Birla Institute of Technology & Science, Pilani, Rajasthan 333 031
First Semester 2022-2023
Course Number: CHEM G553 Course Title: Advanced Physical Chemistry Marks: 18
Mid-Sem Examination Date: November 03.11.2022 Time: 50 mins.
(CLOSED BOOK)

Q.1. (a) Fill up the following table: **[4×1=4M]**

The Chemical Systems	No. of Normal Modes	No. of IR Inactive Modes and its identity (if any)
LiCl		
$BeCl_2$		
NH_3		
Cl_2		

(b) A molecule of the type MX has normalized valence bond wave function of the form $\psi = 0.25\psi_{cov} + 0.968\psi_{ionic}$. What is the chance that in 2000 inspections of the molecule, both electrons of the bond will be found on one atom? **[3M]**

(c) The first ionization potential (I.P.) of atoms A [valence shell electronic configuration, (e.c.) = ns^1] and B (valence shell e.c. = np^1) are given as 13.6 eV and 18.6 eV, respectively. The first and second ionization potentials of the molecule AB are given as 12.8 and 19.3 eV, respectively. Draw the energy level diagram of the atomic as well as molecular orbitals formed by LCAO-MO method. Which molecular orbital will have predominantly A-atom character and which will have B-atom character? **[3+1=4M]**

(d) Suppose that hydrogen is replaced by deuterium in $^1H^{35}Cl$. Show whether the J= 0→1 transition will move to higher or lower wave number? **[3M]**

(e). Fill up the cell of the following Table on the basis of IR and Rotational activity of the molecules. (use '√' for 'active' and 'X' for 'not active') **[3M]**

	N_2	XeF_4	O_3
IR			
Rotational			

(f) Assuming only valence shell atomic orbitals (i.e., s, p and d orbital) take part in molecular orbital formation (M.O.) how many molecular orbitals would be formed in Na_2 molecule according to LCAO-MO approach.

[1M]

END

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Course Number: CHEM G553 **Course Title: Advanced Physical Chemistry** **Marks: 12**
Mid-Sem Examination **Date: November 03.11.2022** **Time: 40 mins.**
(OPEN BOOK)

Useful Data: *Given are commonly used values, notations have usual meanings,* $h = 6.626 \times 10^{-34}$ *Js,* I J = 1 kg m^2 s^{-2}, $Stefan - Boltzmann\ constant\ \sigma = 5.67 \times 10^{-8}\ Wm^{-2}K^{-4}$

Q.1. (a) A hot body radiates power of 4.6 x 10^3 W at a temperature of 2727 ^{0}C. Calculate the area of rectangular surface of the body. **[3M]**

(b) Assume a ball of mass 100 gm, is confined to a one-dimensional box of length 1 m, moves with a velocity of 0.01ms^{-1}. Assuming the ball has only kinetic energy within the box calculate the quantum number n. Is the concept of quantization valid in this case (show all the relevant calculations)? **[3+3 = 6M]**

(c) Which of the following terms cannot be obtained from the ground state electronic configuration $1s^2,2s^2,2p^6,3s^2,3p^3$? Why? Identify the levels (calculate J) corresponding to the valid term(s). **[2+1 = 3M]**

^4F ^4D ^4P ^4S

END