IQF - Trabalho Prático I

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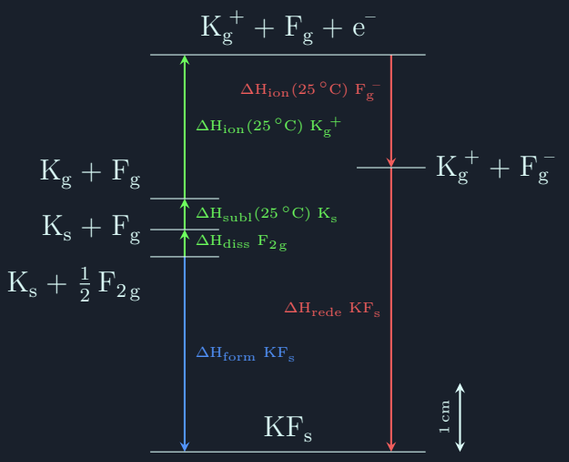
Contents

Question 3 Ciclo Born-Haber KP

Name	Mole	Energy $\mathrm{kJ\,mol^{-1}}$	Scale: $5 * 10^{-3}\,\mathrm{cm/kJ}$ Length (cm)
$\Delta H_{\mathrm{diss}}\ F_{2\,g}$	1/2	+158	0.790
$\Delta H_{\mathrm{subl}}(25\,^\circ\mathrm{C})\ K_s$	1	+90	0.450
$\Delta H_{\mathrm{ion}}(25\,^\circ\mathrm{C})\ K_g^+$	1	+418	2.090
$\Delta H_{\mathrm{ion}}(25\,^\circ\mathrm{C})\ F_g^-$	1	−328	−1.640
$\Delta H_{\mathrm{rede}}\ KF_s$	1	−826	−4.130
$\Delta H_{\mathrm{form}}\ KF_s$	1	−567	−2.835



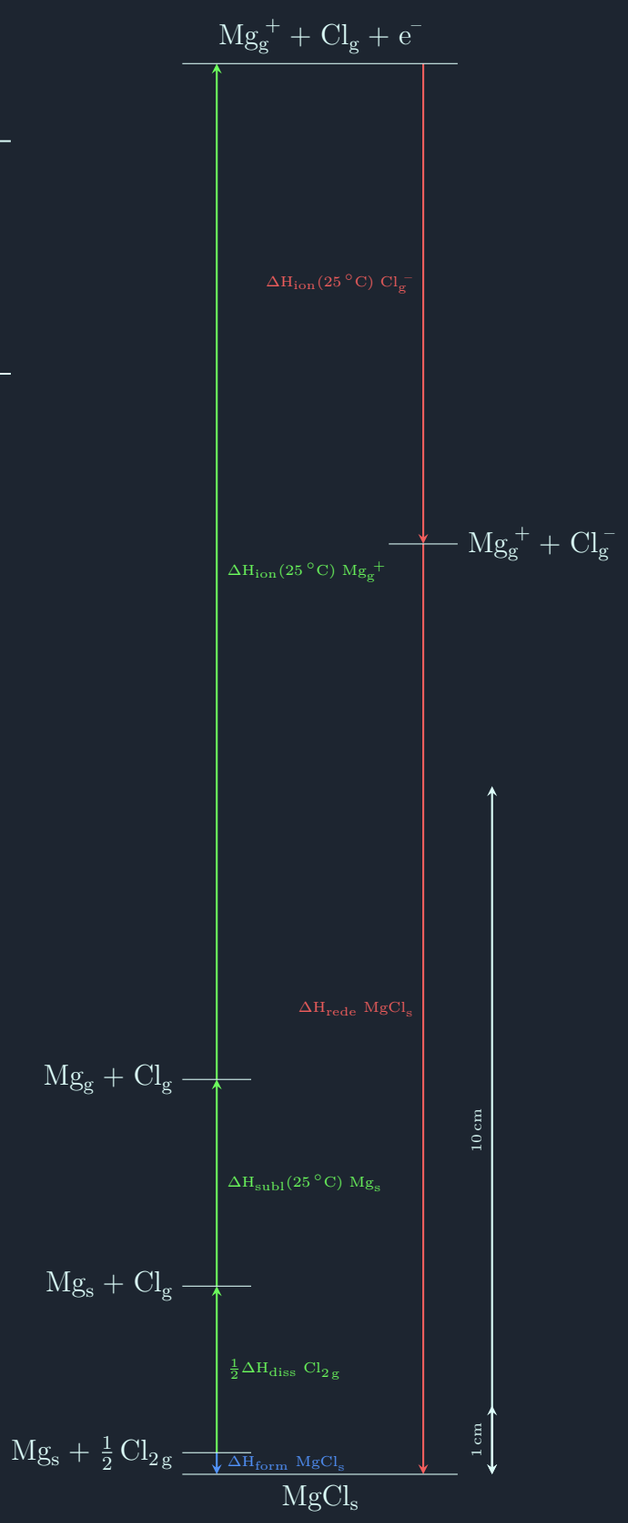
$$KF_s \longleftarrow K_g^+ + F_g^- \longleftarrow K_g^+ + F_g + e^- \longleftarrow K_g + F_g \longleftarrow K_s + F_g \longleftarrow K_s + \tfrac{1}{2} F_{2\,g}$$

Question 4 Ciclo Born-Haber MgCl e $MgCl_2$

(i) MgCl

Name	Mole	Energy $\mathrm{kJ\,mol^{-1}}$	Scale: $2 * 10^{-2}\,\mathrm{cm/kJ}$ Length (cm)
$\Delta H_{\mathrm{diss}}\ Cl_{2\,g}$	1/2	+242.0	2.420
$\Delta H_{\mathrm{subl}}(25\,^{\circ}C)\ Mg_s$	1	+150.2	3.004
$\Delta H_{\mathrm{ion}}(25\,^{\circ}C)\ Mg_g^+$	1	+738.1	14.762
$\Delta H_{\mathrm{ion}}(25\,^{\circ}C)\ Cl_g^-$	1	−349.0	−6.980
$\Delta H_{\mathrm{rede}}\ MgCl_s$	1	−676.0	−13.520
$\Delta H_{\mathrm{form}}\ MgCl_s$	1	−15.7	−0.314

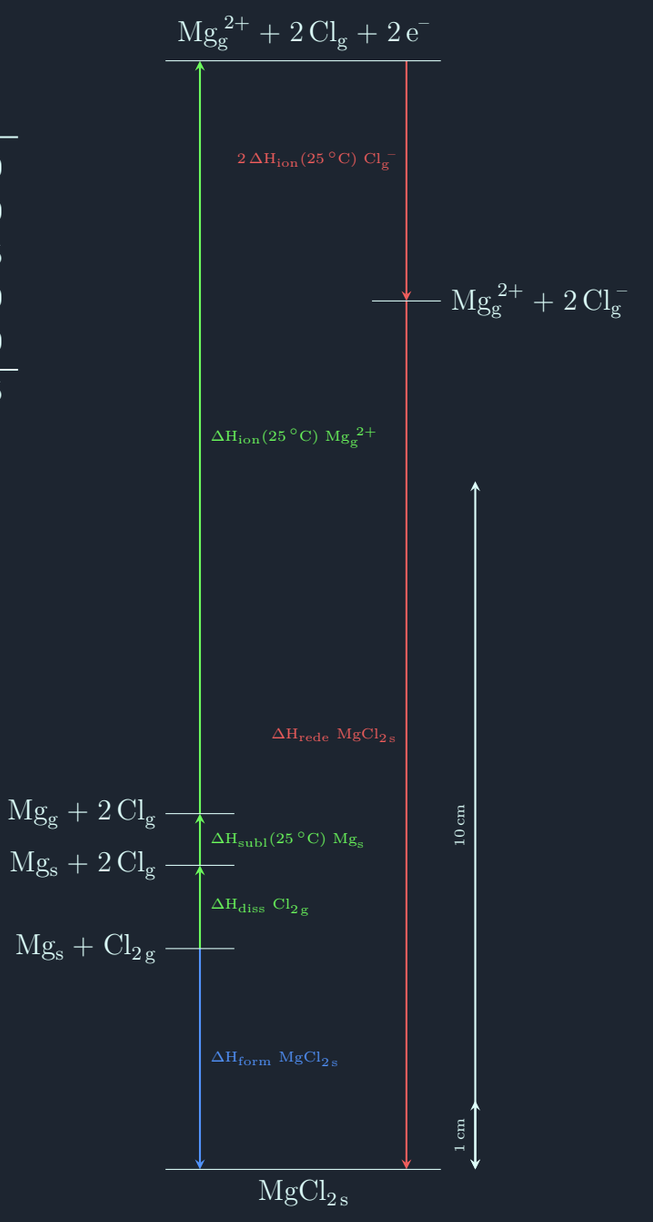
$$
\begin{aligned}
MgCl_s &\longleftarrow Mg_g^+ + Cl_g^- \longleftarrow \\
Mg_g^+ + Cl_g + e^- &\longleftarrow Mg_g + Cl_g \longleftarrow \\
Mg_s + Cl_g &\longleftarrow Mg_s + \tfrac{1}{2}\,Cl_{2\,g}
\end{aligned}
$$



(ii) $MgCl_2$

Name	Mole	Energy $kJ\,mol^{-1}$	Scale: $5 * 10^{-3}$ cm/kJ Length (cm)
$\Delta H_{diss}\ Cl_{2\,g}$	1	+242.0	1.2100
$\Delta H_{subl}(25\,°C)\ Mg_s$	1	+150.2	0.7510
$\Delta H_{ion}(25\,°C)\ Mg_g^{2+}$	1	+2188.1	10.9405
$\Delta H_{ion}(25\,°C)\ Cl_g^-$	2	−349.0	−3.4900
$\Delta H_{rede}\ MgCl_{2s}$	1	−2524.0	−12.6200
$\Delta H_{form}\ MgCl_{2s}$	1	−641.7	−3.2085

$$MgCl_{2\,s} \longleftarrow Mg_g^{2+} + 2\,Cl_g^- \longleftarrow$$
$$Mg_g^{2+} + 2\,Cl_g + 2\,e^- \longleftarrow Mg_g + 2\,Cl_g \longleftarrow$$
$$Mg_s + 2\,Cl_g \longleftarrow Mg_s + Cl_{2\,g}$$



Question 6

Compound	Entropy J/K mol
$Mg\,(s)$	32.68
$Cl_2\,(g)$	223.07
$MgCl_2\,(s)$	89.62
$K\,(s)$	64.18
$F_2\,(g)$	202.78
$KF\,(s)$	66.57

Table 1: Entropy table

Reaction	Δ S	Δ G (298.15 K)
$Mg\,(s) + Cl_2\,(g) \longrightarrow MgCl_2\,(s)$	-0.16613	-592.170
$Mg\,(s) + \frac{1}{2}\,Cl_2\,(g) \longrightarrow MgCl\,(s)$	-0.05459	0.577
$K\,(s) + \frac{1}{2}\,F_2\,(g) \longrightarrow KF\,(s)$	-0.09900	-537.483

We can now use the our calculated properties of the formation enthalpies of both $MgCl_2$ and MgCl to calculate the Gibbs free energy of both systems. We found properties of the entropies, please note here that we use the entropy of $MgCl_2$ for the entropy of MgCl as well, since we do not have the entropy of MgCl because it does not exist naturally. By calculating Gibbs free energy of both systems we can see that the Gibbs Free Energy for the formation of $MgCl_2$ is a negative value which means that the formation of $MgCl_2$ occurs spontaneously while the Gibbs Free Energy for the formation of MgCl is positive, which means that it does not occur's spontaneously.