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.

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.

**(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.

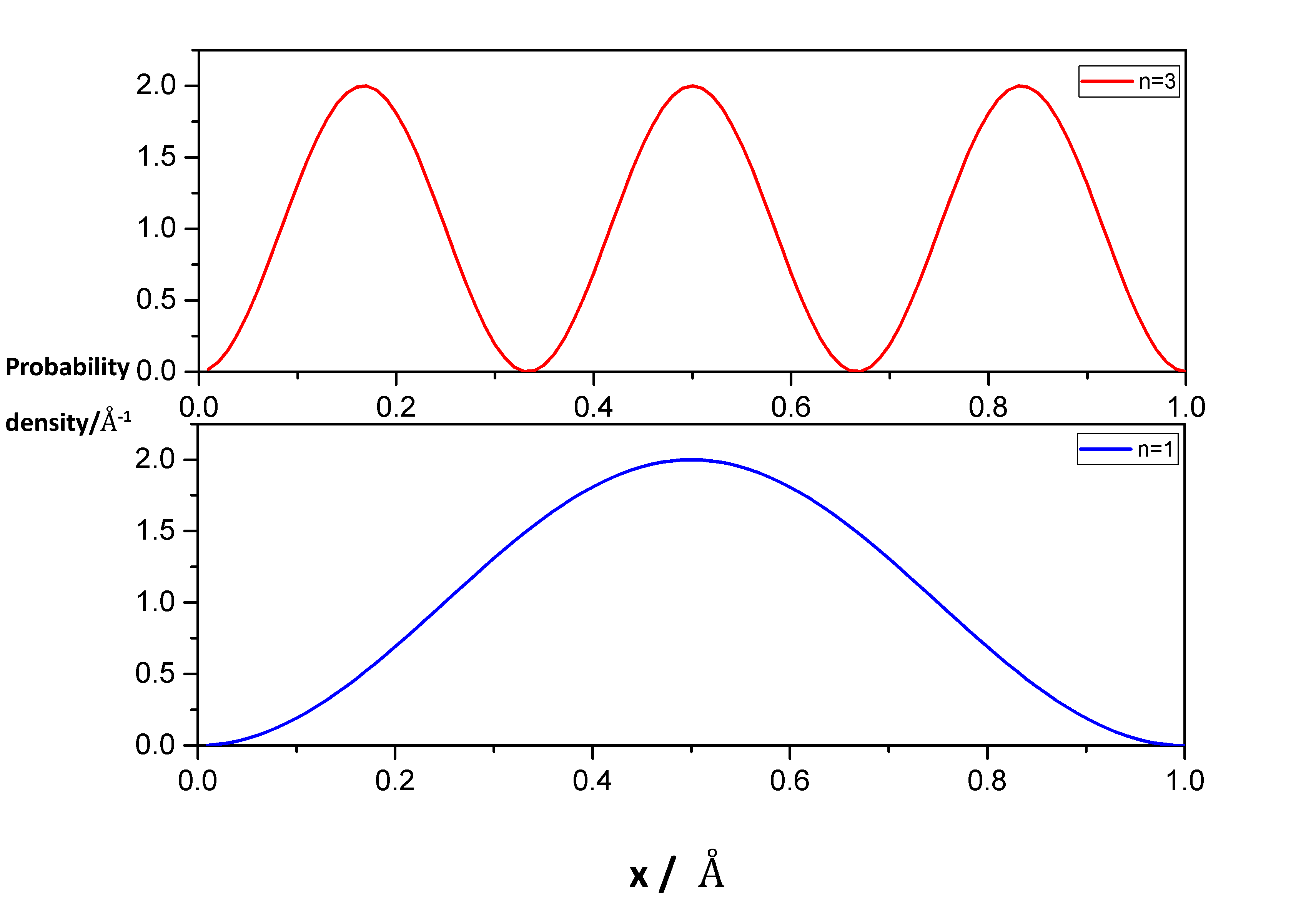
**(11d)** A potassium atom at 1 K (micro Kelvin).

**(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%)

The wavefunction of particle-in-a-box system is solved by Schrodinger equation.

The wavefunction () must satisfy , which means the probability in the whole space is equal to one. So we need this term .

ground state, n=1

second excited state, n=3

**(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.



Peak position:

3 variables --> choose 3 peaks to solve

Here choose 2865, 2906, 2926 cm-1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| No. | Peak (cm-1) | J’ | J” | equation |
| Eq.1 | 2865 | 0 | 1 |  |
| Eq.2 | 2906 | 1 | 0 |  |
| Eq.3 | 2926 | 2 | 1 |  |

Eq.3-Eq.1:

Insert to Eq.2:

Insert to Eq.1:

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

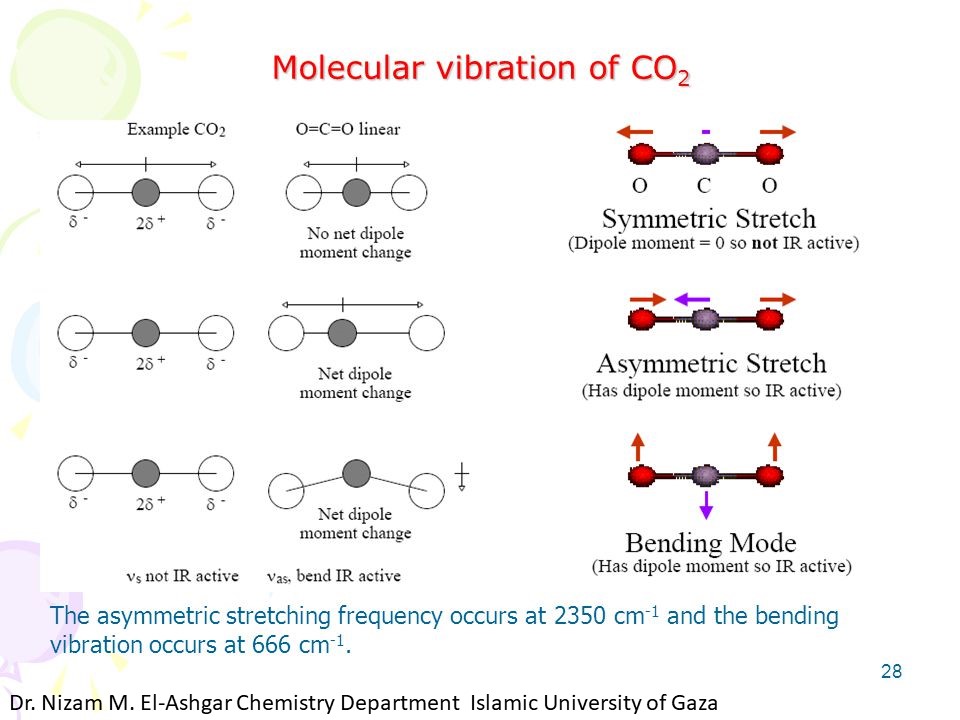
For a diatomic molecule,

For H35Cl,

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

Because there is no dipole moment change when a homonuclear diatomic molecule vibrating.

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

****

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

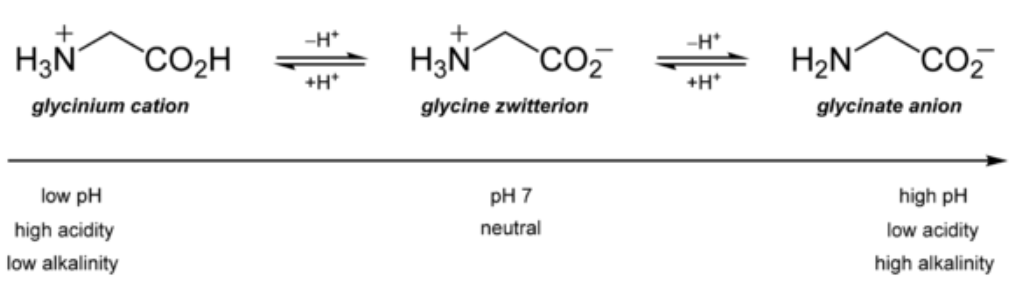
太輕、太軟、強度不夠、不容易焊接、比較貴

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

See : “Chemistry in Life\_0429.pptx” uploaded on ceiba

**(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 …)



pKa1 = 2.34

Ka1 = 102.34

= 4.57 x 103

pKa2 = 9.6

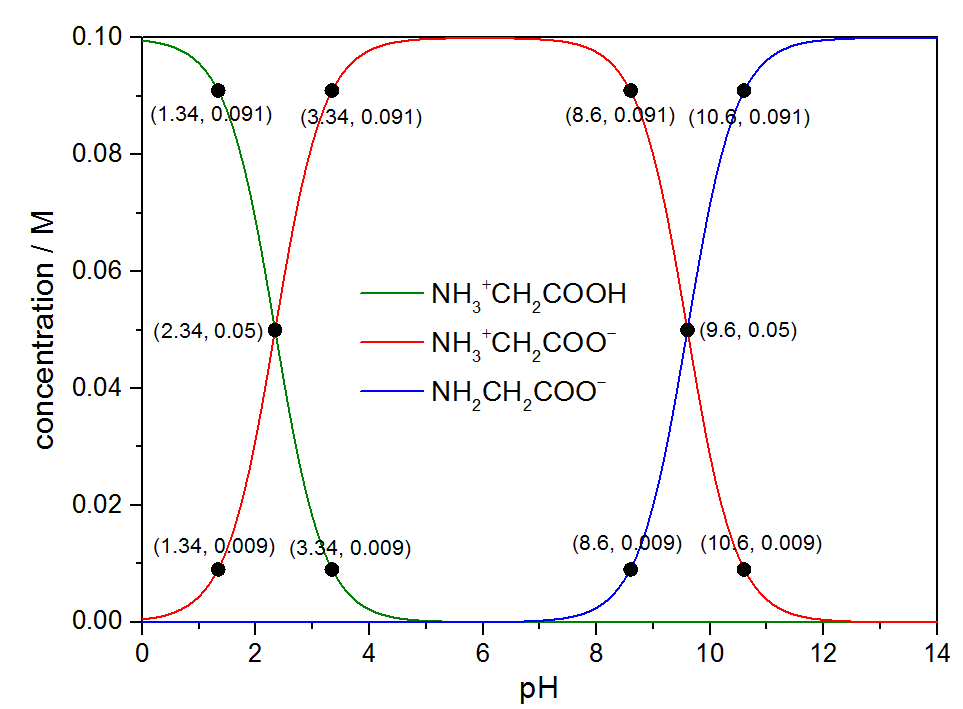
Ka2 = 109.6

= 2.51 x 10

**(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.

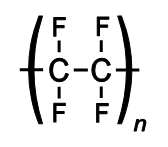
|  |  |  |  |
| --- | --- | --- | --- |
| pH | [NH3CH2COOH]  / M | [NH3CH2COO] / M | [NH2CH2COO] / M |
| 1.34 | 0.091 | 0.009 | 0 |
| 2.34 | 0.05 | 0.05 | 0 |
| 3.34 | 0.009 | 0.091 | 0 |
| 8.6 | 0 | 0.091 | 0.009 |
| 9.6 | 0 | 0.05 | 0.05 |
| 10.6 | 0 | 0.009 | 0.091 |



需標出pH = pKa, pH = pKa ± 1 的點

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

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Abbr. | PE | PP | PS | PVC | Teflon® |
| Full name | Polyethylene | Polypropylene | Polystyrene | Polyvinyl chloride |  |
| Structure |  |  |  |  |  |



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

Ag, Pt, Au …. etc.

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

1. 大部分金屬氧化時會在表面形成緻密氧化層，保護內部金屬不氧化
2. 金屬易導熱，點火時熱量容易分散，難以達到燃點。
3. 融/沸點高(次要原因): 大部分可燃物(汽油、蠟燭等)，是先汽化、再以氣相與氧氣反應，因為氣態的可燃物可與氧氣均勻混和，增加反應速率。