

```

A=1.176
~pst
~c
!
! 1. Výpočet rovnovážného složení z K =====
! CH4 + NH3 --> HCN + 3 H2
K=0.1703
p=80e3 ! [Pa]
pst=101325 ! [Pa]
! CH4 + NH3 --> HCN + 3 H2
! =====
! látka zač. rovn.
! -----
! CH4 1 1-x
! NH3 1 1-x
! HCN 0 x
! H2 0 3x
! -----
! plyny 2 2+2x (=ng)
! =====
def ng=2+2*x
def aCH4=(1-x)/ng*p/pst
def aNH3=(1-x)/ng*p/pst
def aHCN=x/ng*p/pst
def aH2=3*x/ng*p/pst
solve x=0,1 aH2^3*aHCN/aCH4/aNH3-K
xHCN=x/ng
undef ng
undef aH2; undef aCH4; undef aNH3; undef aHCN
!
! 2. Směr reakce =====
! C6H5.CH3 + 3 H2 --> C6H11.CH3
T=520
K=0.644
DrGo=-R*T*ln K
xtol=0.25
xmch=0.45
xH2=0.25
xin=1-(xtol+xmch+xH2) ! inerty (CH4)
pst=101.325
! a) -----
p=1013.25
atol=xtol*(p/pst)*0.945
1.176 amch=xmch*(p/pst)*0.927
1.176 aH2=xH2*(p/pst)
DrG=DrGo+R*T*ln(amch/atol/aH2^3)
! b) -----
p=pst
atol=xtol*(p/pst)
amch=xmch*(p/pst)
aH2=xH2*(p/pst)
DrG=DrGo+R*T*ln(amch/atol/aH2^3)
! c) -----
! =====
! látka začátek rovnováha
! -----
! toluen xtol xtol-x
! H2 xH2 xH2-3*x ! xmax=xH2/3=0.05
! mch xmch xmch+x ! xmin=-xmch=-0.45
! inert xin xin
! -----
! celkem 1 1-3*x
! =====
!
! zde p/pst=1
def atol=(xtol-x)/(1-3*x)*(p/pst)
def amch=(xmch+x)/(1-3*x)*(p/pst)
def aH2=(xH2-3*x)/(1-3*x)*(p/pst)
!
solve x=-.45,.05 amch/atol/aH2^3-K
(xtol-x)/(1-3*x)
(xmch+x)/(1-3*x)
(xH2-3*x)/(1-3*x)
xin/(1-3*x)
!
! 3. Bilance, dvě reakce =====
! =====
! látka začátek 1.krok 2.krok
! -----
! Pb(OH)2 c0 c0-x c0-x
! PbOH+ 0 x x-y
! OH- 0 x x+y
! Pb++ 0 0 y
! =====
!
! (x+y)*(x-y)/(c0-x)=K1
! (x+y)*y/(x-y)=K2
!
c0=6e-3/M(Pb0)
0.1703 101.33 -7524.1 101.33 0.25 0.45 0.25 22425
0.40925 f = 0 0.1452 -0.35103 f = -1.1 · 10-16
0.29274 0.048203 0.6347 0.024353
2.6882 · 10-05

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K1=8.7e-4
K2=1.51e-8
y=0
x=sqrt((K1/2)↑2+K1*c0+y↑2)-K1/2
pHI=14+log (x+y)
y=(x-y)*K2/(x+y)
x=sqrt((K1/2)↑2+K1*c0+y↑2)-K1/2
y=(x-y)*K2/(x+y)
x=sqrt((K1/2)↑2+K1*c0+y↑2)-K1/2
pHII=14+log (x+y)
pHII-pHI
!
! 4. Simultánní reakce =====
! C6H5.CH3 + C2H4 -> o-C2H5-C6H4-CH3 (K1)
! C6H5.CH3 + C2H4 -> p-C2H5-C6H4-CH3 (K2)
! =====
! látka      zač.  rovn.
! -----
! C6H5.CH3  1      1-x1-x2
! C2H4       1      1-x1-x2
! o-isom    0      x1
! p-isom    0      x2
! -----
! celk.pl.  2      2-x1-x2
! =====
!
pst=101.325
p=202.65
K1=1.2
K2=1.7
!
! rov. 1: x1/(2-x1-x2)*(p/pst)/((1-x1-x2)/(2-x1-x2)
) *(p/pst))↑2==K1
! rov. 2: x2/(2-x1-x2)*(p/pst)/((1-x1-x2)/(2-x1-x2)
) *(p/pst))↑2==K2
! rovnice sečteme a označíme x=x1+x2:
solve x=0,1 x/(2-x)*(p/pst)/((1-x)/(2-x)*(p/pst))↑2
-(K1+K2)
! rovnice podělíme ==> x1:x2=K1:K2
x1=x*K1/K2/(1+K1/K2)
x2=x-x1
x2/x1-K2/K1 ! test

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! b) -----
x=0.75
0.75
solve p=200 x/(2-x)*(p/pst)/((1-x)/(2-x)*(p/pst))↑2
-(K1+K2)
524.09
!
! 5. pH a disociace vody =====
! a) -----
! =====
! ion dis.HCl dis.vody
! -----
! H+      c      c+x
! Cl-     c      c
! OH-     0      x
! =====
Kv=1e-14
c=1e-7
solve x=1e-7 (c+x)*x-Kv ! numericky
pH=-log (c+x)
! přesně analyticky (kvadratická rovnice):
pH=-log(√(c↑2/4+Kv)+c/2)
!
! b) -----
! AnH+ --> An + H+ (Kk) rozsah=x (x<0)
! H2O --> H+ + OH- (Kv) rozsah=y
Kk=2.6e-5
! =====
! látka  zač.  rovn.
! -----
! AnH+   0      -x
! An     c      c+x
! H+     0      x+y = z (je malé - num. stabilita)
! OH-    0      y (=z-x)
! =====
! rov.1: (c+x)*z/(-x)=Kk
! rov.2: (z-x)*z=Kv ==> x=z-Kv/z
def x=z-Kv/z
c=1e-4
solve z=0,1e-7 (c+x)*z+x*Kk
pH=-log z
undef x

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