

Supporting information file

Synthesis, Crystal Structures of Two Tri and Tetra Heterometallic Ni (II)-Mn (II)/Ni (II)-Co (III) Complexes from Two Different Ni (II) Containing Metalloligand: Effective Catalytic Oxidase Activity and Schottky Device Approach

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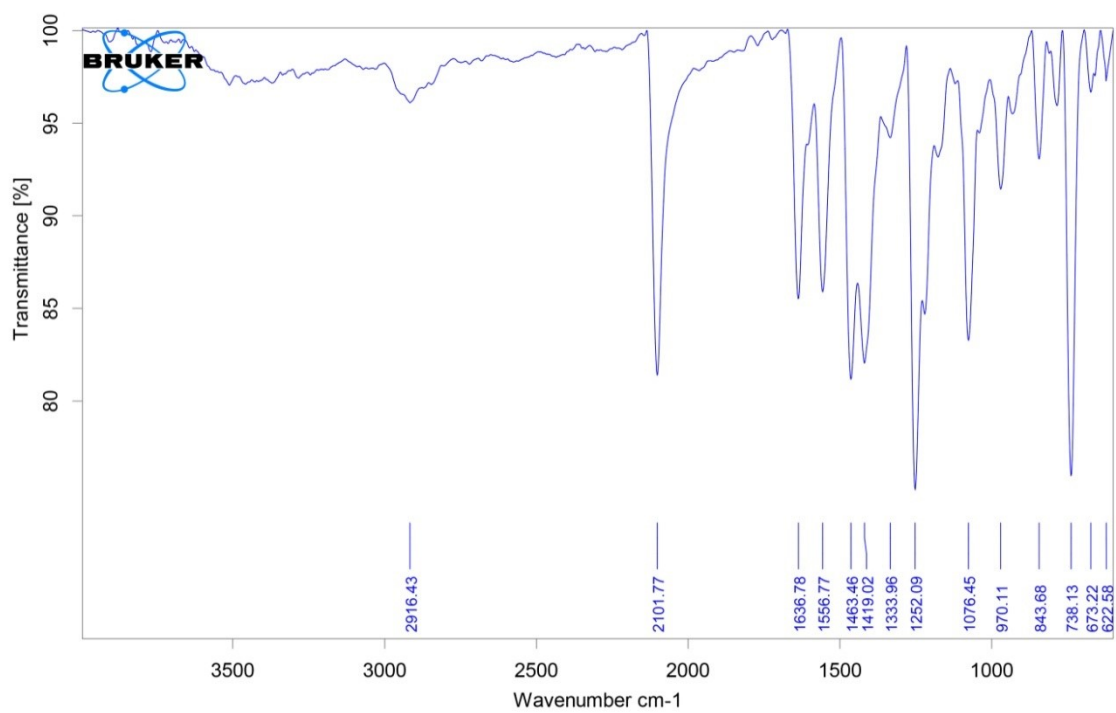


Fig. S1: FT IR spectrum of complex **1**

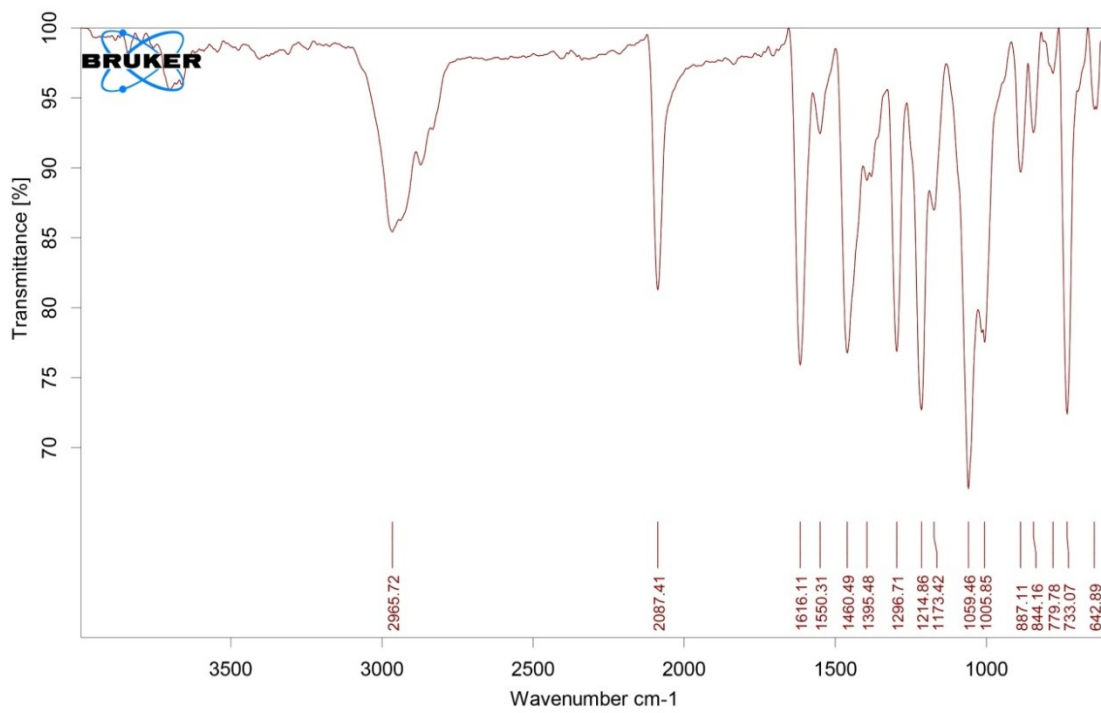


Fig. S2: FT IR spectrum of complex 2

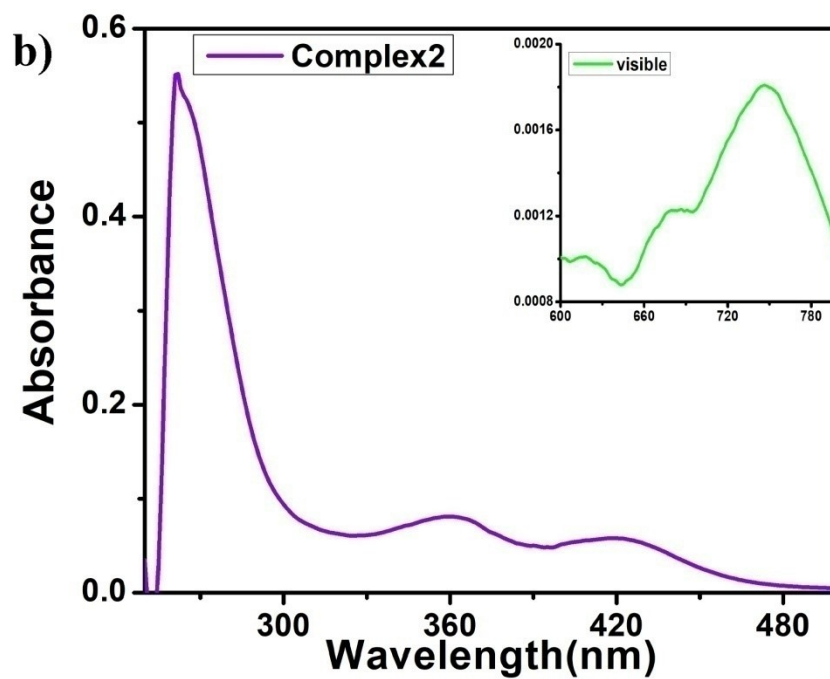
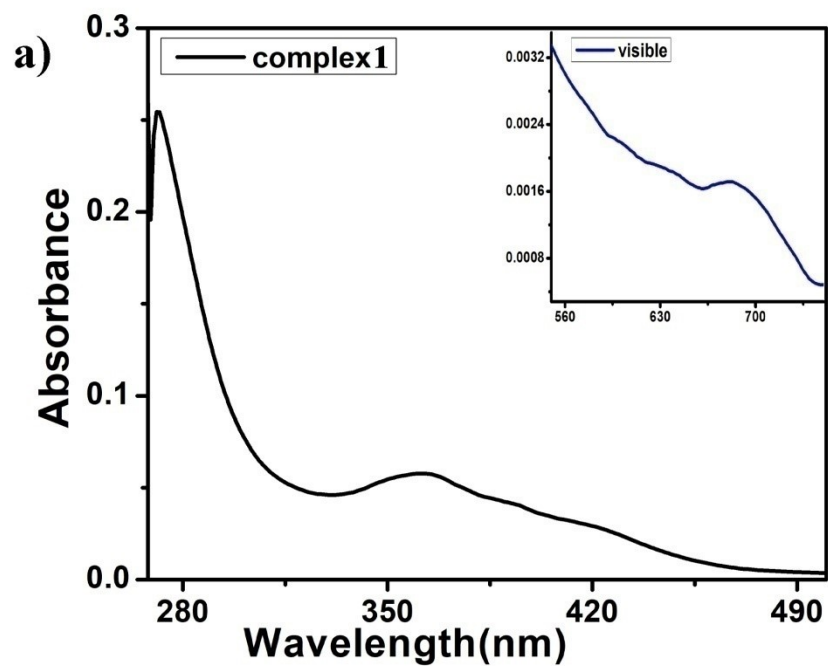


Fig. S3: UV spectrum of a) complex 1 b) complex 2

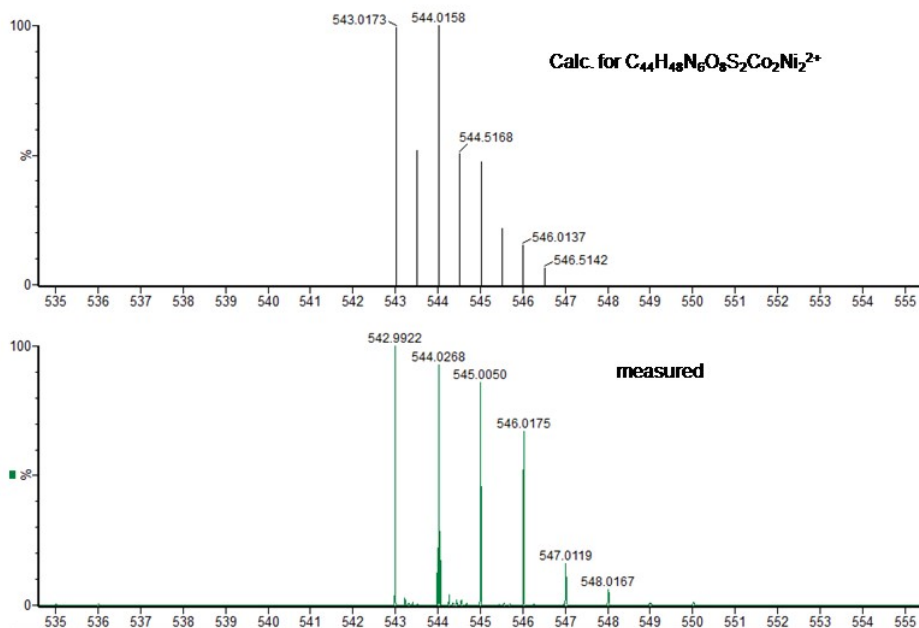


Fig. 4: ESI-MS analyses of complex 1

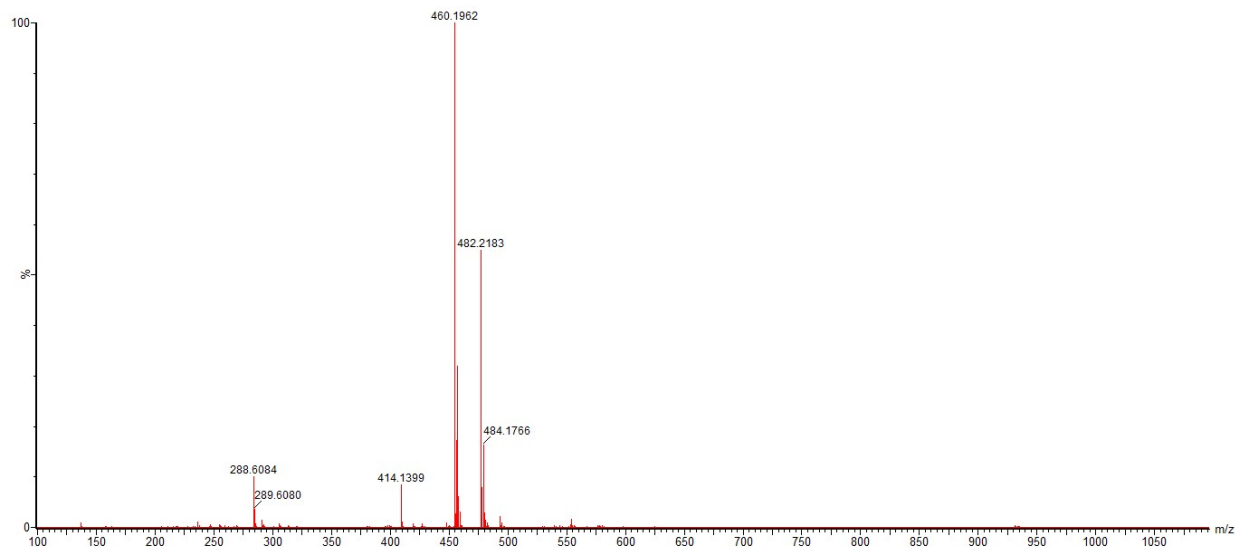


Fig. S5: ESI-MS analyses of complex 2

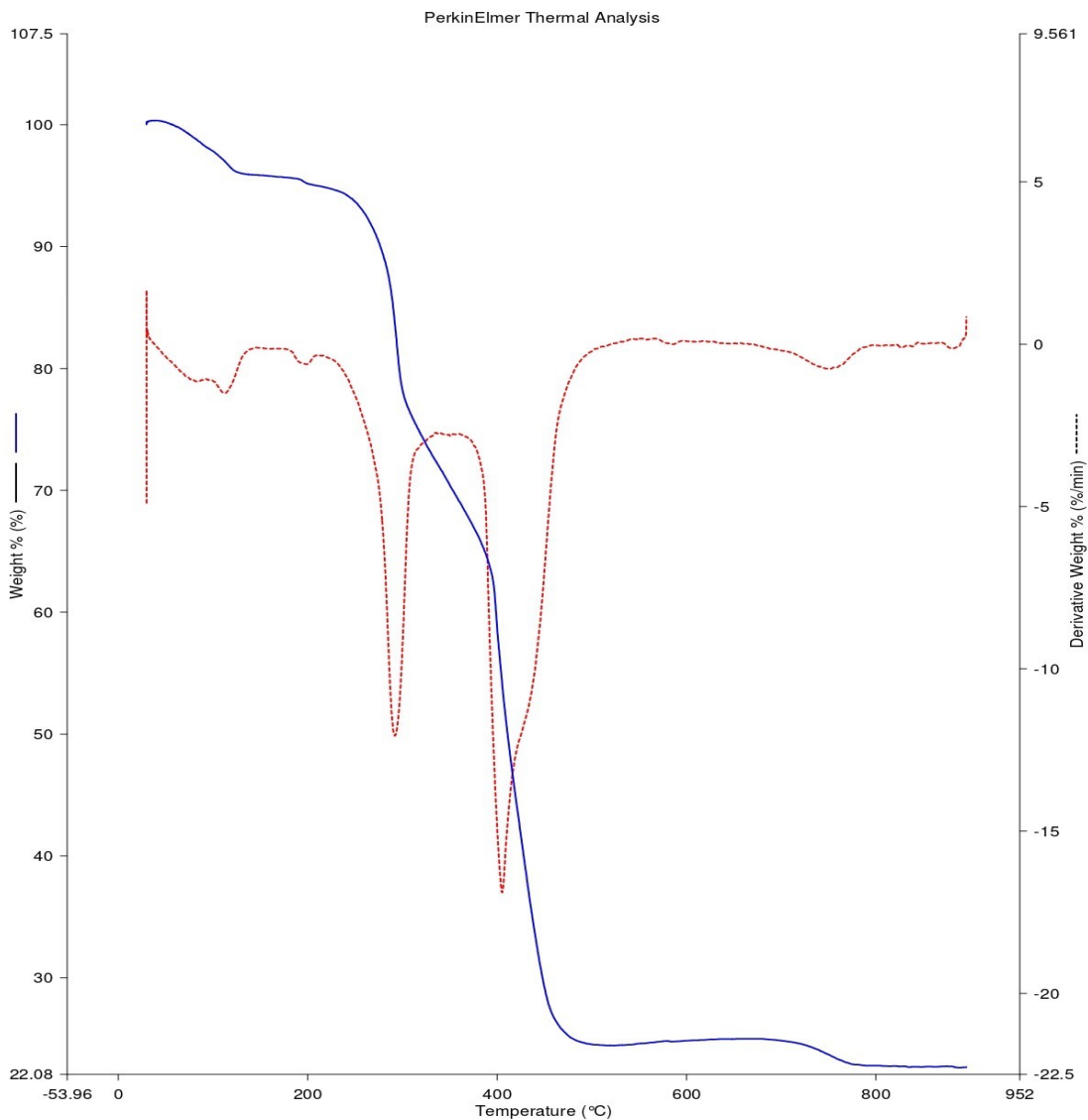


Fig. S6: TGA plot of complex 1

Weight loss calculation:

Orthorhombic Pccn space group, $Z=4$

Therefore $FW = \text{unit cell contents} / Z$

$$= 1206 + 117 \text{ electrons (squeeze results)}$$

$$= 1206 + 4 \text{ water molecules squeezed}$$

$$= 1206 + 4 \times 18$$

$$= 1206 + 72$$

$$= 1278$$

$$\text{Weight loss for four water molecules} = 72/1278 \times 100 \%$$

$$= 5.36 \% \text{ (obtained: } 5.31 \%)$$

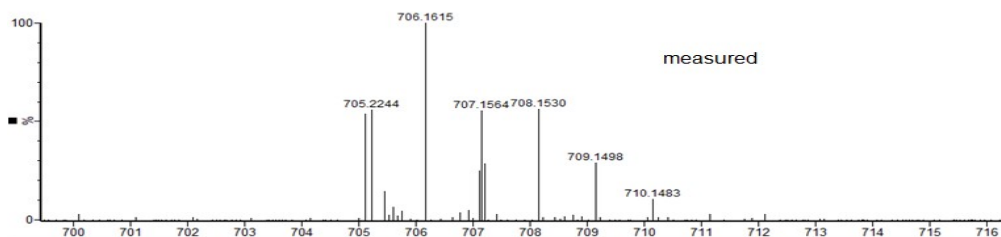
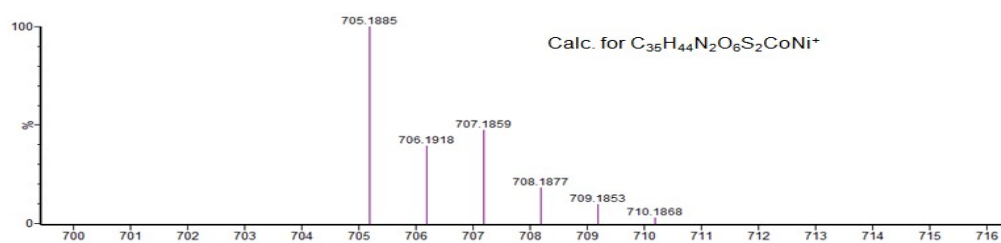
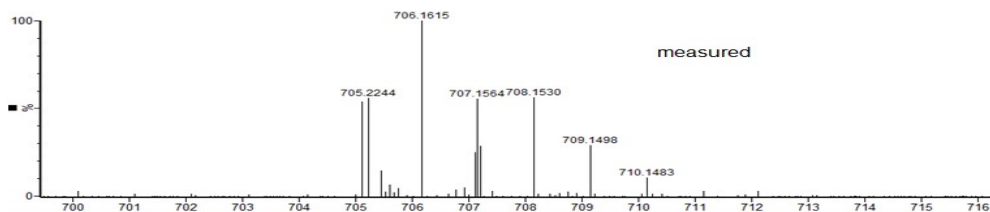
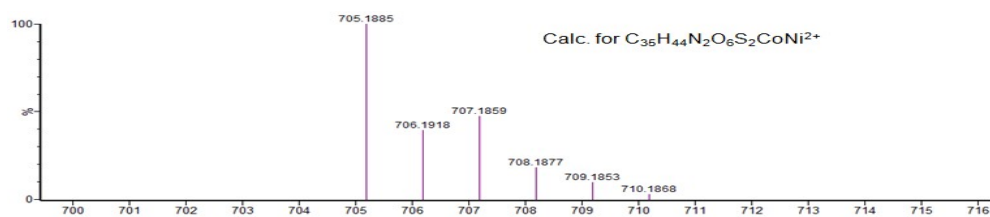
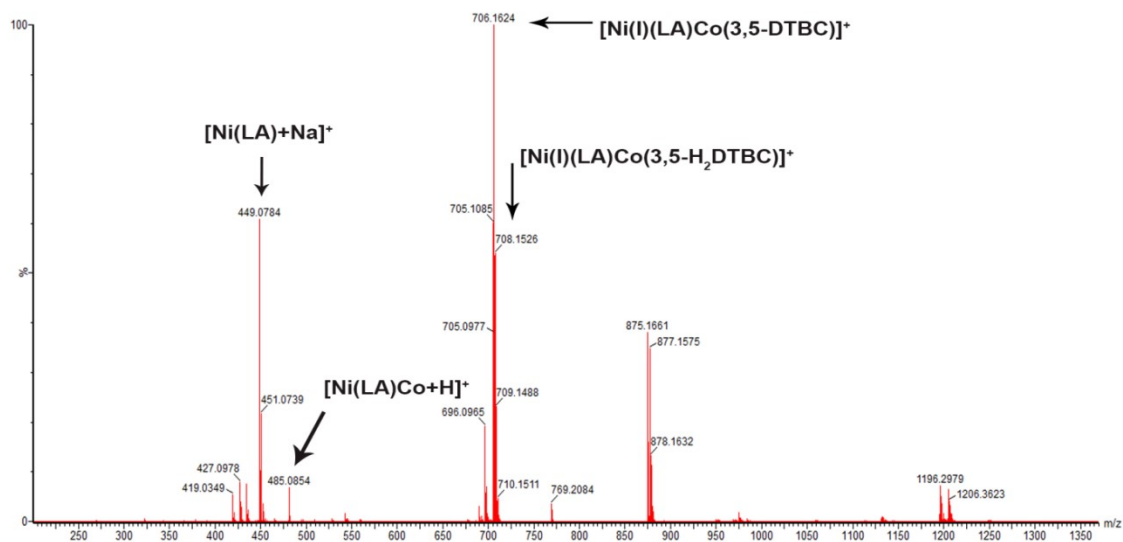


Fig. S7: ESI-MS analyses with isotopic distribution of complex 1 with 3,5-DTBC

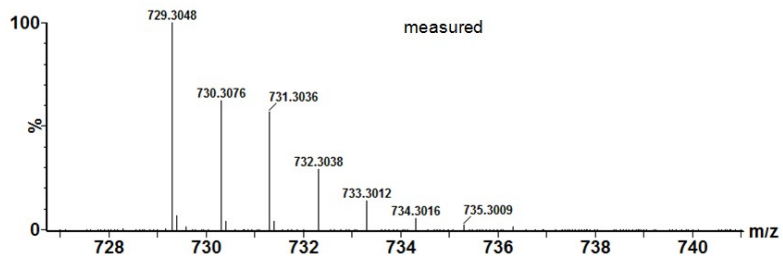
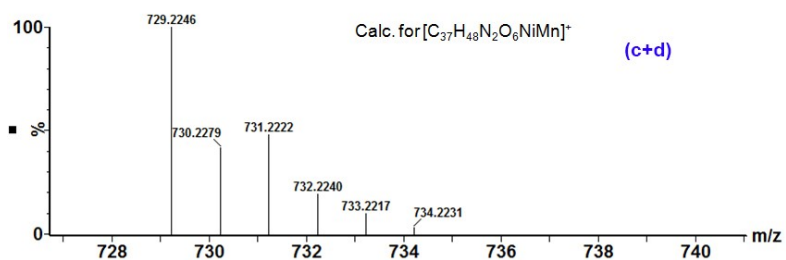
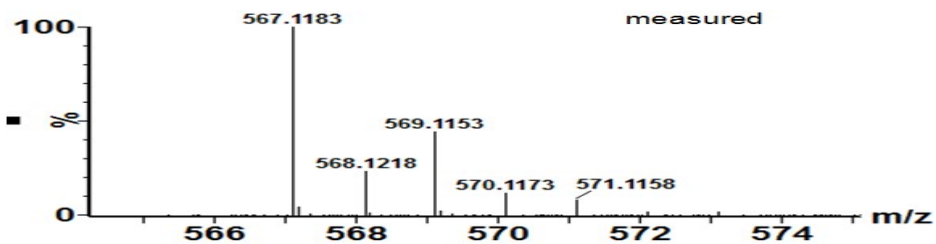
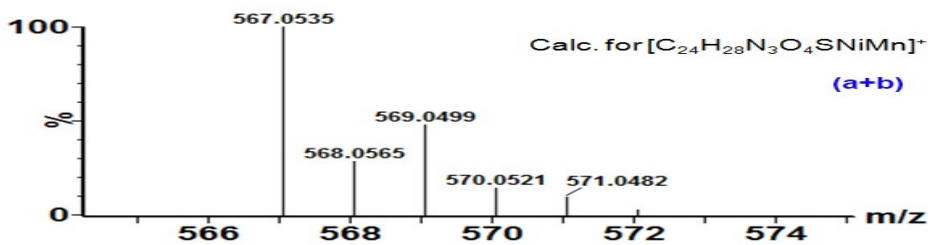
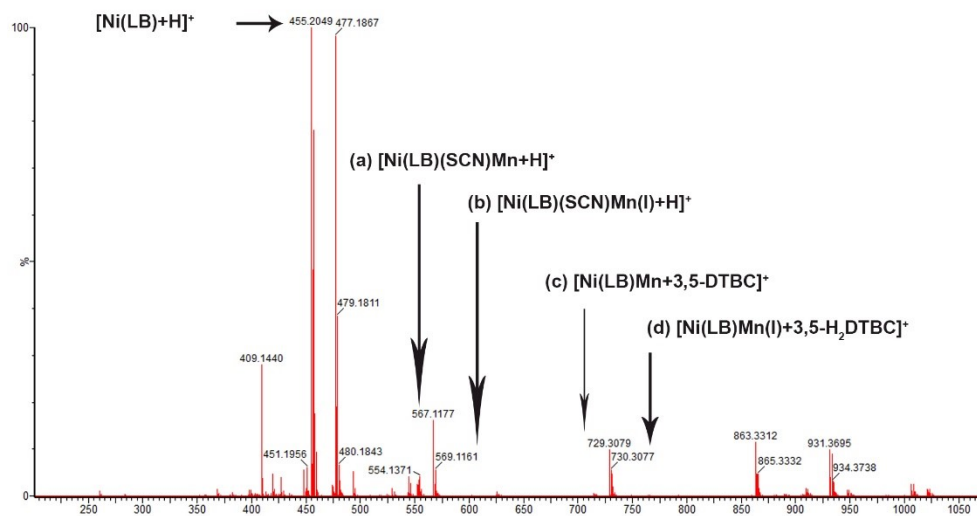


Fig. S8: ESI-MS analyses with isotopic distribution of complex 2 with 3,5-DTBC

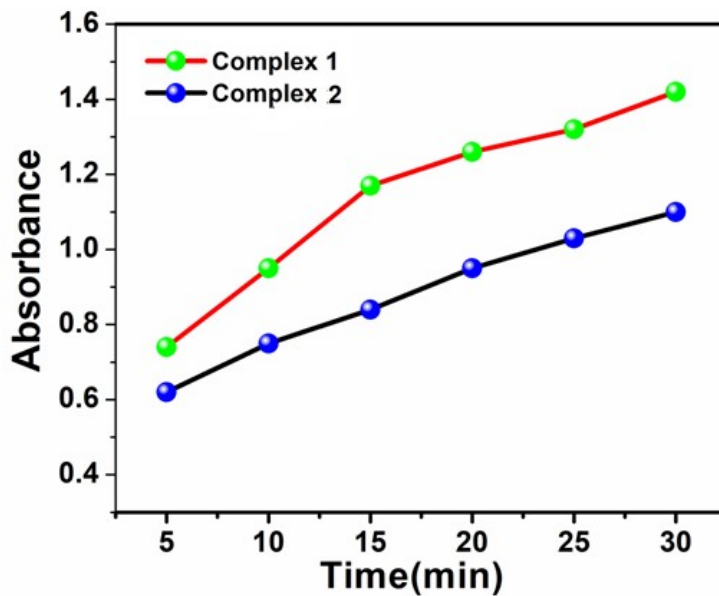


Fig. 9: Change of absorbance plot with respect to time for estimation of H_2O_2 , generated during catalysis in presence of complexes **1** and **2**

Experimental details: Equal volumes of Complex **1**, **2**, and catechol solutions were prepared and mixed as per the requirement to investigate kinetic studies. After an hour, the solution was acidified with H_2SO_4 to convert the pH of the solution to 2 and then an equal volume of water was added to the solution, to prevent any further oxidation. The quinone (3,5-DTBQ) was formed as a product and it was extracted with dichloromethane. After that 1 mL of a 10% solution of KI was mixed with the aqueous layer followed by the addition of three drops of 3% ammonium molybdate solution and the formation of I^{3-} was monitored spectrophotometrically by enhancement of its characteristic absorption band at $\lambda = 353 \text{ nm}$ ($\epsilon = 26000 \text{ M}^{-1}\text{cm}^{-1}$).

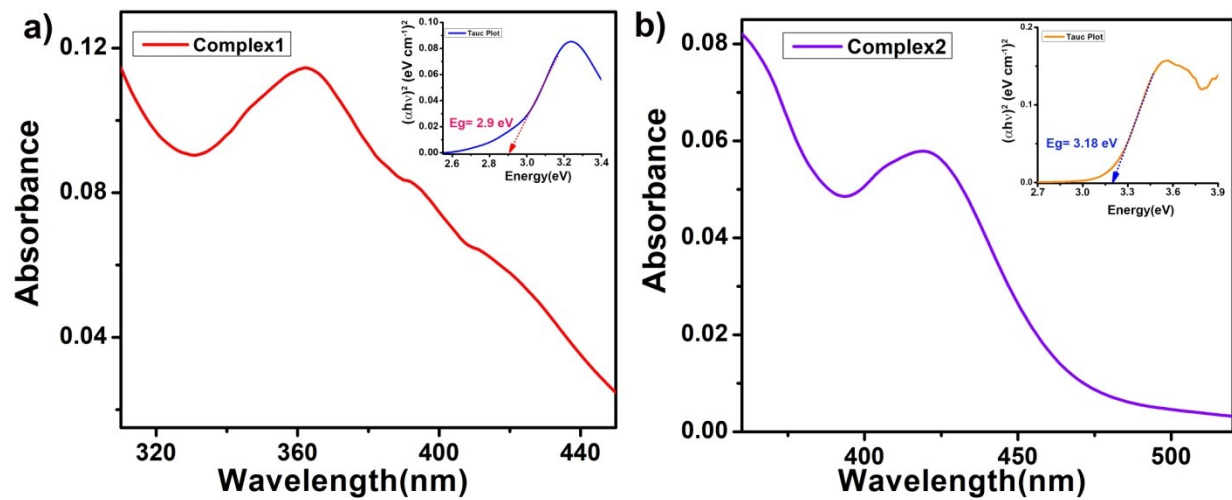


Fig. S10: Band gap energy calculation plot of complex 1, 2