1) $C_v = T\left(\frac{\partial S}{\partial T}\right)_V \qquad C_p = T\left(\frac{\partial S}{\partial T}\right)_p$

$= \left(\frac{\partial U}{\partial T}\right)_V \qquad = \left(\frac{\partial H}{\partial T}\right)_p$

$\cancel{\left(\frac{\partial C_p}{\partial p}\right)_T = \left(\frac{\partial \left(T\frac{\partial S}{\partial T}\right)_p}{\partial p}\right)_T}$

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

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

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

$\left(\frac{\partial C_v}{\partial V}\right)_T = -T\left(\frac{\partial^2 p}{\partial T^2}\right)_V \overset{p = \frac{NkT}{V}}{=} -T\cdot(0) = \underline{\underline{0}}$

$\left(\frac{\partial S}{\partial p}\right)_T = \left(\frac{\partial V}{\partial T}\right)_p$

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

$\left(\frac{\partial}{\partial p}\frac{C_p}{T}\right)_T = \left(\frac{\partial^2 V}{\partial T^2}\right)_p$

$\left(\frac{\partial C_p}{\partial p}\right)_T = T\left(\frac{\partial^2 V}{\partial T^2}\right)_p \overset{V = \frac{NkT}{p}}{=} T\cdot 0 = \underline{\underline{0}}$

2)

$2\,C_7H_5N_3O_6 \rightarrow 3\,N_2 + 5\,H_2O + 7\,CO + 7\,C$

$\frac{\Delta H}{kJ/mol}$ $\quad -80.2 \rightarrow 3\cdot 0 \quad 5\cdot(-241.8) \quad -110.7 + 7\cdot \cancel{716.7}\ 0$

$\Rightarrow -160 \rightarrow \cancel{3037.9} \quad -1982.5 \qquad \Rightarrow \underline{\underline{\Delta H = -1822.5}}$

~~Für~~ H_2O (l) $\Rightarrow \Delta H = \cancel{-2142}\ \underline{\underline{-2042.5}}$

10 2 8 17

$2C_5H_8N_4O_{12} \rightarrow 4N_2 + 1H_2 + 7H_2O + 7CO_2 + \cancel{8}\,3CO$

$-540.2 \rightarrow 0 \quad 0 \quad -7 \cdot 241.8 \quad -7 \cdot 393.5 \quad -110.5 \cdot 3$

$\Rightarrow \Delta H = -3698.6$

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

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

ΔH := -1822. kJ/mol

UnitConvert[ΔH / mTNT * kg, "kJ"]

Out[16]= -8021.77 kJ

In[24]:= mNitro := baritrate CHEMICAL [molar mass]

ΔH := -3698.6 kJ/mol

UnitConvert[ΔH / mTNT * kg, "kJ"]

unit: kilograms

Out[26]= -16 283.9 kJ

3) a) I $CH_3OH + H_2O \to 6H^+ + 6e^- + CO_2$

II $O_2 + 4H^+ + 4e^- \to 2H_2O$

$\Rightarrow 2CH_3OH + \cancel{2H_2O} + \cancel{12H^+} + \cancel{12e^-} + 3O_2 \to \cancel{12H^+} + \cancel{12e^-} + 2CO_2 + \overset{4}{\cancel{6}}H_2O\ (l)$

ΔH	-237.2	0	-393.5	-285.8	$\Rightarrow -1451.8\ \frac{kJ}{mol}$
ΔS	~~209.2~~ 126.8	205.2	213.8	70	$\Rightarrow -161.6\ \frac{J/K}{mol}$
ΔG	-166.6	0	-394.4	-237.1	$\Rightarrow -1404\ \frac{kJ}{mol}$

$\varepsilon = \frac{\Delta G}{\Delta H} \approx 0{,}967...$

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

b) $C_6H_{12}O_6 + 6O_2 \to 6CO_2 + 6H_2O\ (g)$

ΔH	-1271	0	-393.5	~~-285.8~~ 243.6	$\Rightarrow \Delta H = \cancel{-2804.8\ \frac{kJ}{mol}}$ ~~2355~~ $-2551.6\ \frac{kJ}{mol}$
ΔS	209.2	205.2	213.8	~~70~~ 188.8	$\Rightarrow \Delta S = \cancel{-2724.8\ \frac{J/K}{mol}}$ $975.2\ \frac{J/K}{mol}$
ΔG	-910.56	0	-394.4	~~-237.1~~ 228.8	$\Rightarrow \Delta G = \cancel{-2878.44\ \frac{kJ}{mol}}$ $-2828.6\ \frac{kJ}{mol}$

$\Delta Q = \Delta H - \Delta G = \cancel{267}\ \underline{\underline{277.04}}\ \frac{kJ}{mol}$ ⇒ ~~Wärme~~

Freigesetztes ΔQ wärmt Körper

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

ΔG := -2829. kJ/mol

UnitConvert[ΔG / mSugar * 100 g , "kJ"]

Out[37]= -1570.31 kJ
```

a) $H_{0,J} = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j = \cancel{-2J\sum_{\sigma=\pm1}\sigma_i} = -J\sum_i \mu_i$

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

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

$Z = 2\sum_{\{\mu\}}\exp(-\beta(-J\sum_{\langle i,j\rangle}\sigma_i\sigma_j)) = 2\sum_{\{\mu\}}\exp(\beta J\sum_{i=1}^{N-1}\mu_i) =$

$= 2\prod_{i=1}^{N-1}\sum_{\mu=\pm1}\exp(\beta J\mu) = 2\prod_{i=1}^{N-1} e^{\beta J}+e^{-\beta J} = \underline{\underline{2(2\cosh(\beta J))^{N-1}}}$

b) $\langle\sigma_i\sigma_{i+j}\rangle = \frac{1}{Z}\sum_{\Omega}\sigma_i\sigma_{i+j}e^{-\beta H} = \frac{1}{Z}\sum_{\sigma_1=\pm1}\cdots\sum_{\sigma_N=\pm1}\sigma_i\sigma_{i+j}\exp(\beta J_1\sigma_1\sigma_2+\ldots+J_{N-1}\sigma_{N-1}\sigma_N)$

$\sigma_i\sigma_{i+j} = \sigma_i(\sigma_{i+1}\sigma_{i+1})(\sigma_{i+2}\sigma_{i+2})\cdots\sigma_{i+j}$

$= \underbrace{(\sigma_i\sigma_{i+1})}_{\mu_i}\underbrace{(\sigma_{i+1}\sigma_{i+2})}_{\mu_{i+1}}\cdots\underbrace{(\sigma_{i+j-1}\sigma_{i+j})}_{\mu_{i+j-1}}$

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

$= \cancel{\frac{2(\cosh\beta J_1+\sinh\beta J_2+\ldots+\sinh\beta J_j+2\cosh\beta J_{N-1})}{2\cosh(\beta J_1+\cosh(\beta J_2)}}$

$= \tanh(\beta J_2)\cdot\tanh(\beta J_3)\cdot\ldots\cdot\tanh(\beta J_{N-2})$

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

c) $M = mN\sqrt{\lim_{j\to\infty}\langle\sigma_i\sigma_{i+1}\rangle} = mN\sqrt{\lim_{j\to\infty}(\tanh(\beta J))^j} \to \underline{\underline{0}}$

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

e)

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

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

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

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

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

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

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!=0 führt.