Electronic Supplementary Information for Dalton Transactions

Coordination and hydrogen bonded network structures of Cu(II) with mixed ligands: a hybrid hydrogen bonded material, an infinite sandwich arrangement, and a 3-D net.

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$[Cu(phendione)_2(H_2tma)_2].2(H_3tma).1.65(CF_3CH_2OH).2.5(H_2O)$ 5

Thermogravimetric analysis of **5** is shown in Figure 1 and indicates the complex is stable to high temperatures and that full solvent loss occurs in two stages with a 14.2% weight loss corresponding to the loss of all solvent.

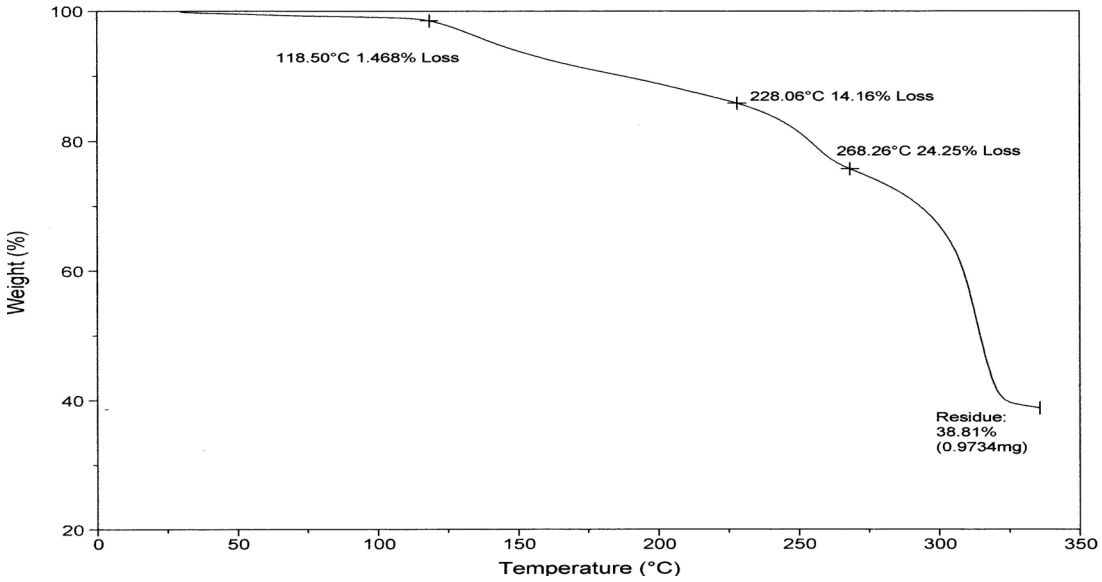
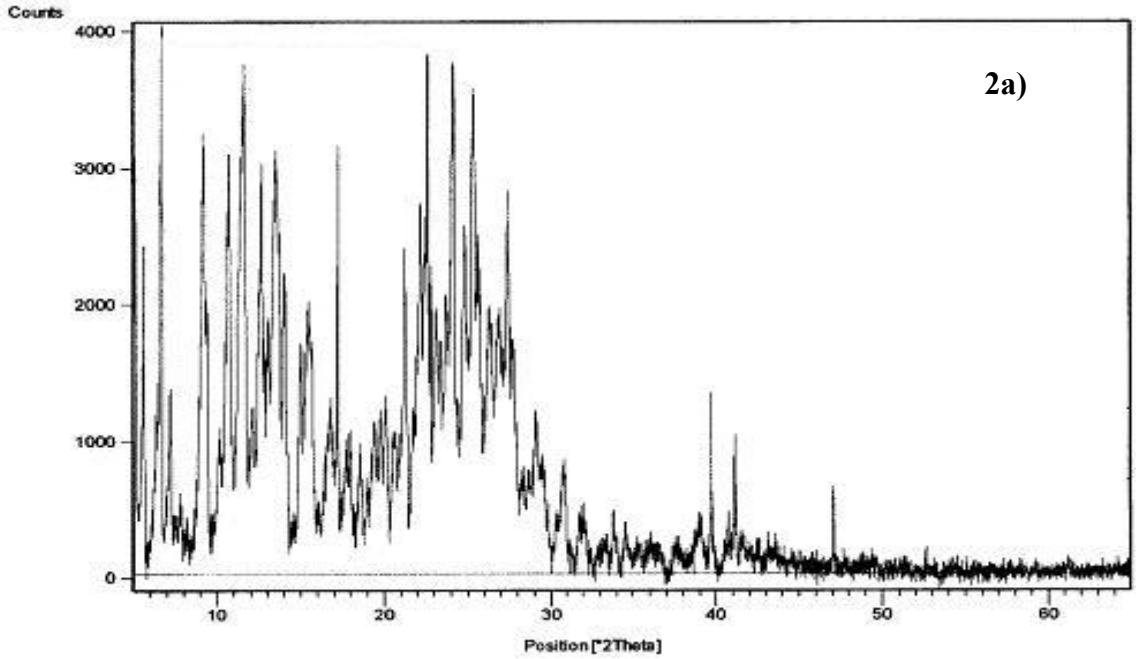
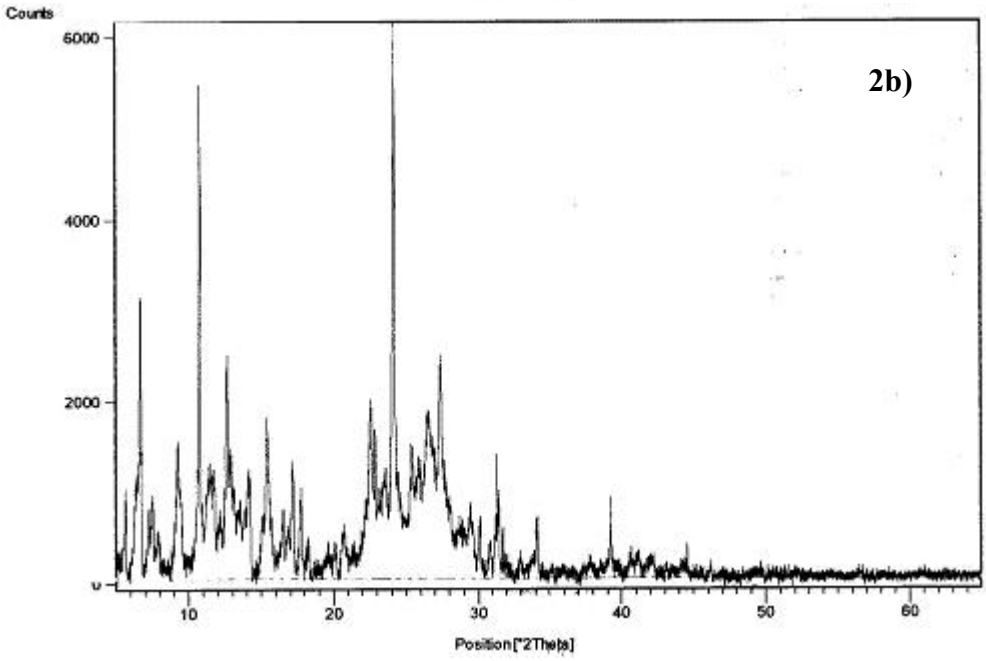


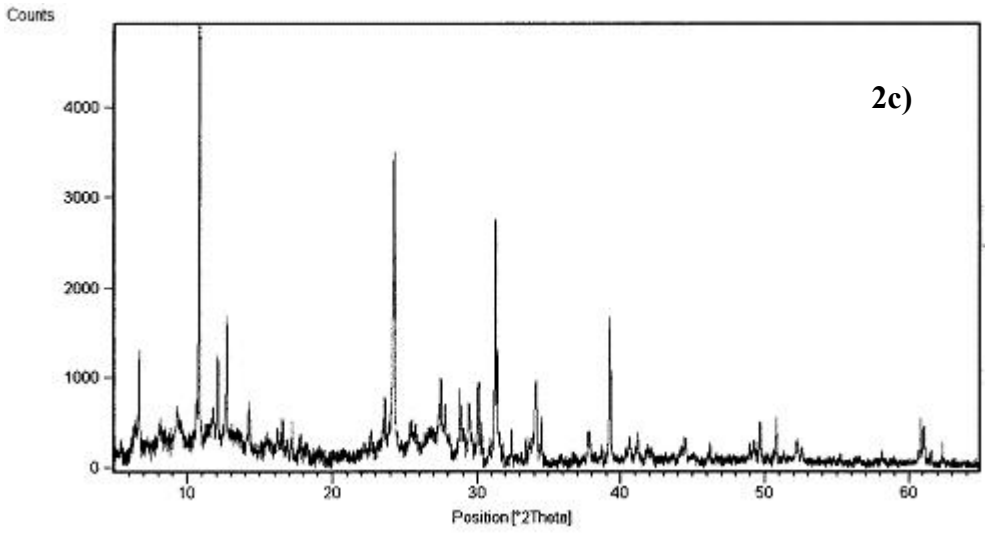
Figure 1: TGA of complex **5**.

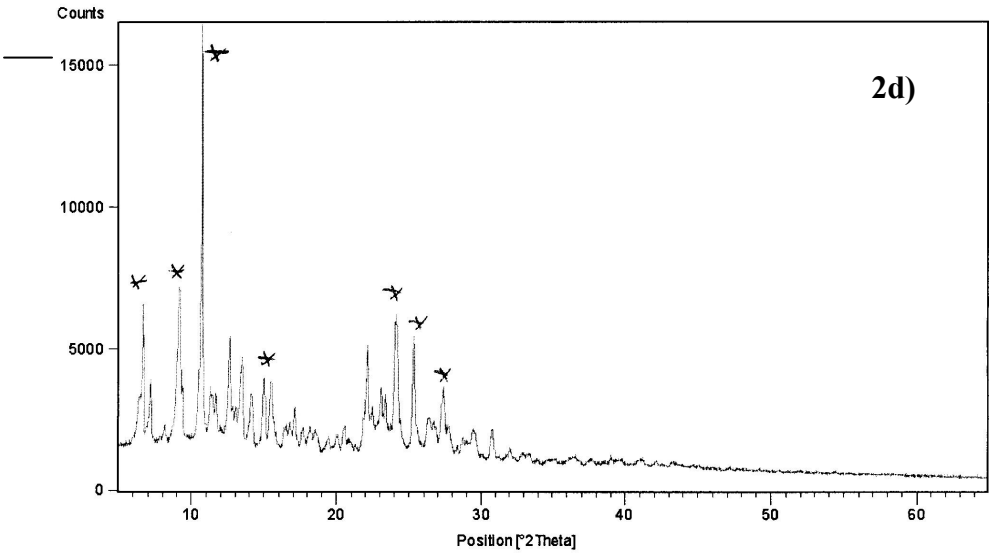
Complexes $[Cu(o\text{-}phen)(H_2tma)_2]_2.2(H_3tma)$ 6 and $[Cu(o\text{-}phen)(H_2tma)_2]$ 7

The formation of complex **6** or the previously reported **7** depends of heating time under solvothermal conditions, Figure 2. Short heating times gives material of poor crystallinity, while at 15, 17 and 19 hrs heating single crystals of **6** were obtained and their identity confirmed by single crystal unit cell determinations. Note that satisfactory refinement of the single crystal structure of **6** employed the SQUEEZE routine; hence the model is missing disordered solvent molecules and a reliable calculated powder pattern cannot be obtained from this structure model. The samples at 15 hrs and 17 hrs all contained some amorphous material as well, and at 19 hrs the powder XRD indicates the presence of some complex **7** (peaks indicated by asterix, Figure 4d) hence TGA was not undertaken. The calculated powder XRD for complex **7** is shown in Figure 3. Minor discrepancies in 2θ values between the calculated and measured patterns will be due to the measured pattern being collected at room temperature, while the single crystal structure was performed at low temperature.









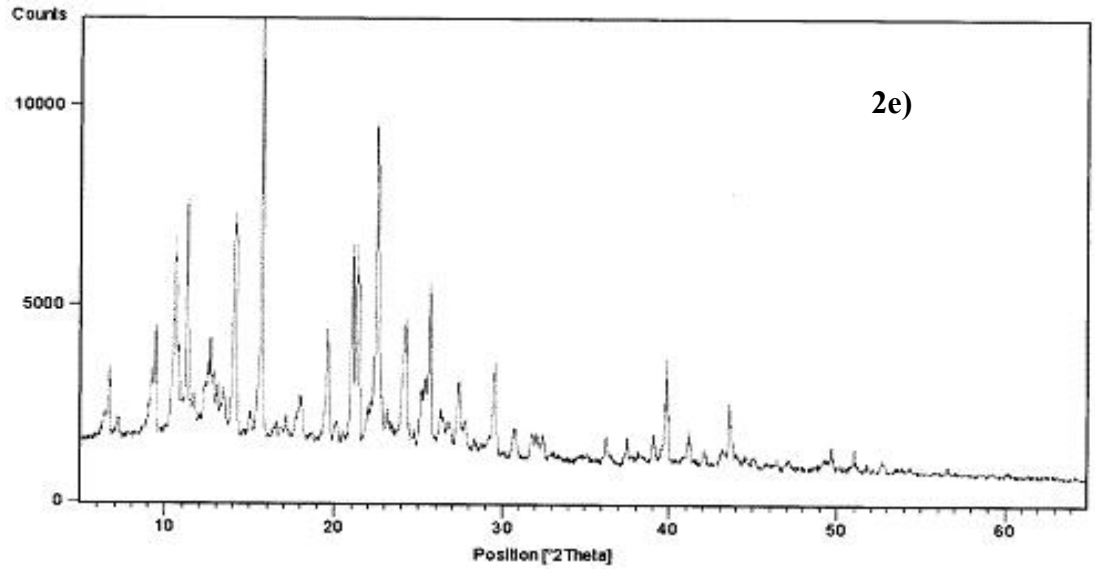


Figure 2: Measured powder XRD patterns (at 298 K) of blue solid obtained from Parr reaction vessels after (a) 13 hrs; (b) 15 hrs; (c) 17 hrs; (d) 19 hrs; (e) 24 hrs heating time.

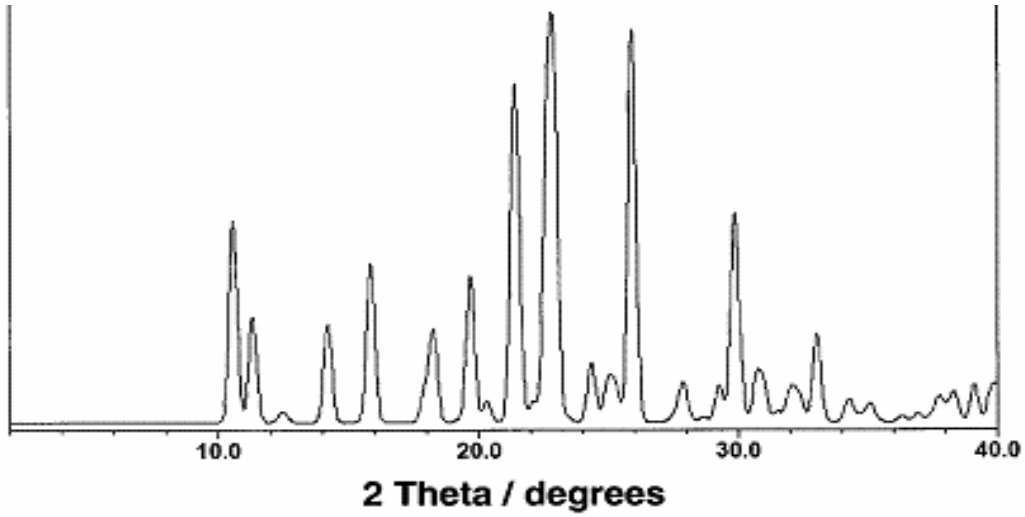


Figure 3: Powder XRD pattern calculated from the single crystal structure of **7** determined from data collected at 150 K.