Help: *R* = 8.314 J mol1 K1; *NA* = 6.022x1023; *h* = 6.626x1034 J sec; c=2.998x108 m/sec;

*e* = 1.602x1019 C; *R*H = 3.290x1015 sec1; *m*p/*m*e = 1836; 1 kcal = 4.184 kJ.

One Dobson Unit is equivalent to 2.687×1016 moleculecm2.

For light of wavelength 1240 nm, the photon energy is 1.00 eV.

Heat capacity: water 1 cal/g∙K, ice 0.5 cal/g∙K; enthalpy of melting of ice = 80 cal/g, enthalpy of evaporation of water = 540 cal/g.

For phase change and chemical reaction, you may assume Ho and So do not depend on T.

**(8)** For 3H2 + N2 ⇌ 2NH3(g) at 298 K,

**(8a)** Find the fHo and So the related species from https://webbook.nist.gov/chemistry/ and calculate the reaction free energy at the standard state. Note: conventionally, the energy is per mol of consumed N2.

**(8b)** If *P*H2 = 30 bar; *P*N2 = 10 bar, estimate *P*NH3 at room temperature.

**(8c)** If *P*H2 = 30 bar; *P*N2 = 10 bar, estimate *P*NH3 at 1000 K.

**(9)** For N2O4(g) ⇌ 2NO2(g),

**(9a)** if *P*total = *P*N2O4 + *P*NO2 = 0.01 bar, what is the ratio of *P*NO2/*P*N2O4? If one hope to have *P*N2O4/*P*NO2 = 103, what *P*total is required?

**(10)** For NH4Cl(s) ⇌ NH3(g) + HCl(g) at 298 K,

**(10a)** Find the values of fHo and So for the related species from https://webbook.nist.gov/chemistry/.

**(10b)** Estimate GoRXN and Keq.

**(10c)** Estimate the equilibrium pressure of NH3(g) if one starts from NH4Cl(s).

-----The above are due May 7th-----------------------------

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**(11)** Estimate the de Broglie wavelength for the following objects. You may use the typical or averaged value if necessary.

**(11a)** A dust particle (assume 1 mg) at 1 m/s speed.

**(11b)** A He atom at 300 K.

**(11c)** An electron of 1 eV energy.

**(11d)** A potassium atom at 1 K (micro Kelvin).

**(12)** For particle-in-a-box system, if the mass is 1 amu (same as that of H atom) and the box size is 1 Å.

**(12a)** Deduce the translational energy of the ground state. (convert your answer to both units of eV and cm1)

**(12b)** Deduce the energy gap between the ground state and the first excited state. (convert your answer to both units of eV and cm1)

**(12c)** Plot the probability densities of the ground state and the second excited state. Remember to show the correct units for the x-axis and y-axis labels.

**(12d)** Estimate the probabilities of finding the particle near the center of the box within ± 0.01 Å (i.e., 0.49 L – 0.51 L) for the ground state and the second excited state. (error < 5%)

**(13a)** Analyze the IR absorption spectrum of HCl(g) (as below. From Wikimedia Commons) and obtain the rotational constants (*B’* and *B”*) and vibrational frequency (**0-1) of HCl molecule. Compare your results with those from the literature.



**(13b)** Using the value of *B”*, estimate the bond length of HCl and compare your answer with that from literature.

**(14a)** Why N2 and O2 have no IR absorption?

**(14b)** Which vibrational modes of CO2 are IR active? Which is IR inactive?

**(15a)** List the disadvantages of aluminum alloy.

**(15b)** What is Anodized Aluminum Oxide? Where can you see it?

**(16)** Glycine is an amino acid which has both acidic functional group (COOH) and basic functional group (NH2).

**(16a)** Find the values of *K*a1 and *K*a2. (from Wiki or …)

**(16b)** Plot the concentration profiles of the related species, [NH3+CH2COOH], [NH2CH2COOH], and [NH2CH2COO], for the system of 0.1 M glycine aqueous solution as a function of pH.

Note: An amino acid changes its charged state (+1, neutral, or -1) depending on the pH value. This property plays a very important role in biology and bioanalysis.

**(17)** Draw the schematic structures of PE, PP, PS, PVC, and Teflon.

**(18a)** Most pure metals are quite reactive towards oxygen. What are the exceptions?

**(18b)** Why it is not often to see a piece of metal burns?

-----The above are due May 21st-----------------------------