```
(*  Isothermen . Beispiel fuer H2O . nach Kripfganz/Perlt,
   zur Physik siehe Landau,Achieser,Lifschitz S.172 *)

In[1]:= kb = UnitConvert[Quantity["BoltzmannConstant"]]
        nA = UnitConvert[Quantity["AvogadroConstant"]]
        RGsi = kb nA
        UnitConvert[Quantity["MolarGasConstant"]]
        (*  Konversion von  kg m^2/s^2  in atm  geht mit:
        9.86923 10^-3 , damit erhaelt man RG in atm l^3/(K mol) *)
        RG = RGsi[[1]] * 9.86923 * 10^-3
        ct = 273.15 (* Verschiebung Kelvin in Celsius *)
```

Out[1]= $1.38065 \times 10^{-23}\ \mathrm{kg\,m^2/(s^2 K)}$

Out[2]= 6.022141×10^{23} reciprocal moles

Out[3]= $8.3145\ \mathrm{kg\,m^2/(s^2 K\,mol)}$

Out[4]= $8.3145\ \mathrm{kg\,m^2/(s^2 K\,mol)}$

Out[5]= 0.0820573

Out[6]= 273.15

```
In[7]:= (* Van der Waals Gas, Zustandsgleichung *)
        Clear[p, a, b, V, T]

In[8]:= p[a_, b_, V_, T_] := RG (T + ct) / (V - b) - a / V^2

        (*  Fuer H2O Gas: a = 5.58 atm l^2 mol^-2
                          b = 0.031 l mol^-1 und V>b ist vorausgesetzt *)

        (* Umstellen der Gleichung zeigt fuer V eine Gl.3.Grades *)

        Expand[p[a, b, V, T] * (V - b) * V^2 - RG (T + ct) * V^2 + a * (V - b)]
```

$-a\,b + a\,V - ct\,RG\,V^2 - RG\,T\,V^2 - b\,V^2\,p[a, b, V, T] + V^3\,p[a, b, V, T]$

```
        (*  Eine oder drei Loesungen sind reell, die Stelle am
         Uebergang ist der kritische Wert. *)

In[9]:= (* Suche kritische Temperatur *)
        dpv = D[p[a, b, V, T], V]
        dpVV = D[p[a, b, V, T], {V, 2}] // Chop
```

Out[9]= $\frac{2\,a}{V^3} - \frac{0.0820573\,(273.15 + T)}{(-b + V)^2}$

Out[10]= $-\frac{6\,a}{V^4} + \frac{0.164115\,(273.15 + T)}{(-b + V)^3}$

```
In[11]:= eq = Eliminate[{dpv == 0, dpVV == 0}, T] // FullSimplify
```

Out[11]= $V \neq 0\ \&\&\ 1.\,b^3 + 3.\,b\,V^2 \neq 3.\,b^2\,V + 1.\,V^3\ \&\&$
$a\left(1.\,b^3 - 2.33333\,b^2\,V + 1.66667\,b\,V^2 - 0.333333\,V^3\right) == 0\ \&\&$
$a\left(1.\,b^4 - 3.33333\,b^3\,V + 4.\,b^2\,V^2 - 2.\,b\,V^3 + 0.333333\,V^4\right) == 0\ \&\&$
$a\left(1.\,b^2 - 1.33333\,b\,V + 0.333333\,V^2\right) == 0$

In[13]:=
```
Solve[eq[[5]], V]
```

Out[13]= $\{\{V \to 1.\, b\}, \{V \to 3.\, b\}\}$

```
Solve[eq[[4]], V] // Chop // FullSimplify (*  very crazy ... *)

Solve[eq[[3]], V] // Chop // FullSimplify (* etwas crazy ... *)
```

$$\Big\{\{V \to 0\},\ \Big\{V \to 1.66667\, b + (0.333333 - 0.57735\, i)\left(-b^3\right)^{1/3} - \frac{(0.333333 + 0.57735\, i)\left(-b^3\right)^{2/3}}{b}\Big\},\ \Big\{V \to 1.66667\, b + (0.333333 + 0.57735\, i)\left(-b^3\right)^{1/3} - \frac{(0.333333 - 0.57735\, i)\left(-b^3\right)^{2/3}}{b}\Big\}\Big\}$$

```
(*  verwende V = 3 b  aus der 1.Zeile weiter,
da V>b ist, berechne kritische Temperatur: *)
```

In[14]:=
```
loesKrit = Solve[(dpv /. V → 3. b) == 0, T]
```

Out[14]= $\left\{\left\{T \to -48.7464\left(-\frac{0.0740741\, a}{b^3} + \frac{5.60349}{b^2}\right) b^2\right\}\right\}$

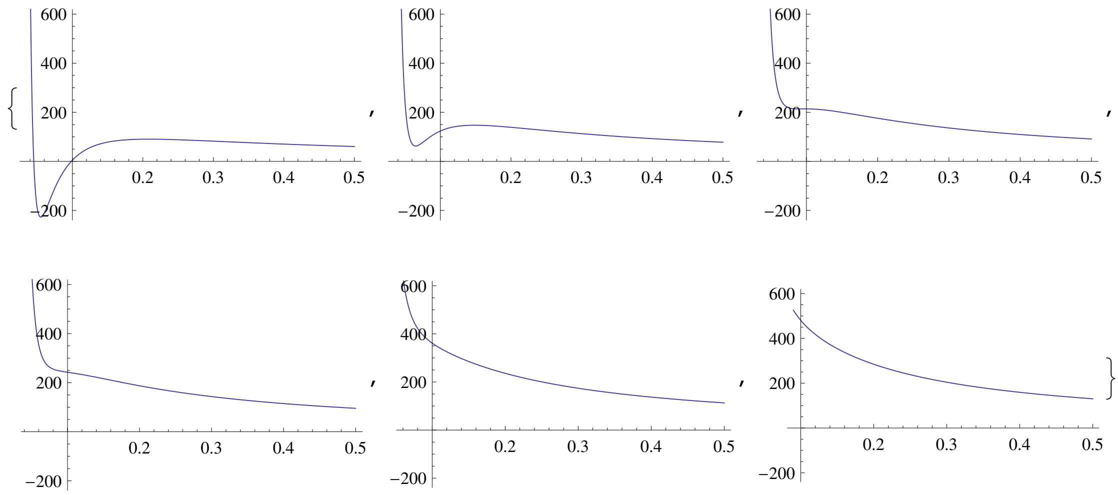
```
Tkrit = loesKrit[[1, 1]] /. {a → 5.58, b → 0.031}
```

$T \to 376.802$

Dann ist entsprechend V_krit → 0.093 und p_krit → 218.5

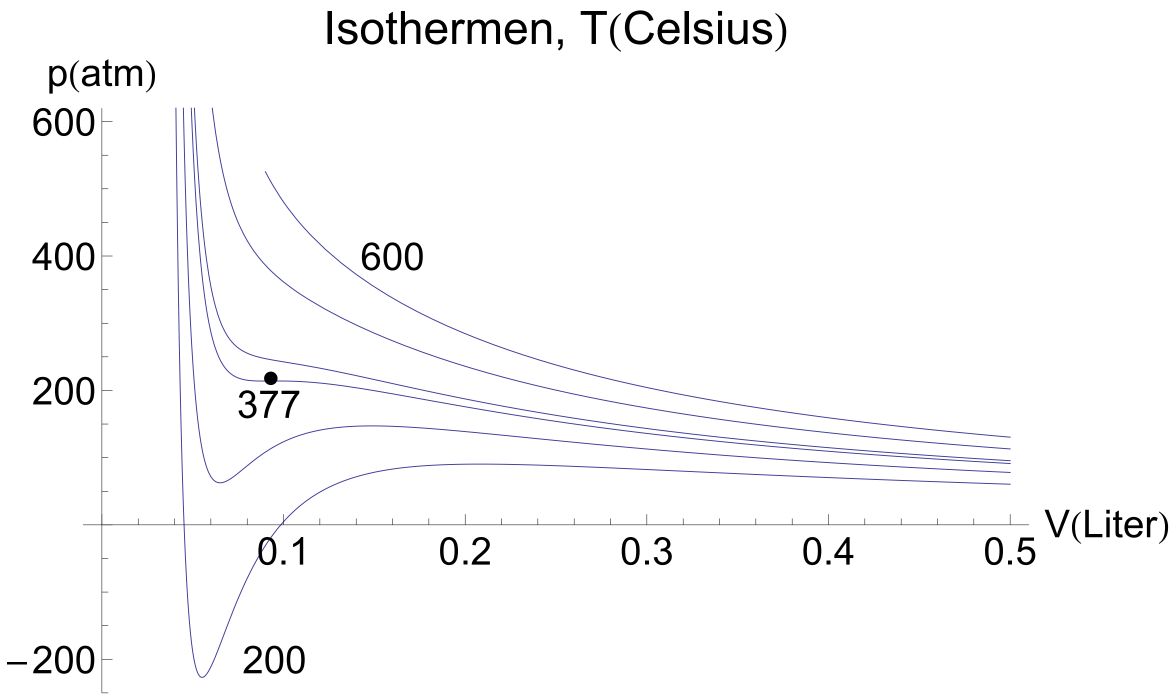
In[16]:=
```
a = 5.58;  b = 0.031;
```

```
(* Erstelle Diagramm *)
temps = {200, 300, 376, 400, 500, 600};
volStart = {0.035, 0.036, 0.04, 0.045, 0.06, 0.09};
Table[pp[i] = Plot[ p[a, b, V, temps[[i]] ],
   {V, volStart[[i]], 0.5}, PlotRange → {-240, 620}], {i, 1, 6}]
```




```
poi = Graphics[{PointSize[Large], Point[{0.093, 218}]}];
```

```
Show[pp[1], pp[2], pp[3], pp[4], pp[5], pp[6], poi,
 PlotRange → {-250, 620}, AxesLabel → {"V(Liter)", "p(atm)"}, AxesOrigin → {0, 0},
 PlotLabel → "Isothermen, T(Celsius)", Epilog → {Text["200", {0.095, -200}],
   Text["600", {0.16, 400}], Text["377", {0.092, 180}] },
 FormatType → TraditionalForm, TextStyle → {FontFamily → "Arial", FontSize → 20}]
```

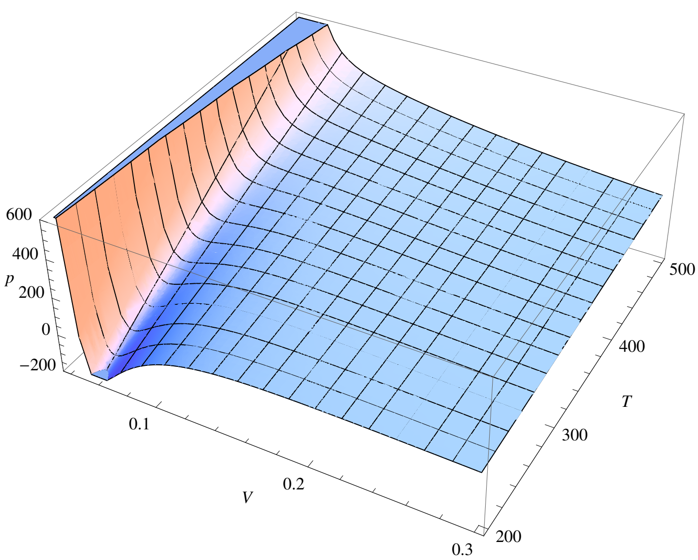



```
(* Globales Bild *)
```

In[17]:=

```
Plot3D[ p[a, b, V, T], {V, 0.04, 0.3}, {T, 200, 500},
 PlotRange → {-200, 600}, AxesLabel → {V, T, p}, PlotPoints → 50]
```

Out[17]=




```
conts = {-100, 0, 100, 150, 200, 218.5, 250, 300, 400};
```

```
ContourPlot[p[a, b, V, T], {V, 0.05, 0.38}, {T, 200, 475}, Contours → conts,
 FrameLabel → {"Volumen", "Temperatur"}, ContourLabels → True]
```