Introduction to Computational Chemistry

Answer all the Questions

Q. No.	Question Description	Marks
1	A student measured the pressure, volume, and temperature for one mole of an ideal gas as 2.560 atm, 275.15 K, and 8.8 L, respectively. Using these values, calculate gas constant, R, to the correct number of significant figures.	8
2	Solve the following with correct number of significant figures: a) 8.2001 + 0.112 - 6.8530 b) $\frac{5.789 + 4.2380 - 5.98}{2.20605}$	8
3	Briefly discuss an experiment which implies that light is made of particles.	8
4	The Balmer series is the name given to a series of spectral emission lines of the hydrogen atom that result from electron transitions from higher levels down to the energy level with principal quantum number 2. Calculate the value of wavelengths corresponding to **first three lines** of the Balmer series in the emission spectrum of atomic hydrogen as per the quantum mechanical model.	10
5	The standard enthalpies of combustion of C(s), $H_2(g)$, and $CH_4(g)$ are -100.5 kJ/mol, -50.4 kJ/mol, and -180.36 kJ/mol, respectively, at 298 K. Using these values, calculate the standard enthalpy of formation of methane, CH_4 (g).	8
6	Iron undergoes oxidation to form Fe_2O_3. $4\,Fe\,(s) + 3\,O_2(g) \rightleftharpoons 2\,Fe_2O_3\,(s)$ Given the data below, calculate the equilibrium constant for the reaction under standard conditions.	8

Substance	$\Delta_f H^\circ$ (kJ/mol)	S° (J/K· mol)

Fe (*s*)	0	27
O_2 (*g*)	0	205
Fe_2O_3 (*s*)	-826	90