Indian Institute of Technology, Guwahati
Guwahati, INDIA 781 039

Department of Chemistry

Date: 20 September 2019; 2:00-4.00 p.m.

CH-101 **Mid Semester Exam** **Maximum Marks = 30**

Name: Division: Signature of Invigilator

Roll No.: Tutorial Group:

Answer only in this sheet. Only fully correct answers will be accepted.
All questions are compulsory. Rough work is mandatory.

1. For a particle-in-a-box of length L, the wavefunction is written as, $\Psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$. If for the first excited state (n = 2), the value of energy is 5.5×10^{-19} J, then the de Broglie wavelength of the particle (in Å) would be, *(Please Tick)* **2.0 Marks**

~~3.32~~	~~4.42~~	6.63 ✓	~~8.84~~	*Use ($h = 6.630 \times 10^{-34}$ Js, $m = 9.11 \times 10^{-31}$ kg)*

2. A proton (1.67×10^{-27} kg) is confined in an infinite one-dimensional square well of width 10 fm (1 fm = 10^{-15} m); h = 6.62×10^{-34} Js; c = 3.0×10^{8} ms^{-1}. The approximate wavelength of the photon (in fm) emitted when the proton undergoes a transition from the second excited state to the first excited state is: *(Please Tick)* **2.0 Marks**

~~242~~	~~303~~	~~151~~	121 ✓

3. If the wave function for an electron circulating on a ring could be written as $\Psi(\varphi) = Ae^{im\varphi}$, then the value of A would be, *(Please Tick)* **2.0 Marks**

~~$\sqrt{2\pi}$~~	~~$1/\sqrt{\pi}$~~	$1/\sqrt{2\pi}$ ✓	~~$\sqrt{2/\pi}$~~

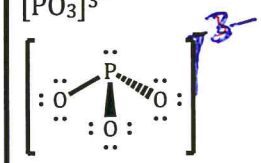
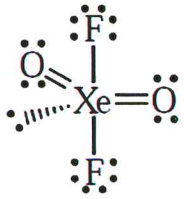
4. The force required to stretch the ^{12}C–H bond (harmonic oscillator) by 0.2 Å is 250 pN (1 pN=10^{-12} N). The vibrational frequency of the ^{12}C–H bond in Hz is: *(Please Tick)* **2.0 Marks**

1.44×10^{13} ✓	~~9.03×10^{13}~~	~~18.06×10^{13}~~	~~4.51×10^{13}~~

5. The hydrogenic Hamiltonian for the electron with mass m_e and nucleus with mass m_N can be rewritten using reduced mass (μ) and total mass (m) as, *(Please Tick)* **2.0 Marks**

	$H = -\frac{\hbar^2}{2m}\nabla^2_{c.m.} - \frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{4\pi\varepsilon_0 r}$

6. Draw the Lewis structure with appropriate molecular geometry for the following. **1 Mark**

$[PO_3]^{3-}$ 	XeO_2F_2 

7. Indicate if the following exhibit Strong (S), Weak (W) or No (N) Jahn-Teller distortion **1 Mark**

	$[Mn(H_2O)_6]^{3+}$	$[CoF_6]^{3-}$	$[Cr(H_2O)_6]^{2+}$	$[Ru(ox)_3]^{3-}$
Strength of Jahn-Teller distortion	S	W	S	W

8. Which of the following statements are true (T) and which are false (F). **0.25 × 8 = 2 Marks**

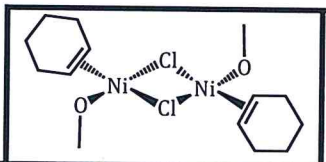
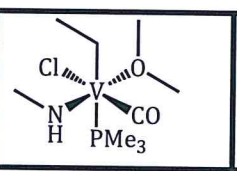
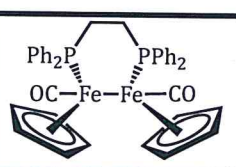
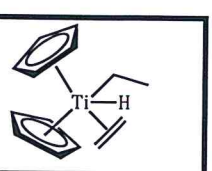
a) Asymmetry in e_g orbital occupancy results in strong Jahn-Teller distortion (T)
b) Using VBT, one can infer that $[CoF_6]^{3-}$ involves d^2sp^3 hybrid orbitals (F)
c) In a square-pyramidal complex, the d_{z^2} orbitals are destabilized (F)
d) In d^4 octahedral complexes with π-donor ligands, the LUMO is e_g* molecular orbital (F)
e) In octahedral complex with CO ligands, the first d electron is filled in t_{2g} (π) bonding molecular orbital (T)
f) The C-H bond energies for the given molecules follows the trend: Acetylene > Ethylene >> Methane (F)
g) There is an large increase in atomic radii as one moves from Al to Ga (F)
h) Cl^- has a larger ionic radius than P^{3-} (F)

9. Which of the following are true when, one compares Molar Extinction Co–efficient (ε) and Wavelength of Absorption (λ) that are highlighted *(Please Tick)* **2 Marks**

ε	
	$[Mn(H_2O)_6]^{2+} < [Ni(H_2O)_6]^{2+} < [NiCl_4]^{2-}$

λ	
	$[CoF_6]^{3-} > [Co(H_2O)_6]^{3+} > [Co(CN)_6]^{3-}$

10. Indicate the number of valence electron on each metal complex. **(0.5 × 4) = 2 Marks**

				
Electron Count	32 or 16	14	36 or 18	18

11. Using CFT, indicate the correct *d*–orbital splitting pattern for octahedral and square–pyramidal complex *(Please Tick)* **1 Mark**

~~a) Octahedral: $d_{z^2} = d_{x^2-y^2} < d_{xy} = d_{xz} = d_{yz}$; Square pyramidal: $d_{xz} = d_{yz} < d_{z^2} < d_{xy} < d_{x^2-y^2}$~~

~~b) Octahedral: $d_{xy} < d_{z^2} = d_{x^2-y^2} < d_{xz} < d_{yz}$; Square pyramidal: $d_{xz} = d_{yz} < d_{z^2} < d_{x^2-y^2} < d_{xy}$~~

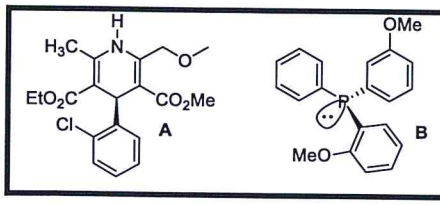
c) Octahedral: $d_{xz} = d_{yz} = d_{xy} < d_{z^2} = d_{x^2-y^2}$; Square pyramidal: $d_{xz} = d_{yz} < d_{xy} < d_{z^2} < d_{x^2-y^2}$

~~d) Octahedral: $d_{xz} = d_{yz} < d_{z^2} < d_{xy} < d_{x^2-y^2}$; Square pyramidal: $d_{xz} < d_{yz} < d_{xy} < d_{z^2} = d_{x^2-y^2}$~~

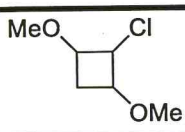
12. The magnitude of the difference in the CFSE (ignoring pairing energy), of $[Fe(CN)_6]^{4-}$ and $[Fe(H_2O)_6]^{2+}$ is *(Please Tick)* **1 Mark**

2.0 Δo	~~1.0 Δo~~	~~0.0 Δo~~	~~3.3 Δo~~

13. Determine the configurations (*R*/*S*) of the chiral centers of the following molecules. **2 Marks**

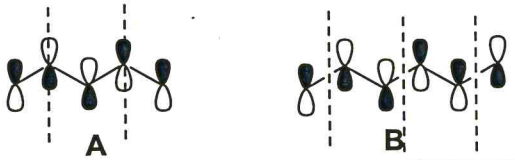
	**A:** (S) **B:** (S)

14. Provide the absolute configuration(s) of optically active isomer(s) of the following compound. **2 Marks**



(R,R) and (S,S)

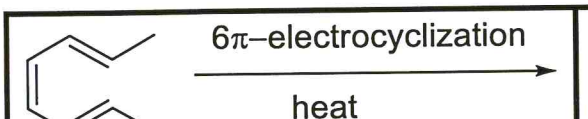
15. Linear combinations of atomic orbitals representing π-molecular orbitals are given below. Place (via dotted line using pen, not with pencil) the appropriate number(s) of nodes at appropriate position (s). **2 Marks**



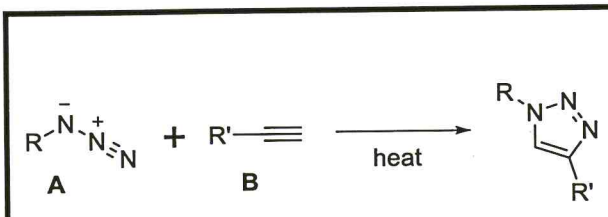
16. Provide the name of the pericyclic reactions involved in the following transformation. **1 Mark**

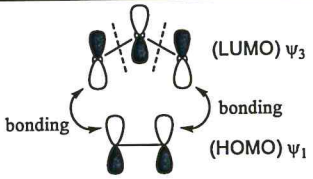
[1,3]-sigmatropic or [3,1]-sigmatropic

17. Provide the structure of the major product formed in the following pericyclic reactions with proper relative stereochemistry. **1 Mark**



18. Present an FMO analysis for following cycloaddition reaction using LUMO of **A** and HOMO of **B** to predict the feasibility of the reaction. Is this reaction symmetry allowed? **2 Marks**





Feasible/ allowed