Supporting Information

Influence of Nitrogen Donor Ligands on the Supramolecular Architecture of Copper (II) 2-Nitrobenzoate Complexes: Structures, DFT Calculations and Magnetic Properties

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Thermogravimetic Analysis.

Thermogravimetric analysis of complexes **1-3** was examined from 33 to 1000° in air to study the thermal stability (Fig. S1-S3). In the TG curve of **1** the first weight loss step (calc = 23.99% , expt = 22.75%) from 74-158 °C corresponds to loss of one molecule of γ-picoline and one nitro molecule from one nitrobenzoate moiety.-In **2,** the first weight loss step (calc = 5.82% , expt = 6.00%) from 70-108 °C corresponds to the loss of two coordinated water molecule whereas the second and the third steps correspond to loss of one □-pic molecule (calc = 15.06%, expt = 14.99% from 108-175 °C) and two nitrobenzoate moieties-(calc = 54.00% , expt = 51.99% from 179-235 °C) respectively. In **3,** the first and second weight loss corresponds to the loss of two lattice water (calc = 4.55%, expt = 4.74% from 30-104 °C) and one 2-nitrobenzoate moiety (calc = 20.99% , expt = 20.52% from 104-198 °C) respectively.

IR and electronic spectroscopy

Infrared spectrum of the newly synthesized complex salts have been recorded in the region 4000-400 cm^{-1} and tentative assignments have been made on the basis of earlier reports in literature [K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, 1997**,** John Wiley & Sons, New York , 5th Ed. , J. Bellamy, The Infrared Spectra of Complex Molecules, 1980, Chapman & Hall, London/ New York, Ed.]. The strong band in the region 3371 cm^{-1} in **2** and 3418- 3225 cm^{-1} in **3** may be attributed to OH(H_2O) stretching and OH of triethanolamine and H_2O stretching, respectively. The bands varying from weak to medium intensity in the region 2877–3167 cm^{-1} and 1607-1601 cm^{-1} in complexes **1**,**2** and **3** may be respectively attributed to CH stretching. In **1-3,** the bands between 1593 -1578 cm^{-1} and 1393- 1385 cm^{-1} may be ascribed to ν_{as}(COO) and ν_s(COO), respectively. The $\Delta\nu$COO = ν_{as}(COO) - ν_{sym}(COO) values are 175 cm^{-1} in **1**, 200 cm^{-1} in **2** and 216 cm-1 in **3** which indicates the presence of bidentate brigding in **1** and monodentate in 2 and 3. The bands between 1340- 1367cm^{-1} and 1524-1537 cm^{-1} in all complexes may be assigned to asymmetric and symmetric stretching mode of nitro group respectively. The bands at 835, 836 and

813 cm^{-1} may be ascribed to δ(NO2) in **1**, **2** and **3** respectively. The bands at 4597, 554 cm^{-1} in **1,** at 463, 538 cm^{-1} in **2** and 466 and 568 cm-1 in **3** are ascribed to ν(Cu-N) and ν(Cu-O) vibrations. The bands at 648, 493 cm^{-1} in **1** and at 649, 513 cm^{-1} in **2** were ascribed to coordinated in plane and out plane ring deformation of γ-picoline and β-picoline, respectively. IR spectra are available as Figures S4-S6 .

The electronic spectra of complex **1, 2** and **3** were recorded in methanol. Complex **1** showed absorption at 732 (ε_{max} = 94.07 mol^{-1} L cm^{-1}) wheras complex **2** and **3** showed maximium absorption 738 nm with ε_{max} = 102.5 mol^{-1} L cm^{-1} and with ε_{max} 63.41 $Lmol^{-1}cm^{-1}$ respectively, due to the d-d transitions. These values are agreement with those observed by O_4N_2 chromophore [F. A Cotton, G. Wilkinson, C. A Muritto, M. Bochmann, *Advanced Inorganic Chemistry*, sixth ed., 1999, John Wiley and Sons, New York, 869; R. P. Sharma, A. Saini, S. Singh, A. Singh, P. Venugopalan, P. Starynowicz, J. Jezierska, *J. Mol. Struct.* 2011**, 994**, 21–28].

Figure S1. The TGA of complex salt **1**

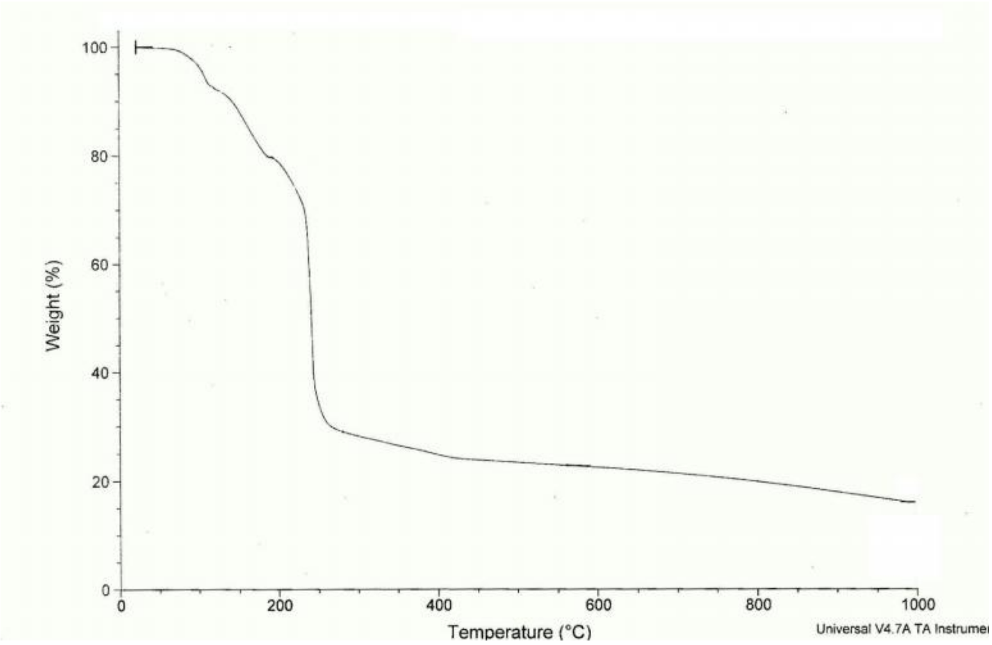

Figure S2. The TGA of complex salt **2**

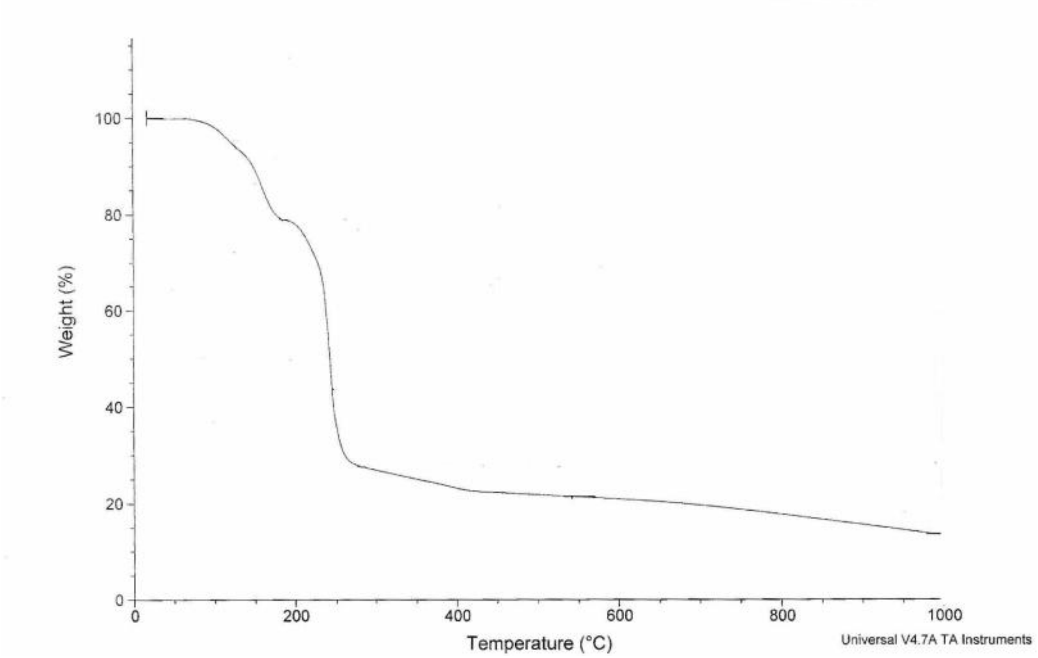

Figure S3. The TGA spectrum of **3**

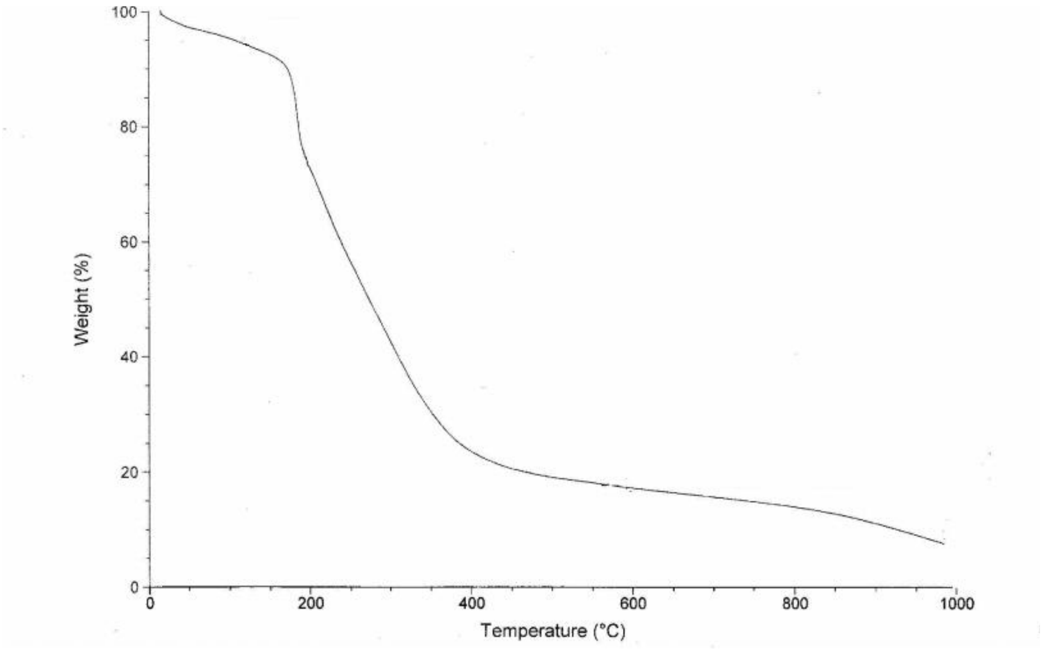

Figure S4. IR spectrum of complex **1**

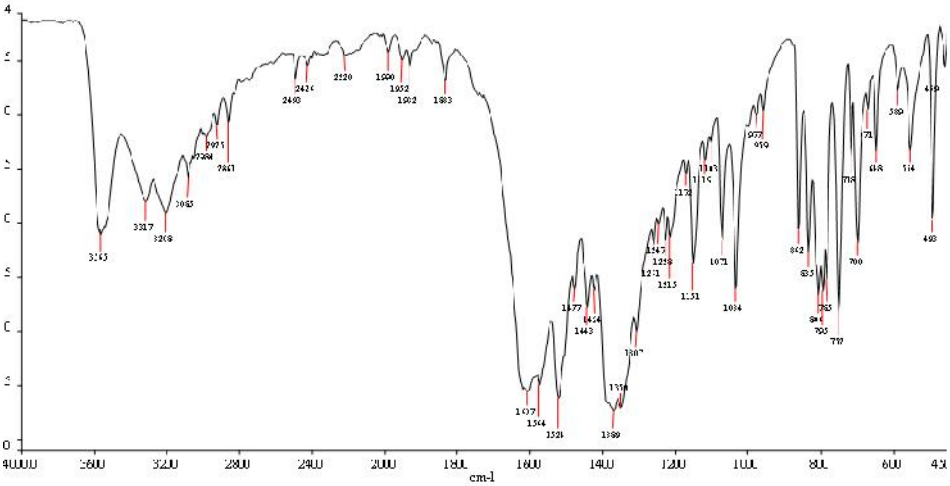

Figure S5. IR spectrum of complex **2**

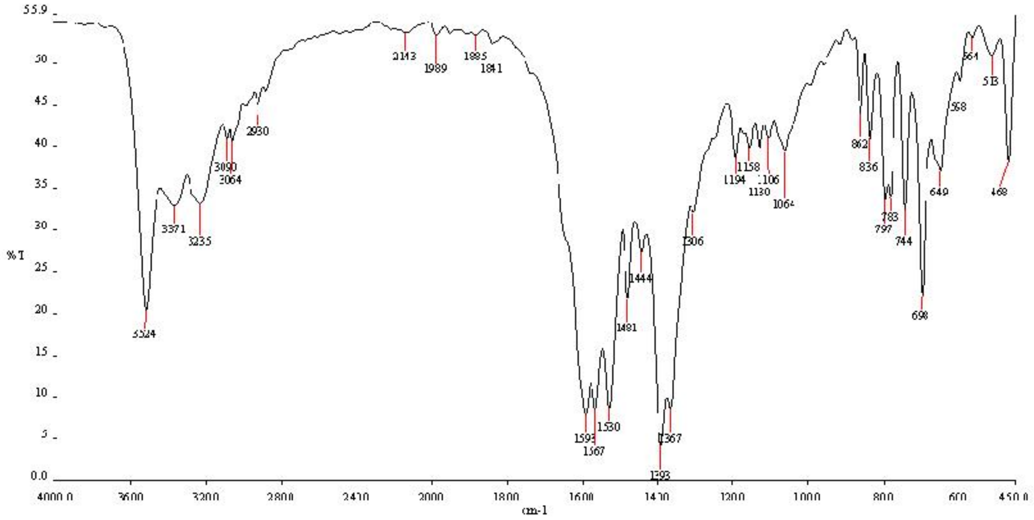

Figure S6. IR spectrum of complex **3**

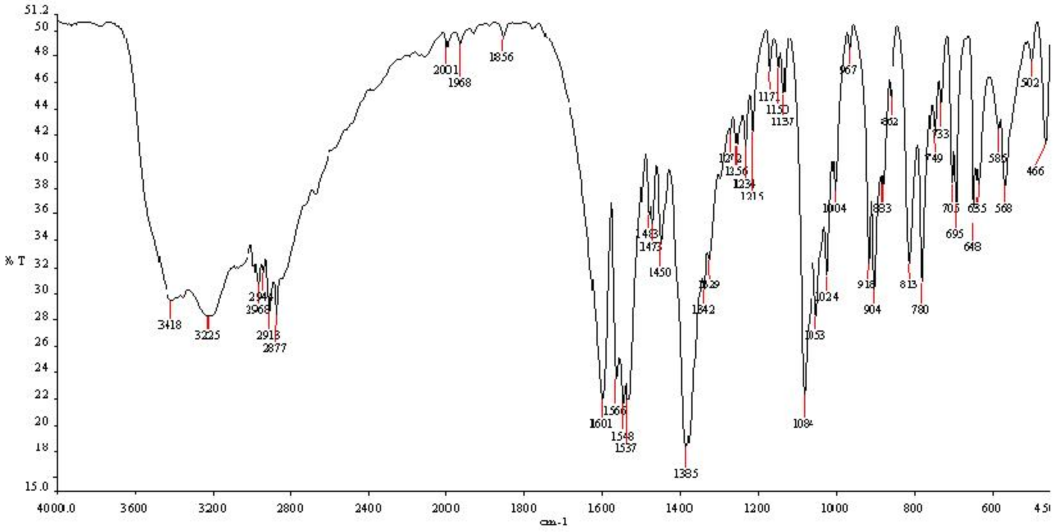

Figure S7. Packing diagram of complex **1** viewed down a axis

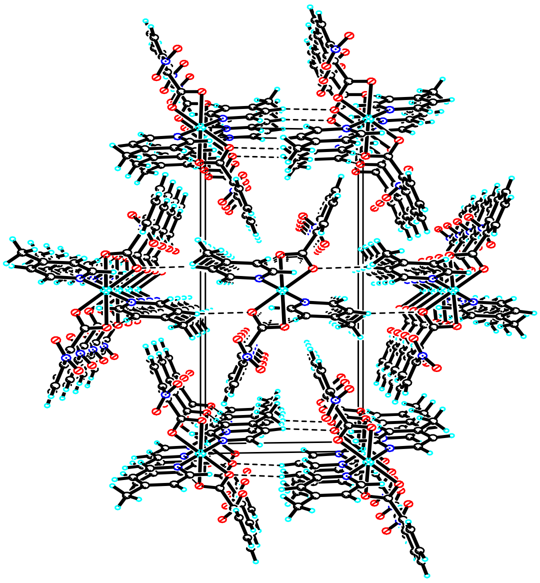

Figure S8. Packing diagram of complex **2** viewed down b axis

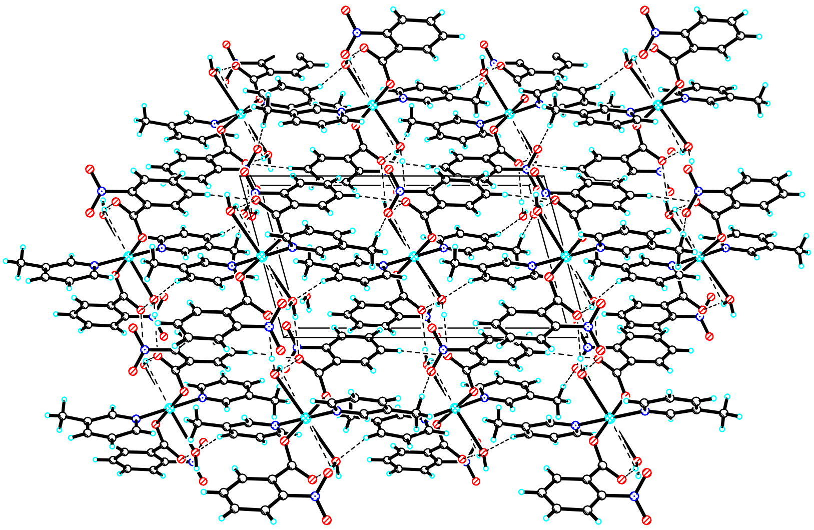

Figure S9. Packing diagram of complex **3** viewed down a axis