Gannon Short

CHEM E 457

CHEM E 457 Project

Problem 1

Part A.

CO2 + 3H2 ⇆ CH3OH + H2O (Reaction 1)

To determine the dissociation energy of a molecule we add up the energy of each of its bonds from Table 2 (D0 at 298K, units are kJ/mol):

CO2 : C + O → CO D0 = 1076.5

CO + O → CO2 D0 = 532.2

Sum the above +\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

C + 2O → CO2 D0,CO2 = 1608.7

H2 : H + H → H2 D0,H2 = 436.0

CH3OH : C + H → CH D0 = 339.0

CH + H → CH2 D0 = 421.7

CH2 + H → CH3 D0 = 473.0

O + H → OH D0 = 428.0

CH3 + OH → CH3OH D0 = 377.0

Sum the above +\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

C + 4H + O → CH3OH D0,CH3OH = 2038.7

H2O : O + H → OH D0 = 428.0

OH + H → H2O D0 = 498.7

Sum the above +\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

O + 2H → H2O D0,H2O = 926.7

ΔDrxn1 = Dprod  – Dreact = D0,CH3OH + D0,H2O – D0,CO2 – 3 × D0,H2

ΔDrxn1 = 2038.7 + 926.7 – 1608.7 – 3 × 436.0 = 48.7 kJ/mol

Part B.

Section I.

Generally: (Eqn 1)

Have CO2 (A), H2 (B), CH3OH (C), H2O (D),

so, a = 1, b = 3, c = 1, d = 1

Now: (Eqn 2)

We now have to find *q0* for each component:

(Eqn 3)

Translational partition function:

(Eqn 4)

where h = 6.63e-34 J·s

k = 1.38e-23 J/K

m = (Mass of molecule in kg)

T = (Temperature in K)

Returns in units of m-3

Rotational partition function:

We have some components that have linear rotation and we have some components that have nonlinear rotation, so there must be separate functions in the code for both. CO2 and H2 rotate linearly. CH3OH and H2O rotate nonlinearly.

Linear: (Eqn 5)

Nonlinear: (Eqn 6)

where h = 6.63e-34 J·s

k = 1.38e-23 J/K

I = (Moment of inertia. Approximately 1D for linear rotation and 3D for nonlinear rotation. Given in Table 1.)

σ = (Symmetry factor. Given in Table 1.)

T = (Temperature in K)

Returns as a unitless number

Vibrational partition function:

We are given θvibration for all components, so we can use the following equation to find *qvibrational* :

(Eqn 7)

where = (Vibrational temperature in K. Given in Table 1)

T = (Temperature in K)

Returns as a unitless number

Electric partition function:

θelectronic is large and T is relatively small for all components, so .

for all of our components (Table 1), so,

(Eqn 8)

We can now substitute Equations 4, 5, 6, 7, and 8 into Equation 3 to get *q0* for each component. Then we can solve Equation 2. For this equation we want to use k with different units than above so that the final units of Kp are atm-2.

(Eqn 2)

where k = 1.36267e-28 m3 atm K-1

R = 0.00184 kJ/mol

ΔDrxn1 = 48.7 kJ/mol

T = (Temperature in K)

Section II.

Plot of Kp for T varying from 50 to 1500 degrees Celsius is attached (Figure 1).

Section III.

The van’t Hoff relation is:

(Eqn 9)

Solving for :

(Eqn 10)

where R = 0.00184 kJ/mol

Attached (Figure 2) is a plot of . The slope of figure 2 is . Two points were chosen near the center of the figure.

Section IV.

from heats of formation () is equal to the heats of formation of the products minus the heats of formation of the reactants:

ΔHrxn1 = ΔHprod  – ΔHreact = ΔH0,CH3OH + ΔH0,H2O – ΔH0,CO2 – 3 × ΔH0,H2

Heats of formation are given in Table 1

ΔH0,CH3OH = –201.0 kJ/mol

ΔH0,H2O = –241.8 kJ/mol

ΔH0,CO2 = –393.5 kJ/mol

ΔH0,H2 = 0 kJ/mol

ΔHrxn1 = (–201.0) + (–241.8) – (–393.5) = –49.3 kJ/mol

**Comment on differences**

Part C.

CO2 + H2 ⇆ CO + H2O (Reaction 2)

Section I.

To determine dissociation energy, we once again add up the energy of each of the bonds in the molecule. We already have D0,CO2, D0,H2, and D0,H2O from part A:

D0,CO2 = 1608.7, D0,H2 = 436.0, D0,H2O = 926.7

D0,CO is provided in Table 2:

CO: C + O → CO D0,CO = 1076.5

ΔDrxn2 = Dprod  – Dreact = D0,CO + D0,H2O – D0,CO2 – D0,H2

ΔDrxn2 = 1076.5 + 926.7 – 1608.7 – 436.0 = –41.5 kJ/mol

Section II.

Using the same procedure as part B, section I:

(Eqn 10)

The properties of

Part D.

Section I.