

Supporting Information

Retention of Cs-Cl bond induces coordination polymer formation over trinuclear chiral assembly of copper(II) complexes of L-leucine derived ligand

Mrigendra Dubey^a and Manabendra Ray*

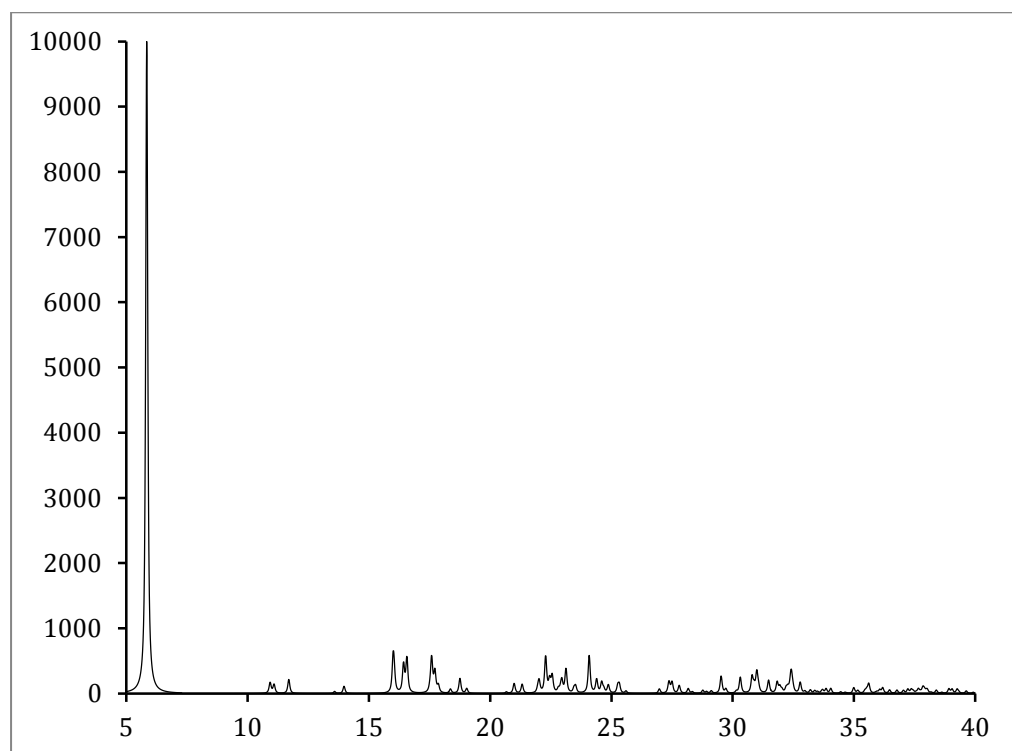
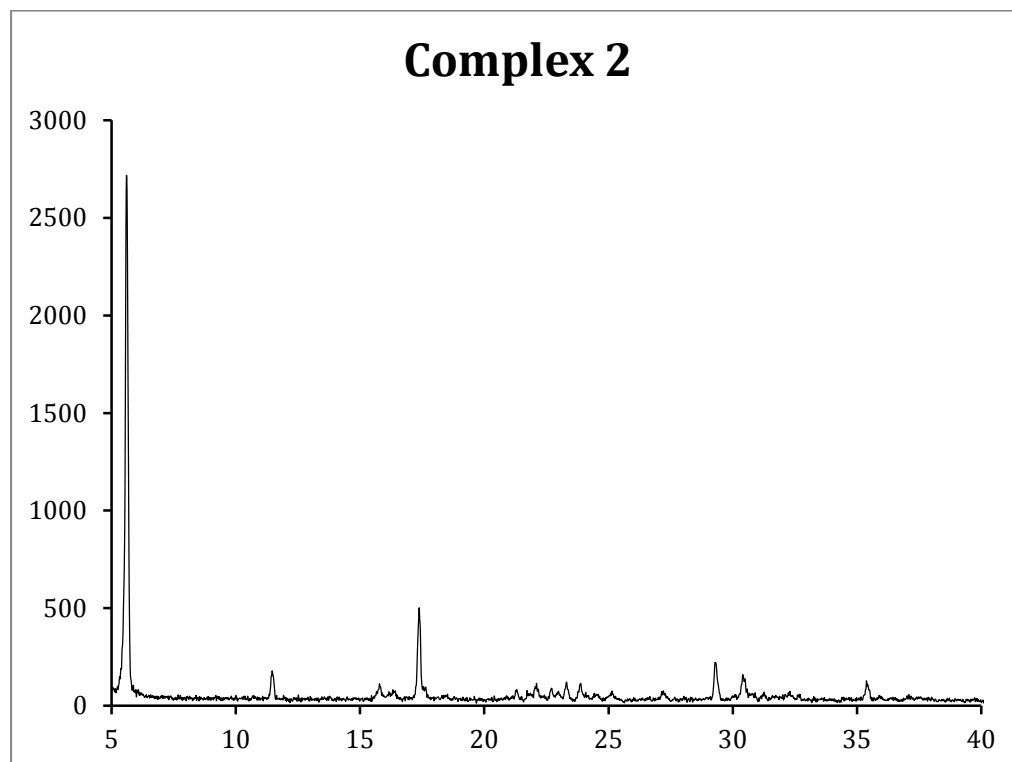


Figure S1. Experimental (top) and simulated (bottom) powder diffraction plot for complex 2.

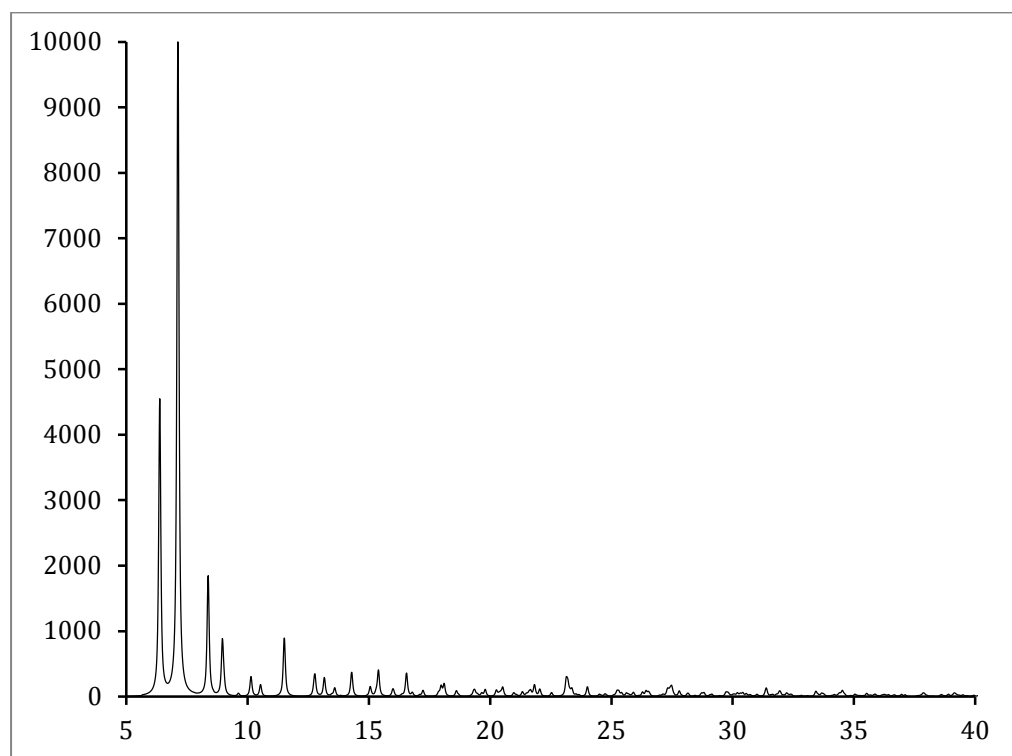
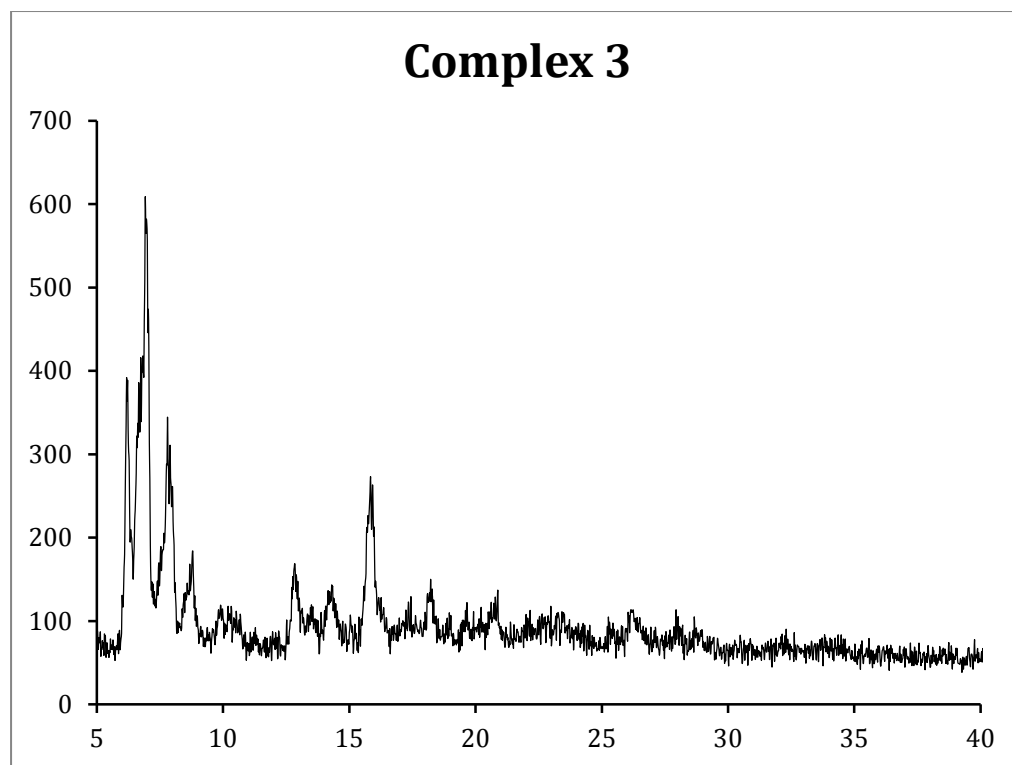


Figure S2. Experimental (top) and simulated (bottom) powder diffraction plot for complex 3.

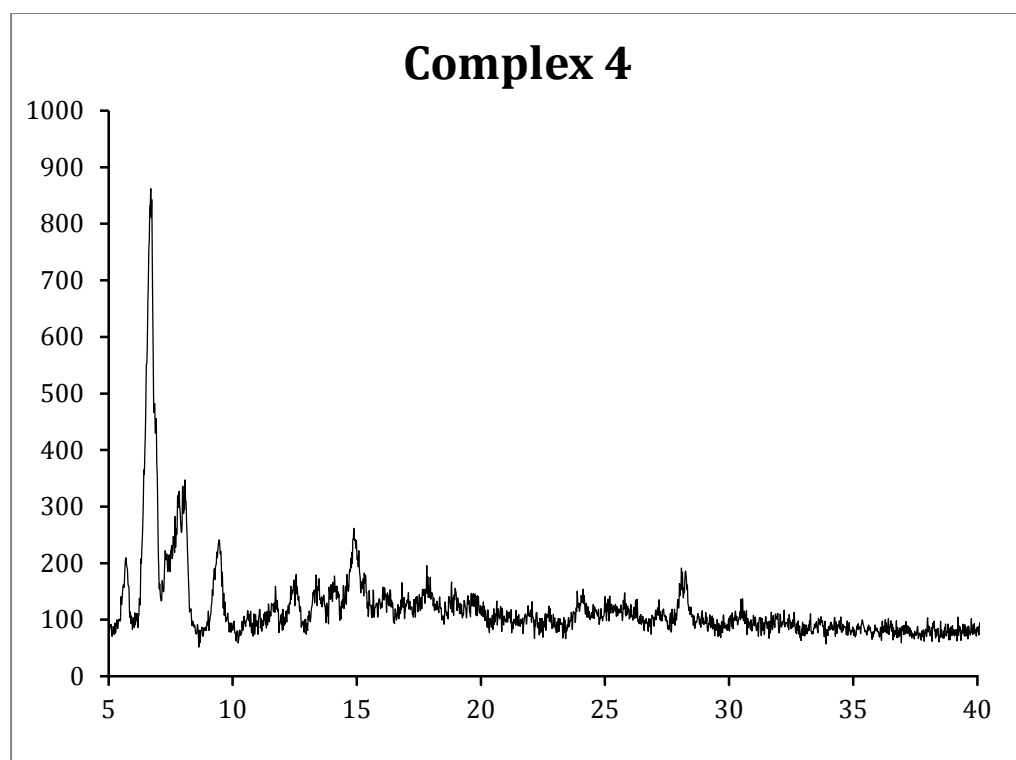


Figure S3. Experimental powder diffraction plot for complex **4**.

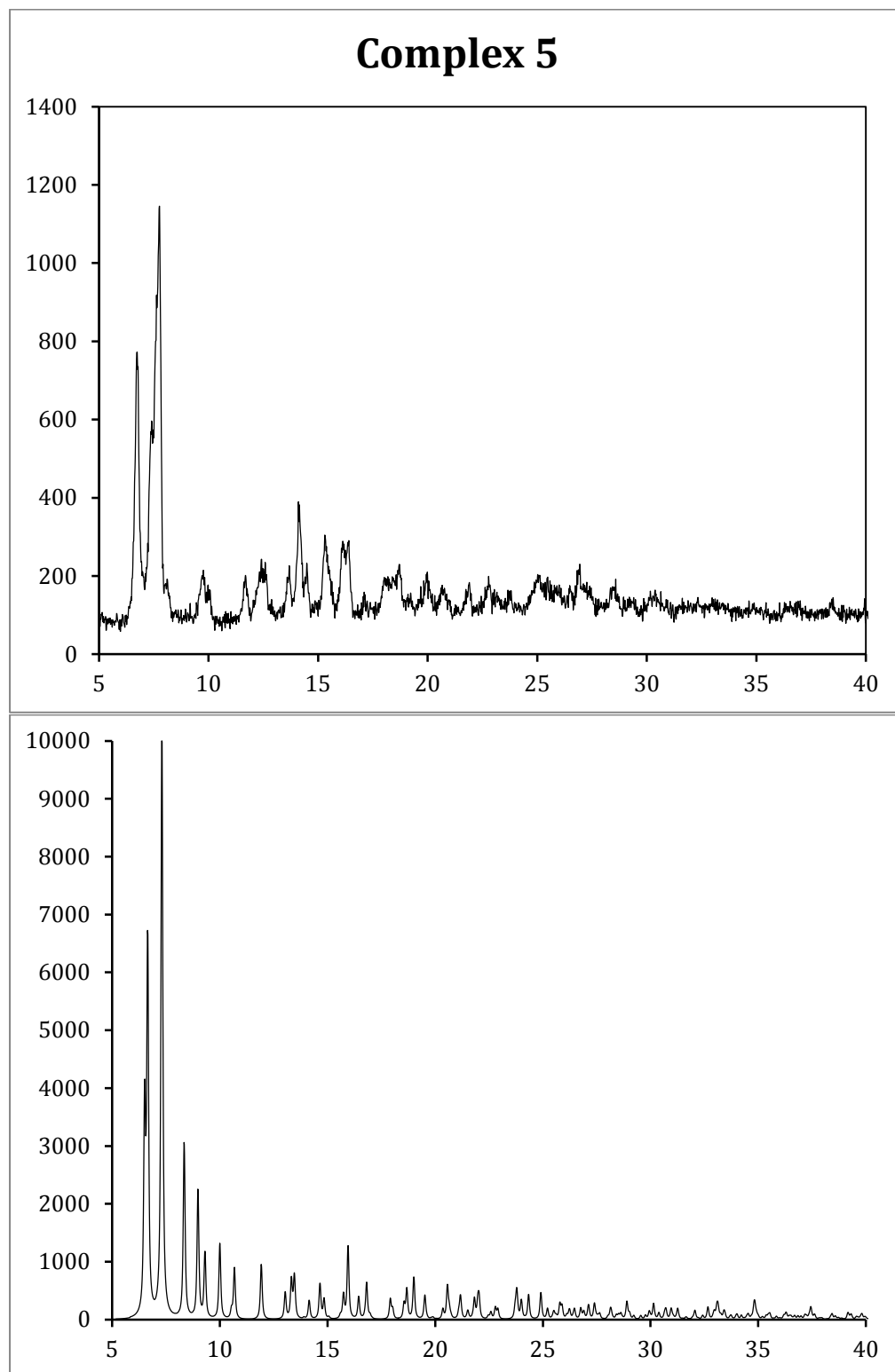


Figure S4. Experimental (top) and simulated (bottom) powder diffraction plot for complex 5.

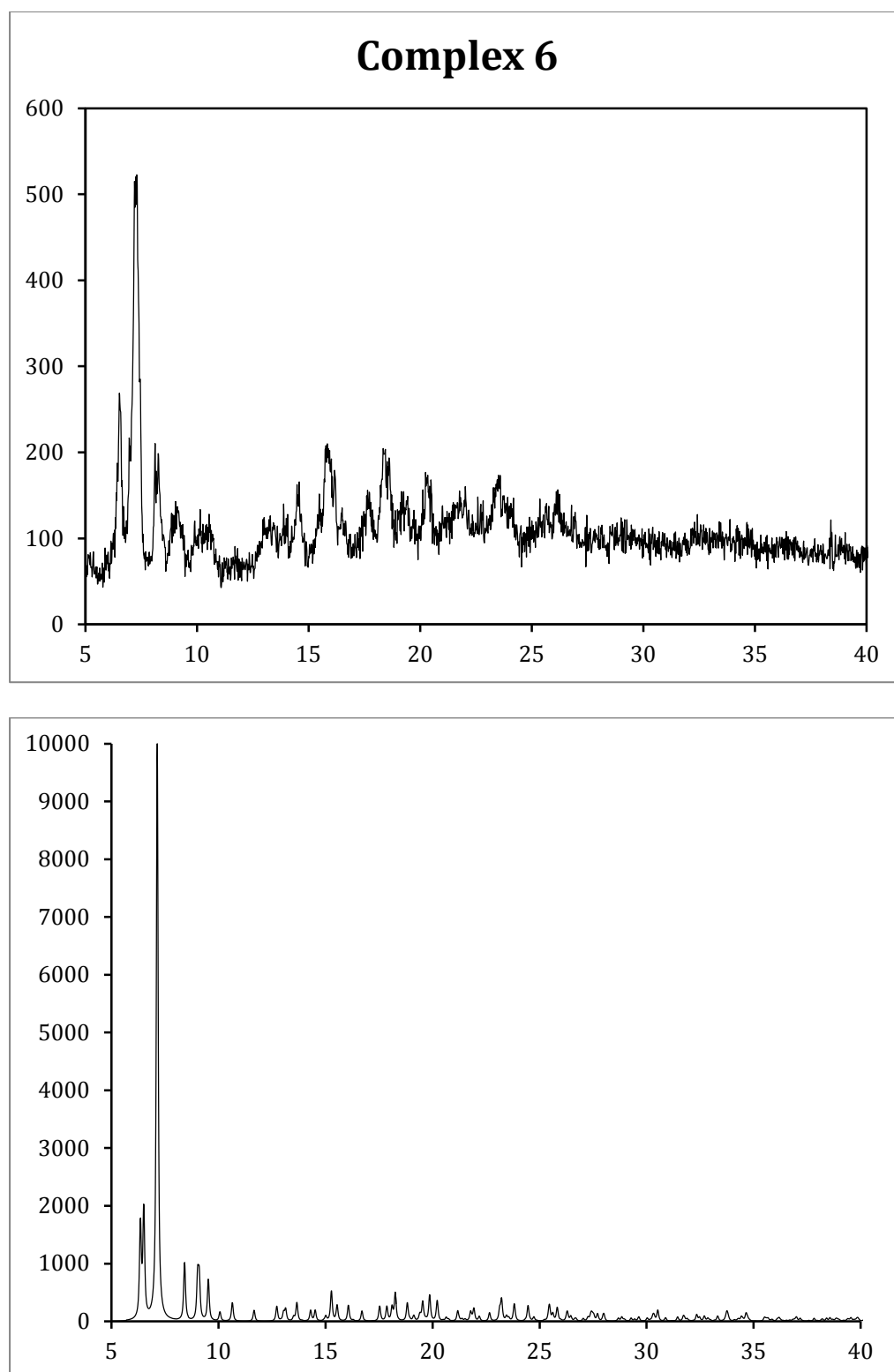


Figure S5. Experimental (top) and simulated (bottom) powder diffraction plot for complex 6.

Thermogravimetric Analysis (TGA)

To determine quantity of water in the crystal, analyses were performed from room temperature to 600 °C at 5 °C/min heating rate. Considerable weight losses (>12%) for complex 3, 4 and 6 occur over a wide range in multiple overlapping slopes. This suggests partial decomposition followed by loss of water of crystallization (or solvent). Thus determination of quantity of solvent loss is difficult. For complex 2 and 5 this is not the case. In the table below we have tabulated the experimental loss along with expected loss for number of water/solvent molecules used in the formulation based on elemental analysis. Estimation for complex 2 and 5 supports the formulation obtained from elemental analysis. It should be noted that the values obtained from TGA could vary based on a particular batch, nature of the complex and heating rate used. Thus for the formulation of the bulk material we have used elemental analysis preferentially.

| Complex | experimental weight loss % | Calculated weight loss % |
|---------|----------------------------|-----------------------------|
| 2 | 5.3 % (between 25-150 °C) | 7.1% for 3 H ₂ O |
| 5 | 6% (between 25-150°C) | 6.8% for 7 H ₂ O |

TGA Plots

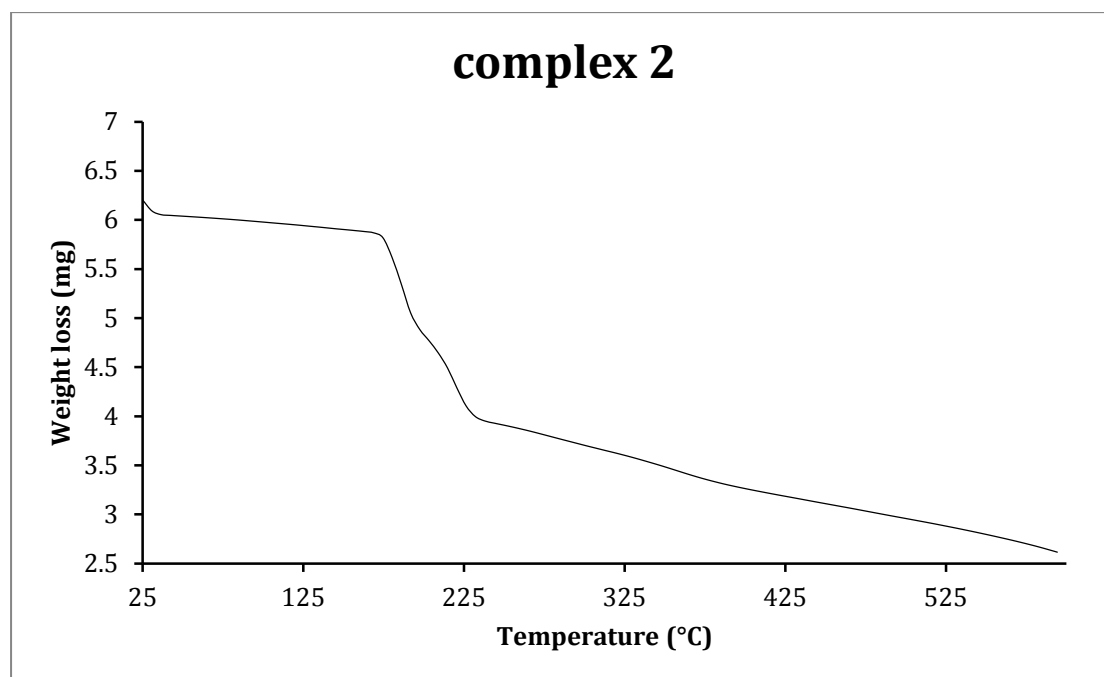


Figure S6. TGA plot for complex 2.

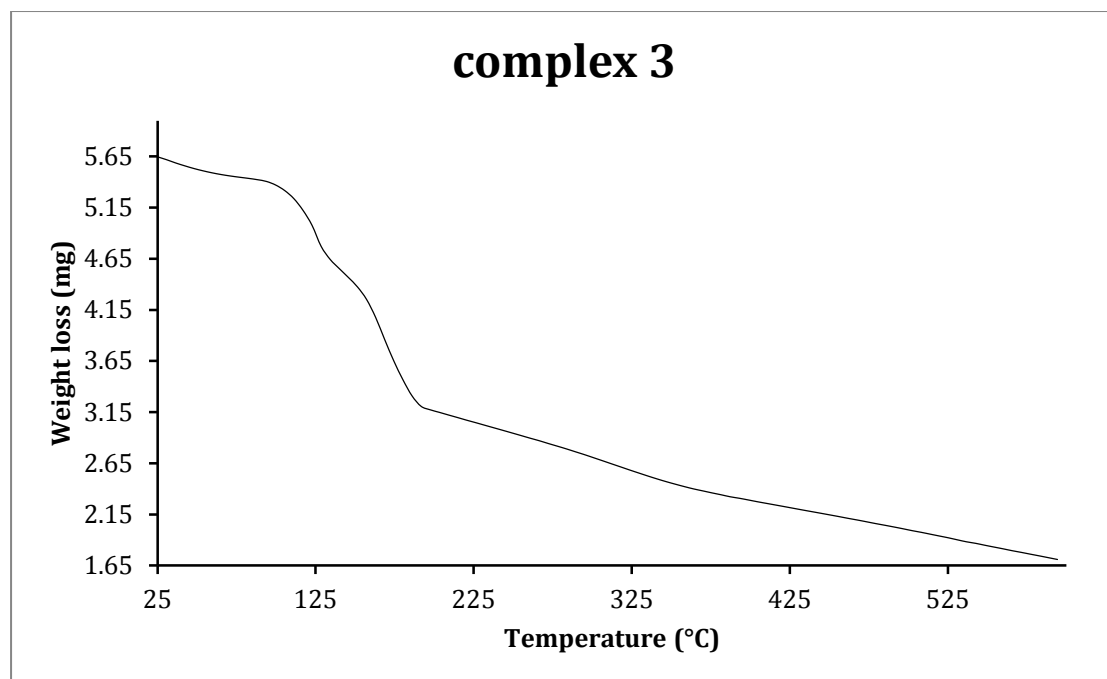


Figure S7. TGA plot for complex 3.

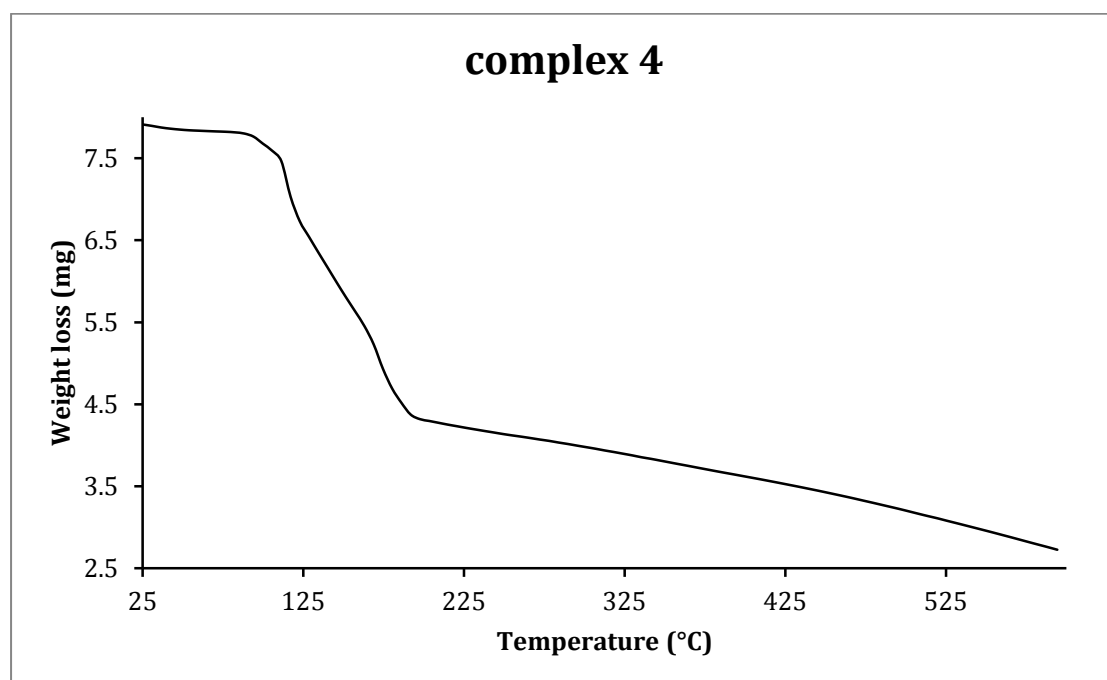


Figure S8. TGA plot for complex 4.

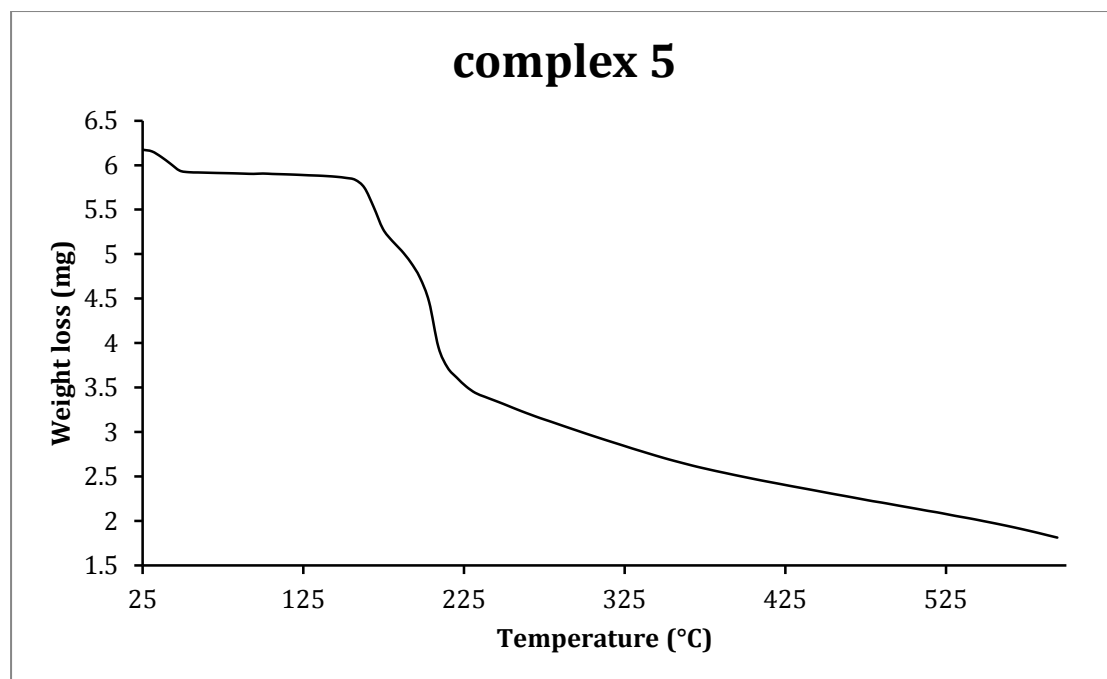


Figure S9. TGA plot for complex 5.

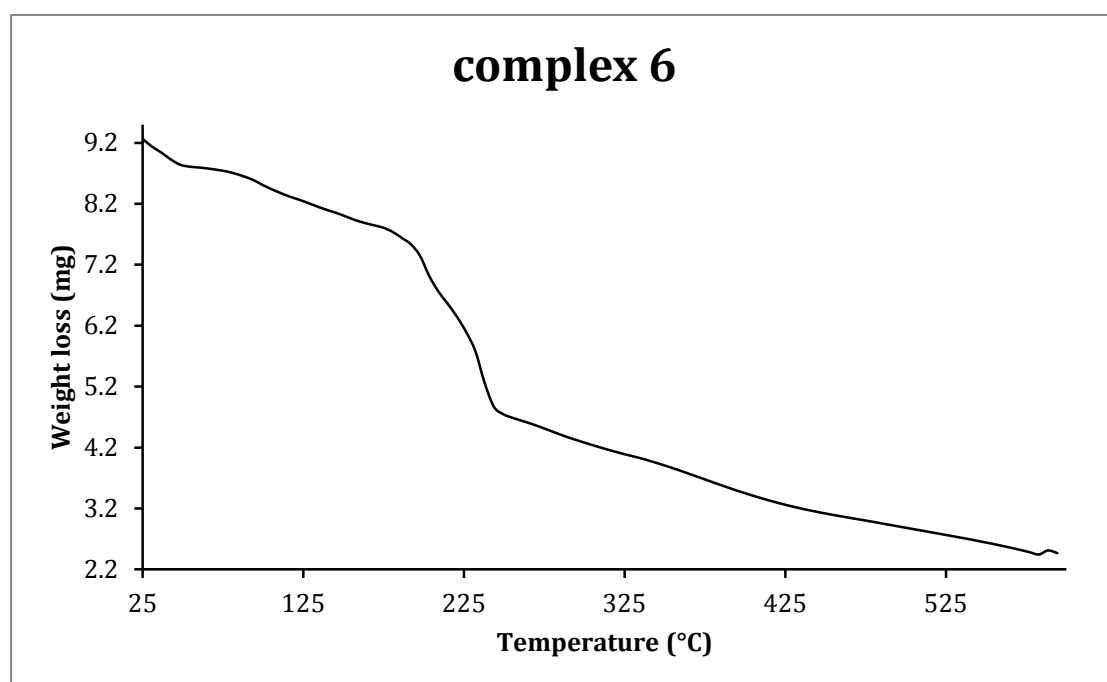


Figure S10. TGA plot for complex 6.