

Electronic Supporting Information (ESI)

Nuclearity versus oxidation state in catalytic efficiency of Mn^{II/III} azo Schiff base complexes: Computational study on supramolecular interactions and phenoxazinone synthase like activity

Saikat Banerjee,^a Paula Brandão,^b Antonio Bauzá,^c Antonio Frontera,^{*c} Miquel Barceló-Oliver^c, Anangamohan Panja,^d and Amrita Saha,^{*a}

^aDepartment of Chemistry, Jadavpur University, Kolkata- 700032, India.

E-mail: amritasahachemju@gmail.com; asaha@chemistry.jdvu.ac.in; Tel. +91-33-2457294.

^bDepartamento de Química, CICECO, Universidade de Aveiro, 3810-193 Aveiro, Portugal.

^cDepartament de Química, Universitat de les Illes Balears, Crta. De Valldemossa km 7.5, 07122 Palma (Balears), Spain.

E-mail: toni.frontera@uib.es.

^dPostgraduate Department of Chemistry, Panskura Banamali College, Panskura RS, WB 721152, India.

CONTENTS:

| | |
|--|----|
| Fig. S1: ¹ HNMR Spectrum of the ligand, H ₂ L ¹ | S2 |
| Fig. S2: ¹ HNMR Spectrum of the ligand, H ₂ L ² | S3 |
| Fig.S3: FTIR spectrum of H ₂ L ¹ showing sharp peak at 1610 cm ⁻¹ for C=N bond..... | S4 |
| Fig.S4: FTIR spectrum of H ₂ L ² showing sharp peak at 1616 cm ⁻¹ for C=N bond..... | S5 |
| Fig.S5: FTIR spectrum of complex 1 showing sharp peak at 1625 cm ⁻¹ for C=N bond..... | S6 |
| Fig. S6: FTIR spectrum of complex 2 showing sharp peaks at 1622 cm ⁻¹ and 2070 cm ⁻¹ for C=N bond and μ _{1,1} azido bridging, respectively..... | S7 |
| Fig. S7: View of the coordination environment of complex 2 | S8 |
| Fig. S8: ESI mass spectrum of complex 1 | S9 |

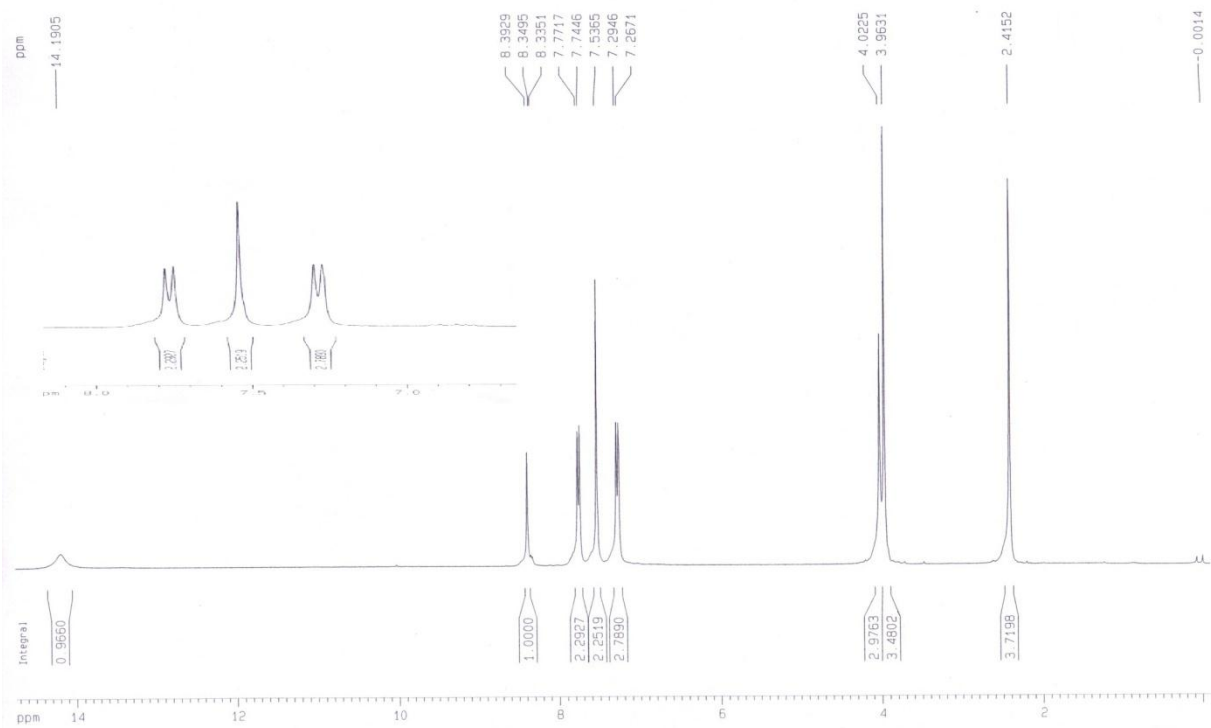


Fig. S1. ^1H NMR(CDCl_3 , 300 MHz) spectrum of H_2L^1 .

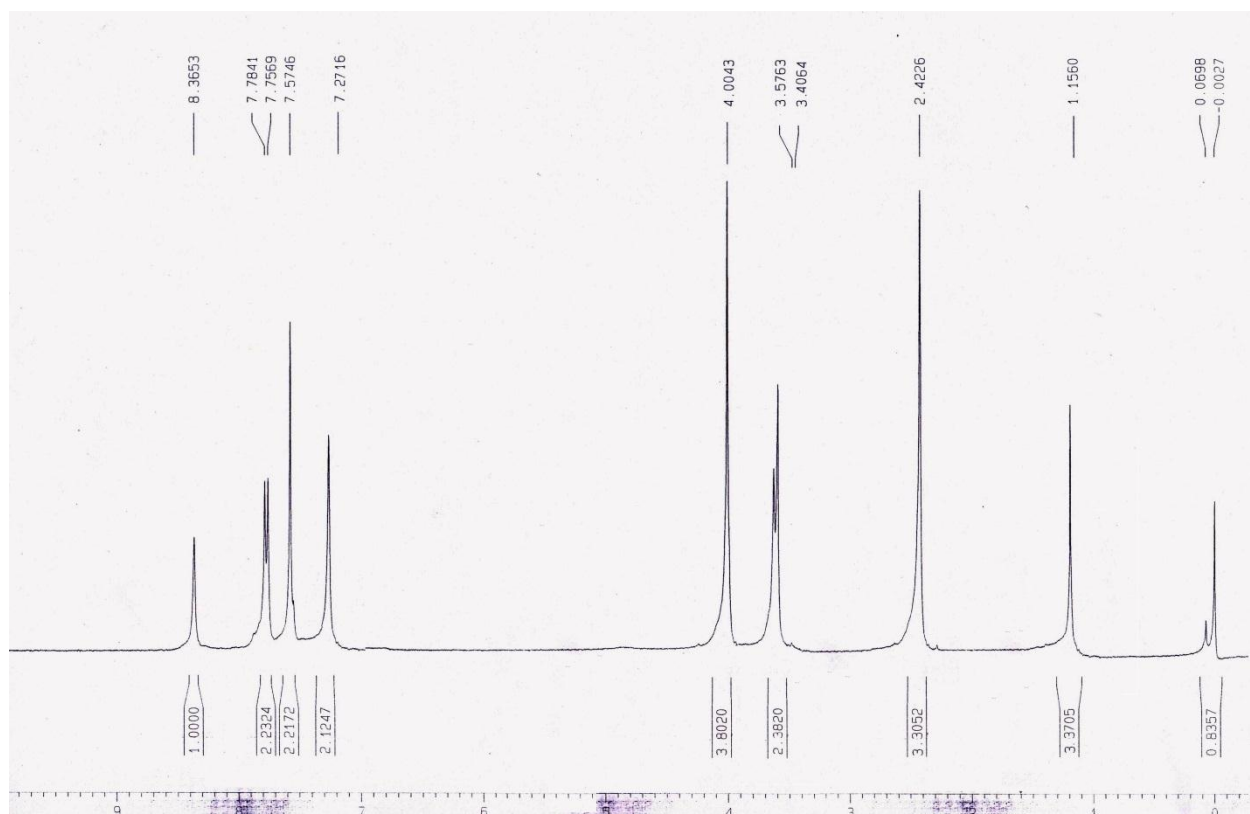


Fig. S2. ¹H NMR(CDCl₃, 300 MHz) spectrum of **H₂L²**.

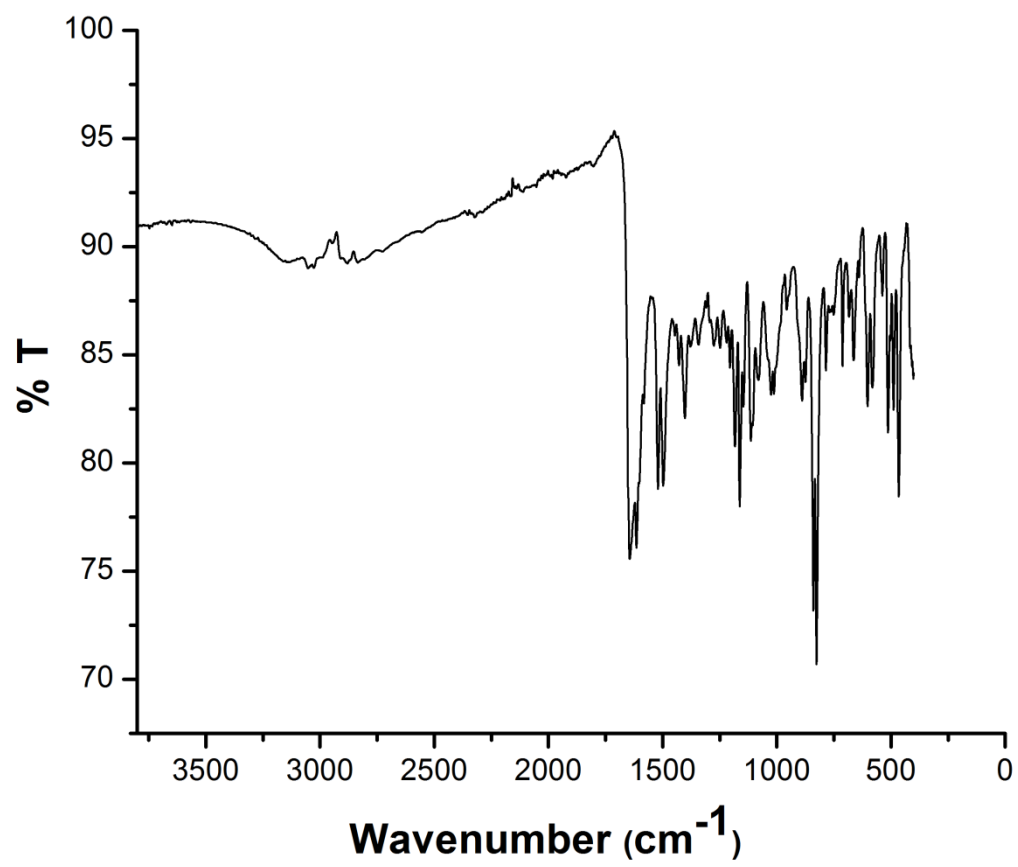


Fig. S3. FTIR spectrum of **H₂L¹**.

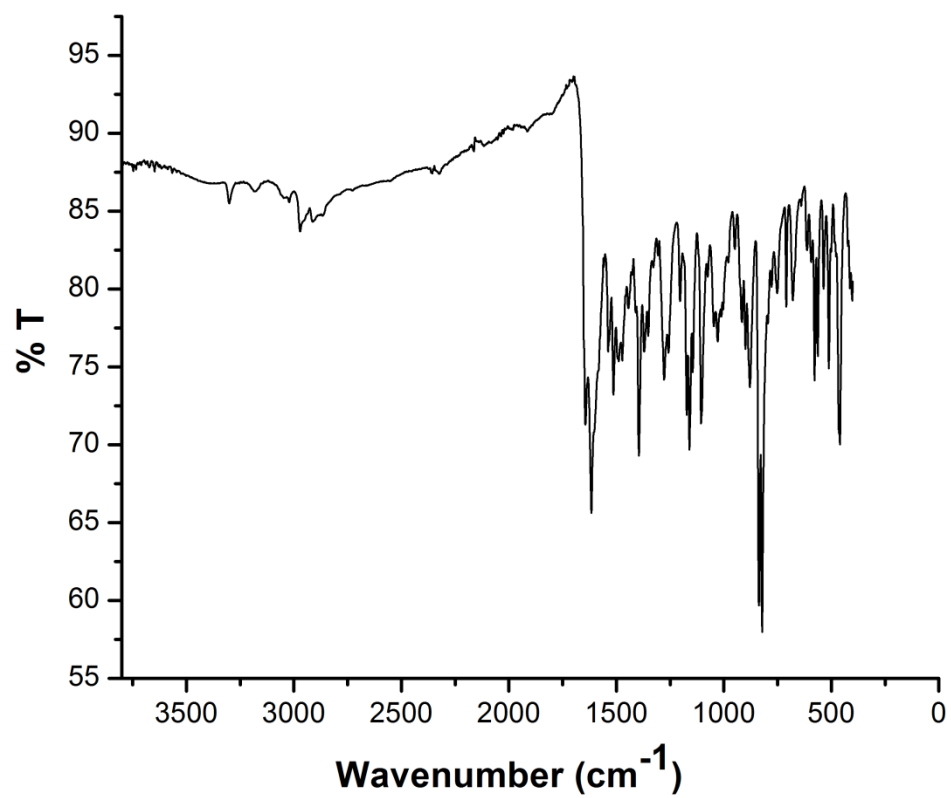


Fig. S4. FTIR spectrum of H_2L^2 .

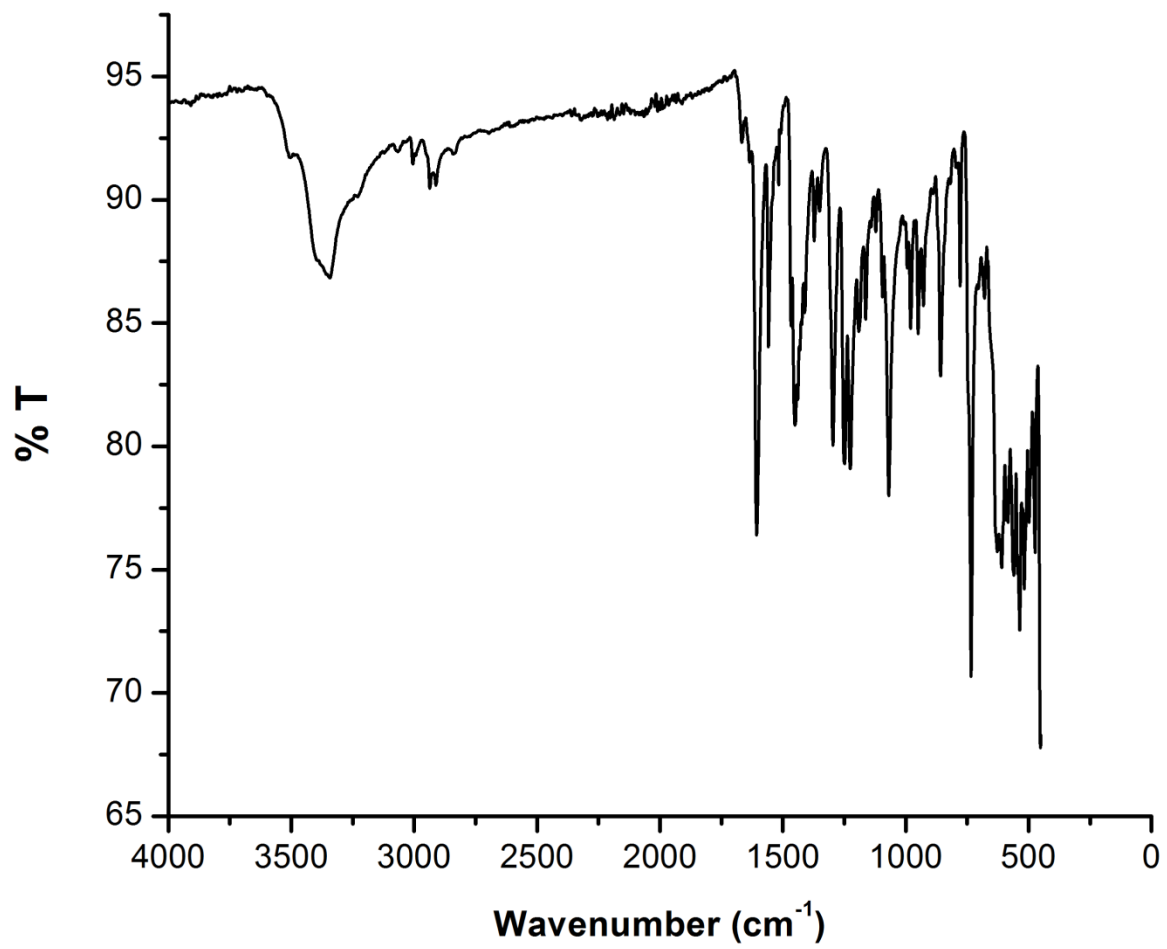


Fig. S5. FTIR spectrum of complex **1**.

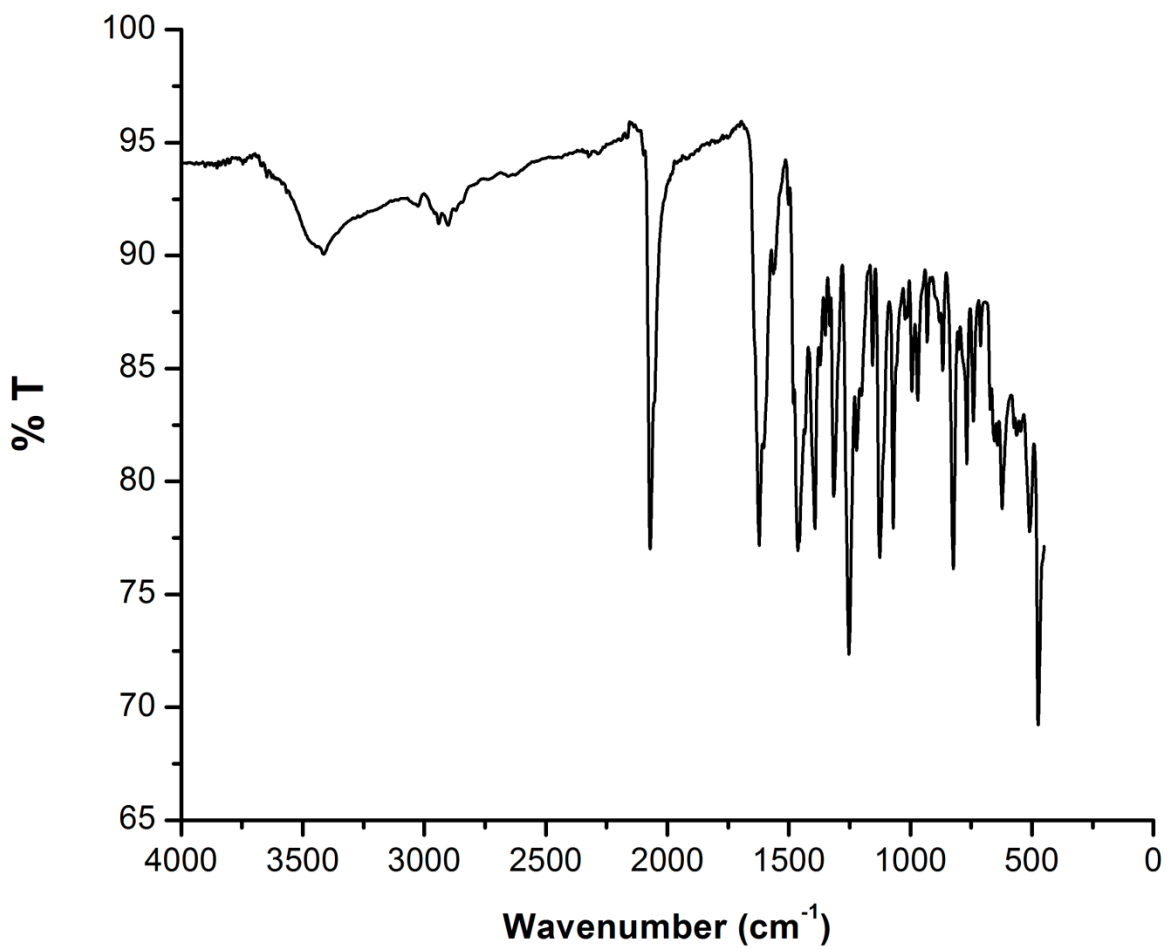


Fig. S6. FTIR spectrum of complex 2.

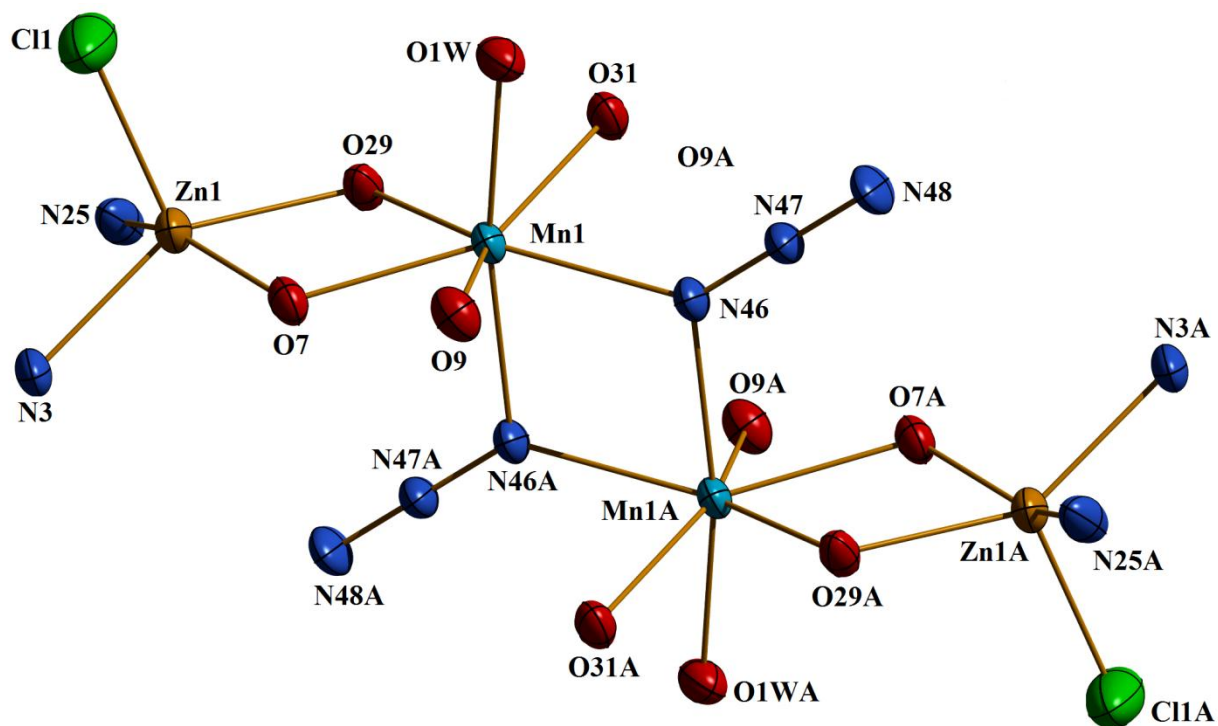


Fig. S7. View of the coordination environment of the Zn(II) and Mn(II) in complex 2.

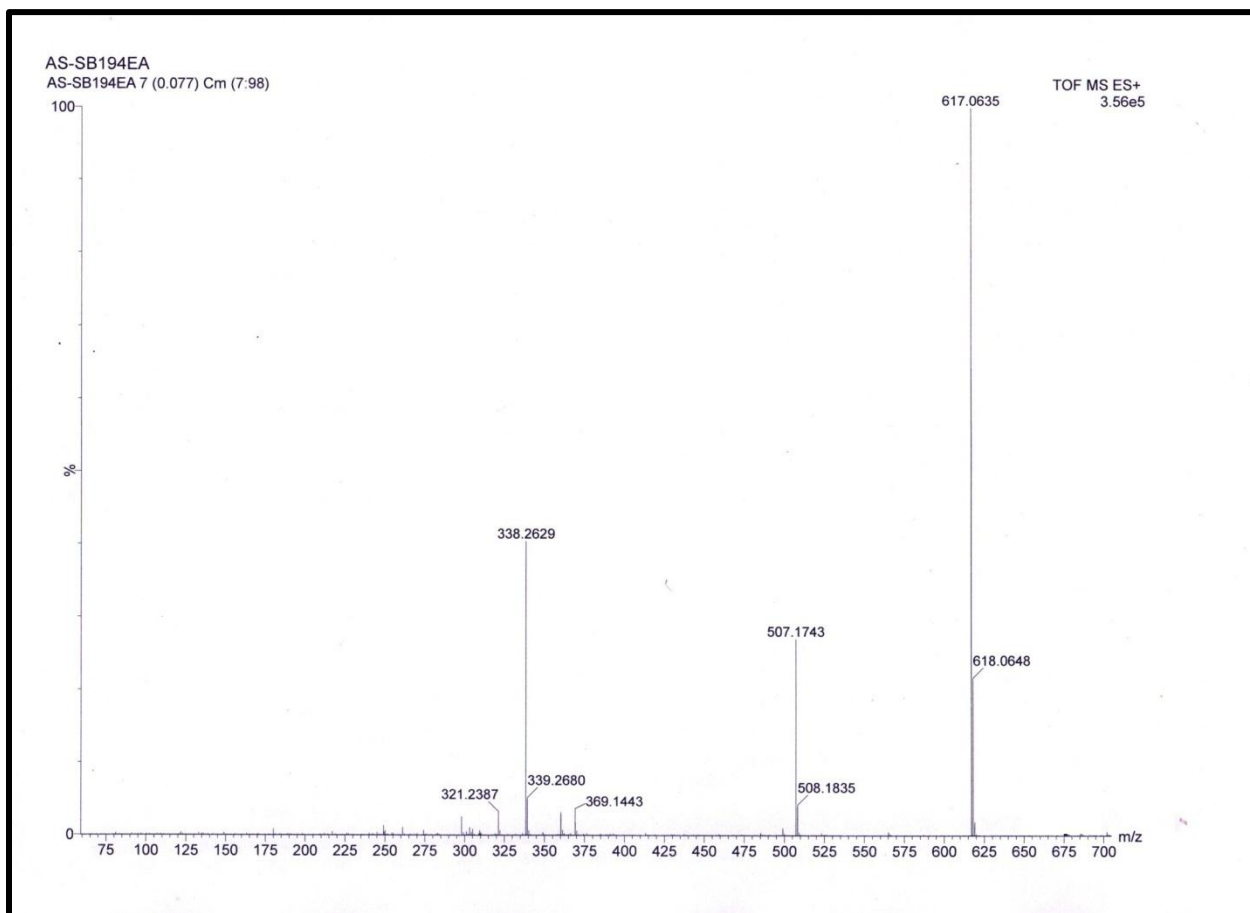


Fig.S8. ESI mass spectrum of complex 1.