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A=1.176 ! [dm3/2 mol-1/2]
1.176
!
! 1. (8.37) Střední aktivitní koef. z E článku ===
! P: Cl2 + 2 e- -> 2 Cl- (redukce)
! EP= E.Cl -R*T/2/F*ln(aCl-↑2/(p/pst))
! L: Fe -> Fe3+ + 3e- (ox)
! EL=-E.Fe -R*T/3/F*ln(aFe3+)
! E=EL+EP
! p/pst=1
! E = E.Cl-E.Fe -R*T/3/F*ln(aCl-↑3*aFe3+)
! = E.Cl-E.Fe -R*T/3/F*ln(gamma↑4*27*mm↑4)
T=298.15 ! [K]
298.15
c=0.01 ! [mol dm-3]
0.01
solve gamma=0,1 1.36+0.036-R*T/3/F*ln(gamma↑4*27*c
↑4)-1.5515
0.46859 f = -2.2 · 10-16
gamma=(exp((1.36+0.036-1.5515)*3*F/R/T)/27)↑0.25/c
0.46859
!
! 2. pH a Debye-Hückel =====
I=0.03+0.001 ! [mol dm-3]
0.031
gamma=exp(-A*√I/(1+√I))
0.83857
pH=-log(0.001*gamma)
3.0765
gamma=exp(-A*√I) ! limitní
0.81297
pH=-log(0.001*gamma)
3.0899
gamma=1 ! ideální
1
pH=-log(0.001*gamma)
3
!
! 3. Součin rozpustnosti =====
! Mg(OH)2 --> Mg++ + 2 OH-
m=11.5e-3 ! [g]
0.0115
c=m/M(MgO2H2) ! [mol dm-3]
0.00019719
I=1/2*(2↑2*c+1↑2*(2*c)) ! =3c
0.00059157
! Debye-Hückel:
gammaaa=exp(-1*2*A*√I/(1+√I))
0.94568
Ks=c*(2*c)↑2*gammaaa↑3
2.5939 · 10-11
gamma=exp(-1↑2*A*√I/(1+√I))
0.97246
aOH=2*c*gamma
0.00038352
aH=1e-14/aOH
2.6074 · 10-11
pH=-log aH
10.584
! limitní Debye-Hückel:
gammaaa=exp(-1*2*A*√I)
0.9444
Ks=c*(2*c)↑2*gammaaa↑3
2.5833 · 10-11
gamma=exp(-1↑2*A*√I)
0.9718
aOH=2*c*gamma
0.00038326
aH=1e-14/aOH
2.6092 · 10-11
pH=-log aH
10.583
! ideální:
Ks=c*(2*c)↑2
3.067 · 10-11
aOH=2*c
0.00039438
aH=1e-14/aOH
2.5356 · 10-11
pH=-log aH
10.596
!
! 4. m-0/2 s Debyem-Hückelem =====
! R: E=0.3338 V
! L: 0.5 H2 -> H+ + e-
T=298.15 ! [K]
298.15
p=119.4 ! [kPa]
119.4
~pst ! (zruš konstantu pst)
pst=101.3 ! [kPa]
101.3
c=0.015 ! [mol dm-3]
0.015
! E=0.3338 - R*T/F*ln(aH/(p/pst)↑0.5) = 0.449
aH=exp((0.3338-0.449)*F/R/T)*(p/pst)↑0.5
0.012258
pH=-log aH
1.9116
gamma=1 ! 1.iterace
1
cH=aH/gamma ! zde Ic=cH
0.012258
gamma=exp(-A*√cH/(1+√cH)) ! 2.iterace
0.88939
cH=aH/gamma
0.013782
gamma=exp(-A*√cH/(1+√cH)) ! 3.iterace
0.88377
cH=aH/gamma
0.01387
gamma=exp(-A*√cH/(1+√cH)) ! 4.iterace
0.88346
cH=aH/gamma
0.013875
Kdis=aH↑2/(c-cH) ! (špatně podmíněné: c-cH << c)
0.13354

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!
! 5. Výpočet koncentrace z pH =====
Kd=1e-14/2.28e-11
pH=11.8
a=1e-14/10↑-pH ! aktivita OH
!
! ideálně:
gamma=1
c=a/gamma
c0=a↑2/Kd+a/gamma ! [mol dm-3]
! limitní Debye-Hückel (1. iterace)
gamma=exp(-A*√c)
c=a/gamma
c0=a↑2/Kd+a/gamma
!
! limitní Debye-Hückel (2. iterace)
gamma=exp(-A*√c)
c=a/gamma
c0=a↑2/Kd+a/gamma
!
! limitní Debye-Hückel (3. iterace)
gamma=exp(-A*√c)
c=a/gamma
c0=a↑2/Kd+a/gamma
!
! 6. Neideální roztok =====
mm=6 ! [mol kg-1]
nsach=mm ! [mol] v 1 kg
nvoda=1000/M(H2O) ! [mol]
xvoda=nvoda/(nvoda+nsach)
p=516 ! [Pa]
ps=611 ! [Pa]
gammavoda=p/(xvoda*ps)
!
!
!
!
! 7. Regulární roztok =====
b=0.42
ps1=42.4 ! všechny tlaky v [kPa]
ps2=26.4
x1=0.2
x2=1-x1
gamma1=exp(b*x2↑2)
gamma2=exp(b*x1↑2)
p1=ps1*x1*gamma1
p2=ps2*x2*gamma2
p=p1+p2
y1=p1/(p1+p2)
! azeotrop:
x2a=(ln(ps2/ps1)/b+1)/2
!
! 8. Slivovice =====
! 15 hm. proc.
! C6H12O6 -> 2 C2H5OH + 2 CO2
n1=2*15/M(C6H12O6) ! [mol]
n2=85/M(H2O) ! [mol]
n=n1+n2 ! [mol]
x1=n1/n; x2=n2/n ! složení kvasu
! kontrola -- objemová proc. alkoholu v kvasu
rho=M(C2H5OH)/58.1 ! [g cm-3]
X=x1*M(C2H5OH)/rho/(x1*M(C2H5OH)+x2*M(H2O))
X*100 ! [%]
!
T=89.5+273.15
!
! *** a) Raoult
A1=10.23347; B1=1591.28; C1=-47.055
A2=10.19621; B2=1730.63; C2=-39.724

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