Supplementary Information

Synthesis, Characterization, and DFT Computational Study of Cu(II) Complex with 3-Hydroxybenzoate

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Calculation of Cu Content in AAS Analysis

The concentration of Cu(II) in each sample can be determined using the following Equations 1 and 2.

$$\text{Weight of Cu (mg)} = \text{Cu Concentration (ppm)} \times \text{Volume (L)} \quad (1)$$

$$\%\text{Cu} = \frac{\text{Weight of Cu (mg)}}{\text{Weight of complex sample (mg)}} \times 100\% \quad (2)$$

Table S1. Calculation of Cu(II) content in the Cu(II)-3HBA complex.

Sample Weight (mg)	Volume (mL)	Concentration (ppm)	Cu^{2+} mass (mg)	% Cu^{2+}	Average %Cu^{2+}
7	10	3.6864	0.9216	13.1657	13.168 ± 0.03
		3.6878	0.9219	13.1707	
		3.6875	0.9218	13..169	

Thermogravimetric Analysis

Table S2. Calculation of H_2O release in the Cu(II)-3HBA complex.

Temperature (°C)	Weight loss (%)	Estimated H_2O (482.756 g/mol)	Cu(3-hydroxybenzoic acid)$_2Cl_2 \cdot 4H_2O$
30 – 110	14.913	Experiment $14.91\% \times 482.756 = 65.36 \sim 4H_2O$	Theory $\frac{0}{482.756} \times 100\% = 14.914\%$