H2+M=H+H+M 4.577E+19 -1.40 1.0438E+05

H2/2.5/ H2O/12/

function [fwdk,revk]=getkfkr5(P,T,X)

%reaction number

I=5;

RU=83145100; %erg/(mol\*K)

[A,B,E]=getabe; %-units of E are cal/mol , 1 calorie = 41 840 000 erg

%-units of A are cgs (cm, sec, K, mole), the exact units

% depending on the reaction.

[nuf,nur]=getnu;

kf=A(I)\*T^B(I)\*exp(-E(I)\*41840000/(RU\*T));

%molar concentration c=X\*P/(RU\*T)

findnuf=find(nuf(:,I));

fwdk=kf;

for i=1:length(findnuf)

fwdk=fwdk\*(X(findnuf(i))\*P/(RU\*T))^(nuf(findnuf(i),I));

end

%Kp(T)=exp{-[sum i=1:N of (vi''-vi')\*mu0,i(T)]/(RU\*T)}

g=getg(T);

Kp=exp( -dot(nur(:,I)-nuf(:,I),g) / (RU\*T) );

%kf/kb=Kc=Kp/(RU\*T)^[sum i=1:N of vi'' - vi']

Kc=Kp/(RU\*T)^sum(nur(:,I)-nuf(:,I));

kb=kf/Kc;

%molar concentration c=X\*P/(RU\*T)

findnur=find(nur(:,I));

revk=kb;

for i=1:length(findnur)

revk=revk\*(X(findnur(i))\*P/(RU\*T))^(nur(findnur(i),I));

end

%third body efficiences

%H2/2.5/ H2O/12/

a=ones(9,1);a(1)=2.5;a(3)=12;

c=X\*P/(RU\*T);

fwdk=fwdk\*dot(a,c);

revk=revk\*dot(a,c);

end



function [fwdk,revk]=getkfkr5b(P,T,X)

%reaction number

I=5;

RU=83145100; %erg/(mol\*K)

[A,B,E]=getabe; %-units of E are cal/mol , 1 calorie = 41 840 000 erg

%-units of A are cgs (cm, sec, K, mole), the exact units

% depending on the reaction.

[nuf,nur]=getnu;

kf=exp(log(A(I))+B(I)\*log(T)-E(I)\*41840000/(RU\*T));

%molar concentration c=X\*P/(RU\*T)

findnuf=find(nuf(:,I));

fwdk=kf;

for i=1:length(findnuf)

fwdk=fwdk\*(X(findnuf(i))\*P/(RU\*T))^(nuf(findnuf(i),I));

end

EG=exp(getsmh(T));

RU=8.31451D7;

PATM=1.01325D6;

PFAC1 = PATM / (RU\*T);

EQK=EG(4)\*EG(4)/EG(1)\*PFAC1;

small=1e-200;

kb=kf/max(EQK,small);

%molar concentration c=X\*P/(RU\*T)

findnur=find(nur(:,I));

revk=kb;

for i=1:length(findnur)

revk=revk\*(X(findnur(i))\*P/(RU\*T))^(nur(findnur(i),I));

end

%third body efficiences

%H2/2.5/ H2O/12/

a=ones(9,1);a(1)=2.5;a(3)=12;

c=X\*P/(RU\*T);

fwdk=fwdk\*dot(a,c);

revk=revk\*dot(a,c);

end

