5. (*a*) Calculate the energy of Helium atom using first order degeneration perturbation theory.

***OR***

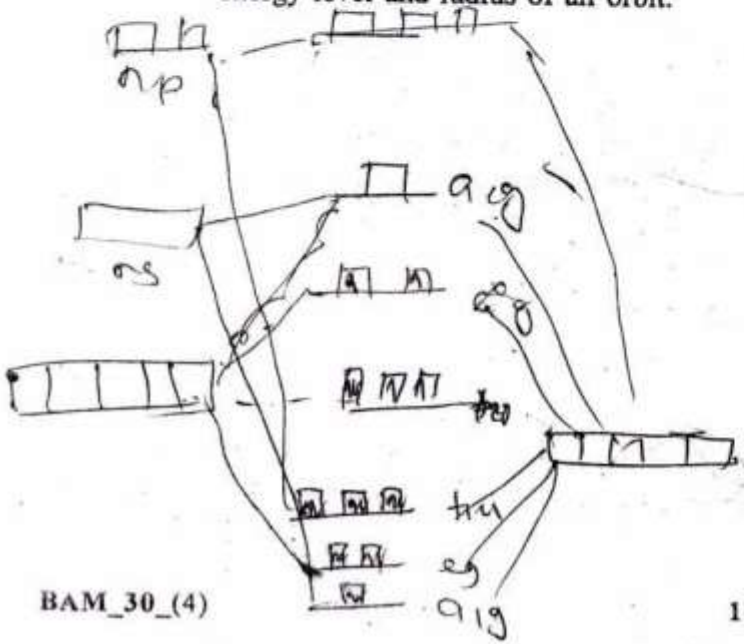
(*b*) Set up secular determinant for Ethylene. Find out electron density, charge density and bond order of ethylene.

6. (*a*) Discuss the application of computers in chemistry. Write a programme to calculate the rate constant.

***OR***

(*b*) (*i*) Write a C programme to find largest and smallest of two numbers.

(*ii*) Write a programme for evaluation of energy level and radius of an orbit.







# MSc-Chem-IS–(403)

**January, 2017**

## BASIC PHYSICAL CHEMISTRY-I

*Time* : Three Hours] [*Maximum Marks* : 80

**Note** : Answer from both the Sections as directed. The figures in the right-hand margin indicate marks.

### SECTION-A

**1.** Answer any **four** of the following : 4×4

(*a*) Give the hierarchy operations used in C Programme.

(*b*) Show that the order of a group is the integral multiple of the order of its subgroups.

(*c*) Show that for a particle moving in a one dimensional box of length $a$, average value of $p$, $\langle p \rangle = 0$.

(*d*) Show that average value of $r$ in $2s$ state is $6a_0$.

(e) A symmetry point group consists of the following operators E, $2C_3$, $3C_2$, $\sigma_h$, $2S_3$ and $3\sigma_v$.

(i) What is the order of the group ?

(ii) How many classes are in the group ?

(f) Write different types of instructions used in C programme.

*OR*

2. Answer **all** of the following questions : 2×8

(a) What do you mean by Spherical Harmonics ?

(b) State important properties of irreducible representation.

(c) List the symmetry elements for the following molecules :

(i) $C_6H_6$

(ii) $[PtCl_4]^{-2}$

(d) List out the pairs of atomic orbitals for which allowed overlaps are possible.

(e) What happens to the energy of a particle in one dimensional box if the length of the box is made larger ?

(f) State the linear variation theorem.





(g) What is the difference between input and output devices ?

(h) What are the basic elements of computer language ?

## SECTION-B

Answer **all** of the following questions : 16×4

3. (a) For the $H_2O$ molecule, carry out the following :

(i) Determine all the symmetry operations and set up a multiplication table, ascertain that this constitutes a group.

(ii) Use the 1*s* atomic orbitals of the two H atoms to generate a representation of the symmetry group of the molecule.

*OR*

(b) What do you mean by group multiplication table ? Construct a group multiplication table for $C_{3v}$ point group by taking $NH_3$ as an example.

4. (a) Construct a molecular orbital energy level diagram for the $[PtCl_4]^{-2}$ species.

*OR*

(b) Construct a molecular orbital energy level diagram for the $[CoF_6]^{-3}$ species and account for its paramagnetic nature.