Introduction to Computational Chemistry

Answer ALL the Questions

Q. No.	Question Description	Marks

PART - A – (3 x 10 = 30 Marks)

1 (a) The IC_{50} value of a drug candidate was measure using five different researchers and was found to be equal to : **10**

44.3, 47.9, 34.0, 44.8, 45.6

Calculate the average, mean absolute error and the standard deviation for these measurements.

OR

(b) Calculate the the maximum wavelength of light that can remove an electron from a hydrogen atom in its **a) ground state, b) third excited state**. **10**

2 (a) Given the following data: **10**

$3\ N_2O(g) + 2\ NH_3(g) \rightarrow 4\ N_2(g) + 3\ H_2O(l)$ $\Delta H = -254$ kJ

$N_2O(g) + 3\ H_2(g) \rightarrow N_2H_4\ (l) + H_2O\ (l)$ $\Delta H = -75$ kJ

$2H_2\ (g) + O_2(g) \rightarrow 2\ H_2O\ (l)$ $\Delta H = -72$ kJ

$N_2H_4(l) + O_2\ (g) \rightarrow N_2(g) + 2\ H_2O(g)$ $\Delta H = -154$ kJ

Calculate the ΔH for the following reaction:

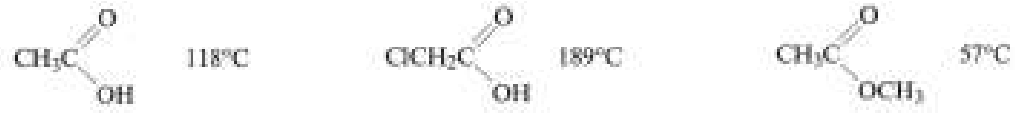
$2\ NH_3(g) + ½\ O_2\ (g) \rightarrow N_2H_4\ (l) + H_2O\ (l)$

OR

(b) The bonded and non-bonded parameter for a molecule are needed to perform its molecular dynamics simulations. Discuss the procedure to obtain these **10**

parameters. Discuss why the quality of force-field parameters is important for MD simulations.

3 **(a)** The boiling points for the following substances are given below. Justify the differences in the boiling points. **10**



OR

(b) Describe the Born-Oppenheimer approximation and its importance for the classical molecular dynamics simulations. **10**

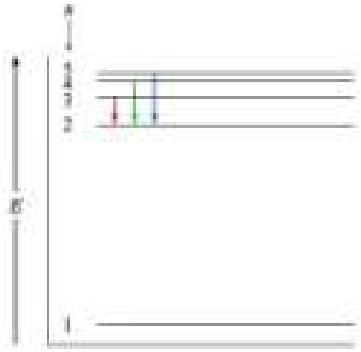
Part - B – (2 x 10 = 20 Marks)

4 Given the emission spectrum for a He^+ ion, **10**

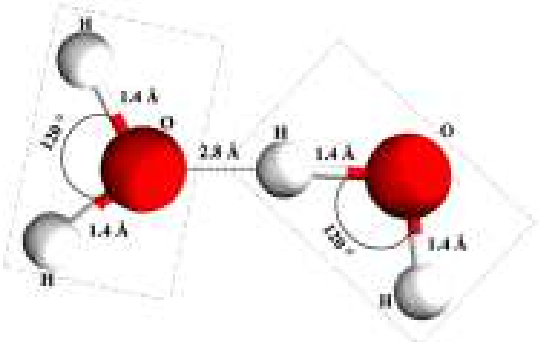
a. *"As the value of principle quantum number increases, the energy levels get closer."*

Justify the statement with mathematical support.

b. Calculate the wavelengths associated with the electronic transitions shown in the figure.



5 Given the following force-field parameters, write the expression for the potential energy H_2O dimer: **10**



#Charge: $Q_O = -0.834$, $q_H = 0.417$

#Bond:

O-H: $r^o = 0.9$ Å, $K_b = 450$ kcal/mol/Å^2

O-O: $r^o = 1.9$ Å, $K_b = 700$ kcal/mol/Å^2

H-H: $r^o = 3.5$ Å, $K_b = 500$ kcal/mol/Å^2

#Angle: H-O-H: $\theta^o = 109.5$ Å, $K_\theta = 105$ kcal/mol/degree^2

#L-J parameters: O-H: $\sigma = -0.5$ Å, $\varepsilon = 0.0104$ kcal/mol

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