M\}} \exp(-\beta (-J \sum_{\langle i,j \rangle} \sigma_i)) = Z \sum_{\{M\}} \exp(\beta J \sum_{i=1}^{N-1} m_i) =$$

$$= 2 \prod_{i=1}^{N-1} \sum_{M_i=1}^{\infty} \exp(\beta J M_i) = 2 \prod_{i=1}^{N-1} e^{-\beta J} + e^{\beta J} = 2(2 \cosh(\beta J))^{N-1}$$

$$b) \langle \sigma_i, \sigma_{i+j} \rangle = \frac{1}{2} \sum_{\Omega} \sigma_i \sigma_{i+j} e^{-\beta H} = \frac{1}{2} \sum_{\Omega_{i+1}} \dots \sum_{\Omega_{N-1}} \langle \sigma_i, \sigma_{i+j} \exp(\beta J_1 \sigma_{i+1} + \dots + J_{N-1} \sigma_{N-1} \sigma_N) \rangle$$

$$\begin{aligned} \sigma_i \sigma_{i+j} &= \sigma_i (\sigma_{i+1} \sigma_{i+1}) (\sigma_{i+2} \sigma_{i+2}) \dots \sigma_{i+j} \\ &= \underbrace{\sigma_i}_{m_i} \underbrace{(\sigma_{i+1} \sigma_{i+1})}_{m_{i+1}} \dots \underbrace{(\sigma_{i+j-1} \sigma_{i+j-1})}_{m_{i+j-1}} \end{aligned}$$

$$\Rightarrow \langle \sigma_i, \sigma_{i+j} \rangle = \frac{1}{2} (2 \cosh(\beta J_1) + 2 \sinh(\beta J_2) + \dots + 2 \sinh(\beta J_i) + \dots + 2 \cosh(\beta J_{N-1}))$$

~~$$= \frac{2(\cosh(\beta J_1) + \sinh(\beta J_2) + \dots + \tanh(\beta J_i) + \cosh(\beta J_{N-1}))}{\cosh(\beta J_1) + \cosh(\beta J_2)}$$~~

~~$$= \tanh(\beta J_2) \cdot \tanh(\beta J_3) \cdot \dots \cdot \tanh(\beta J_{N-1})$$~~

~~$$= \prod_{m=1}^{i-1} \tanh(\beta J_{i+m-1})$$~~

$$c) M = m N \sqrt{\lim_{j \rightarrow \infty} \langle \sigma_i \sigma_{i+j} \rangle} = m N \sqrt{\lim_{j \rightarrow \infty} (\tanh(\beta J))^j} \xrightarrow{=} 0$$

$$d) S = k_B \ln 2 + k_B T \frac{\partial \ln Z}{\partial T} = -k_B \beta F - k_B T \left(\frac{\partial \beta F}{\partial T} \right)_V = -k_B \beta F - k_B T \beta \frac{\partial F}{\partial T} - k_B T F \frac{\partial \beta}{\partial T} = \beta^2 \frac{\partial F}{\partial T} - k_B \beta^2 \frac{\partial F}{\partial \beta}$$

e)

$$S = k_B \ln z + k_B T \left(\frac{\partial \ln z}{\partial T} \right)_V$$

$$z = 2(2 \cosh(\beta J))^{N-1}$$

$$\frac{\partial \ln z}{\partial T} = -\frac{1}{2} N k_B (N-1) \tanh(J\beta)$$

$$-k_B \ln 2 e^{\beta J} + (N-1)k_B \ln(2 \cosh \beta J) + \beta J k_B (N-1) \tanh \beta J =$$

$$= k_B \ln 2 + k_B (N-1) (\ln(2 \cosh \beta J) + \beta J \tanh \beta J)$$

$$T \rightarrow 0 \quad S \rightarrow k_B \ln 2$$

Ohne Magnetfeld pendeln sich die Spins zufällig ein und frieren aus mit $M=0$. Mit Magnefelt richten sich die Spins vermehrt parallel aus, was zu $M \neq 0$ führt.

