Lecture 31 Wed 16 April

31.0 Finish First law part 1 exercises

Correction on Problem 1.2:

there is no temperature or mole count listed, so if we used isothermal compression we can’t compute work. ..so the assumption must be that it is a constant P process (see problem 19.2)

1. How much work gets done ? (make sure to indicate + or -)

PΔV = 10 bar\*(1-10) = 90 \*100 joules =9000 J (recall 1 bar \* 1 dm3 = 100 J)

35.2. Review enthalpy idea

H=E+PV is a state function=> at constant P, ΔHp =Qp…can measure reaction heats at constant P and be assured that it is independent of how reaction run.

35.3. Exercise 2…warm up by predicting reaction heats

2.2 Given the data in the table provided, use Hess’ Law to ΔrHo for:

ΔrHo

1. OH(g) 🡪H(g) + O(g) **428.2 kJ**
2. H2O(g) 🡪 2H(g) + O(g) **926.98**
3. H2O(g)🡪 H(g) + OH(g) **498.76**

Final answers

reaction known ΔrHo

½ H2(g) + ½ O2(g) 🡪 OH(g) 38.95 kJ/mol  
 H2(g) + ½ O2(g) 🡪 H2O(g) -241.814 kJ/mol

H2(g) 🡪2 H(g) +435.994 kJ/mol

O2(g) 🡪 2O(g) +498.34 kJ/mol

(see also problems 19.35-19.36 pp 804-5)

b) H2O(g)🡪H2(g) + ½ O2(g) +241.814

H2(g) 🡪2 H(g) 435.994

½ O2(g) 🡪 O(g) ½ (498.34)

**H2O(g) 🡪 2H(g) + O(g) 926.98**

1. OH(g) 🡪½ H2(g) + ½ O2(g) -38.95

½ H2(g) 🡪 H(g) ½ (435.994)

½ O2(g) 🡪 O(g) ½( 498.34)

½ H2(g) + ½ O2(g) 🡪 OH(g) **+428.2 kJ**

c)H2O(g)🡪H2(g) + ½ O2(g) +241.814

½ H2(g) + ½ O2(g) 🡪 OH(g) 38.95

½ H2 (g)🡪 H(g) ½ (435.994)

1. **H2O(g)🡪 H(g) + OH(g) 498.76**

35.3. Graphical rationale for bond energies

**Example: finding ε(O-H)**

2H + O

½ O2🡪 O 249.17

2ε(O-H) H2🡪 2H (2\*217.9)

H2 + ½ O2 element reference line

+241.8 kJ/mol ΔHf =-241.8 kJ/mol H2 + ½O2🡪 H2O

H-O-H

H2O(g)

∴2ε(O-H) = 241.8 + 2\*217.9 + 249.17 = 926.77

ε(O-H) = ½ (926.77) = 463.4 vs. 459.8 obs.

**Example: finding ε(H-Cl)**

H + Cl

½ Cl2🡪 Cl 121.02

½ H2🡪H 217.9 kJ ε(H-Cl) = 92.3 + 217.9 + 121.02 = 431.22 vs 430.9 obs

½ H2 + ½ Cl2

-ΔHf = 92.3 kJ/mol

HCl \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

H

Can figure out bond energies given a basis set and compound ΔHf

Can figure out ΔH(T) given Cp

**35.4 Computing ΔH(T ≠25 C) ….powerpoint**

0 T2

* ΔH(T) = ∫Cp dT for 0🡪T2 =H(T) –H(o) no phase change

Standard state case is that T2 = 298, 1 atm

* If there is a phase transition, heat comes out or goes in at constant T

ΔH(T) = ∫Cp dT + ΔHtransition  + ∫Cp’ dT …

* Finish part 2 exercises with Cp