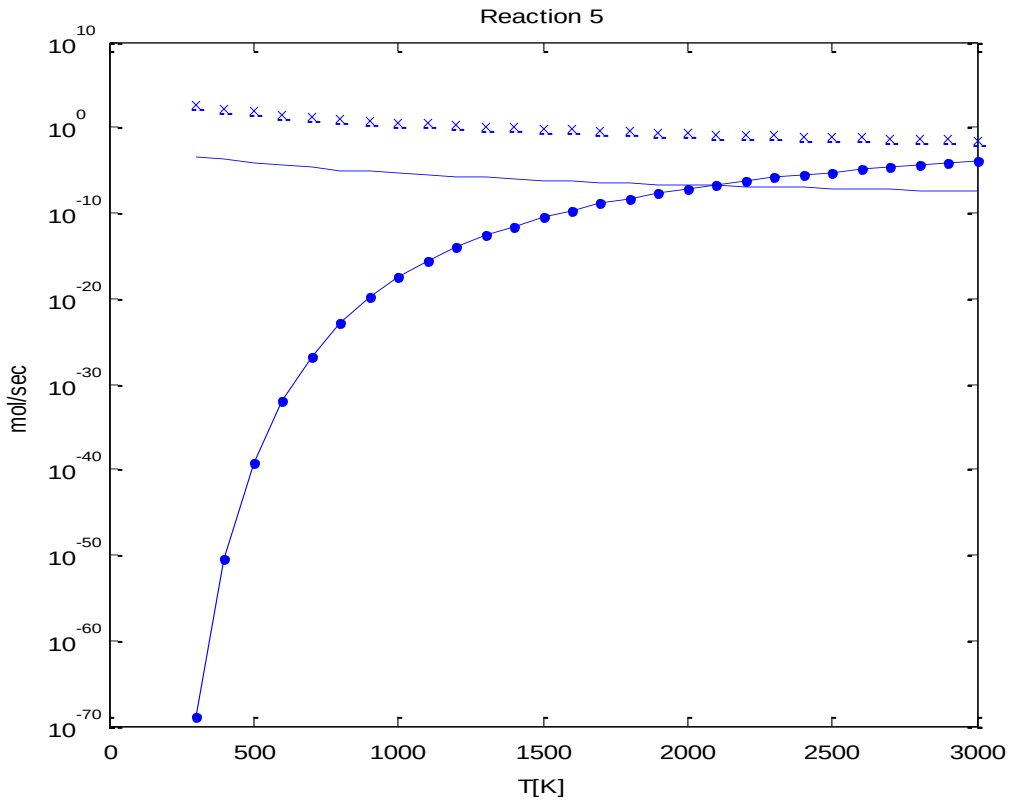
```
H2+M=H+H+M                4.577E+19 -1.40  1.0438E+05
   H2/2.5/ H2O/12/
```

$$K_p(T) = \exp\left\{-\frac{\left[\sum_{i=1}^{N}(v_i'' - v_i')\bar{\mu}_i^0(T)\right]}{R^0 T}\right\}$$

$$K_c(T) = K_p(T) \,/\, (R^0 T)^{\sum_{i=1}^{N}(v_i'' - v_i')}$$

$$\frac{k_f}{k_b} = K_c$$

```
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
```