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! ===== rotace CO =====
Mred=1/(1/M(O)+1/M(C))
6.8605251
mred=Mred*1e-3/NA ! [kg]
1.1392168 · 10-26
l=0.1128e-9
1.128 · 10-10
I=mred*l2
1.4495212 · 10-46
def Erot=h2/8/pi2/I*J*(J+1)
def g=2*J+1
T=300
300
! semiklasická partiční funkce
qclass=8*pi2*I*k*T/h/h
107.97107
! kvantová partiční funkce
q=sum J=0,10000 g*exp(-Erot/k/T)
108.30502
plot J=0,50,1 g*exp(-Erot/k/T)/q
! +++ tepelna kapacita kvantove a klasicky
T0=100
100
d=1e-4
0.0001
T=T0+d
100.0001
q=sum J=0,10000 g*exp(-Erot/k/T)
36.325587
Ep=sum J=0,10000 g*Erot*exp(-Erot/k/T)/q
1.3678406 · 10-21
T=T0-d
99.9999
q=sum J=0,10000 g*exp(-Erot/k/T)
36.325515
Em=sum J=0,10000 g*Erot*exp(-Erot/k/T)/q
1.3678379 · 10-21
Crot_q=(Ep-Em)/2/d
1.3806746 · 10-23
Crot_clas=k
1.3806504 · 10-23
Crot_q/Crot_clas
1.0000175

! ===== rotace acetylenu =====
CC=120.3e-12
1.203 · 10-10
CH=106e-12
1.06 · 10-10
mC=12e-3/NA
1.9926465 · 10-26
mH=1.008e-3/NA
1.6738231 · 10-27
I=2*((CC/2)2*mC+(CC/2+CH)2*mH)
2.3660333 · 10-46
B=hbar2/(2*I*h*c)
118.31088
Throt=h*B*c/k
1.7022275
def Erot=h2/8/pi2/I*J*(J+1)
def g=(2*J+1)*(1+4*frac(J/2))
T=300
300
qclass=8*pi2*I*k*T/h/h*2+2/3
353.14599
q=sum J=0,10000 g*exp(-Erot/k/T)
353.14675
plot J=0,25,1 g*exp(-Erot/k/T)/q

! ===== tepelna kapacita CO2 =====
def x=exp(-E/k/T)
def Cvibx=1/T2*E2/k*x/(1-x)2
! nejpomalejší vibrace -----
E=667e2*h*c ! [J]
1.3249591 · 10-20
plot T=50,2000 Cvibx/k
T=500 ! [K]
500
E=2349e2*h*c ! [J]
4.6661605 · 10-20
Cvib=Cvibx ! [JK-1 mol-1]
7.3341283 · 10-25
E=1320e2*h*c
2.6221081 · 10-20
Cvib=Cvib+Cvibx
5.4037905 · 10-24
E=667e2*h*c
1.3249591 · 10-20
Cvib=Cvib+2*Cvibx
2.5899405 · 10-23
! translace 3/2*R, rotace R, Mayer R
Cpm=Cvib*NA+3/2*R+R+R
44.697641

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