

# Synthesis and Characterization of Hematite-Based Nanocomposites as Promising Catalysts for Indigo Carmine Oxidation

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The concentrations of H<sub>2</sub>O<sub>2</sub> at the end of the catalytic tests were determined by the spectrophotometric methods 209 and 210 developed on Aqualytic spectrophotometer AL 800/SpectroDirect (Dortmund, Germany) using the specific reagent kits for the concentrations range of 0.01–0.5 mg/L and 0.03–1.5 mg/L H<sub>2</sub>O<sub>2</sub>.

Method 209 uses Hydrogen peroxide LR reagent tablets allowing the determination of concentrations in the range of 0.01–0.5 mg/L H<sub>2</sub>O<sub>2</sub>. Zero is determined with 50 mm cells filled with the water samples. After zero determination, the cell is emptied into a beaker, and the cell is dried completely. After rinsing the beaker with the water sample and emptying it, a few drops of water should remain in the beaker and the Hydrogen peroxide LR reagent tablets has to be crushed inside the beaker using a clean stirring rod. After the tablet is crushed, 10 mL of water sample are added to dissolve the tablet. After dissolution the sample is transferred into the 50 mm cell of the spectrophotometer and after 2 minutes reaction time the measurement starts automatically.

Method 210 – uses Hydrogen peroxide LR reagent tablets allowing the determination of concentrations in the range of 0.03–1.5 mg/L H<sub>2</sub>O<sub>2</sub>. The procedure is similar to the above described one, but instead of 50 mm cells the samples are poured in spectrophotometer vials (24 mm diameter).

The Mössbauer spectra as well as the associated NORMOS fits are presented in Figure S1.

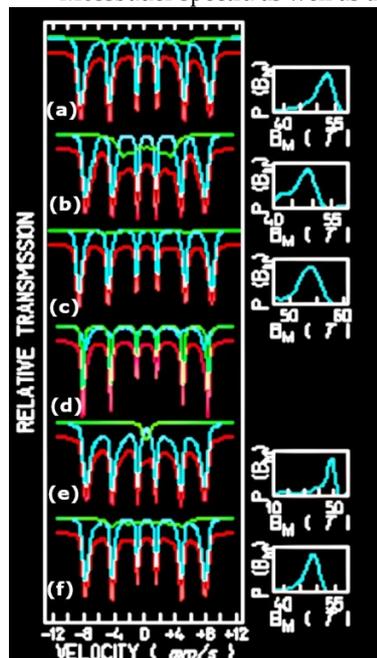


Figure S1. Mössbauer spectra and associated NORMOS fits.

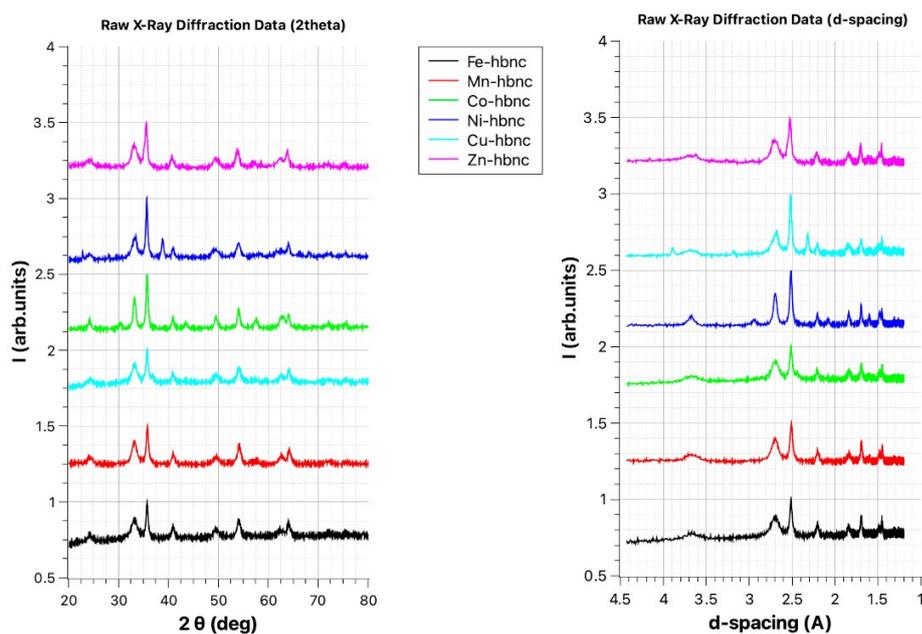
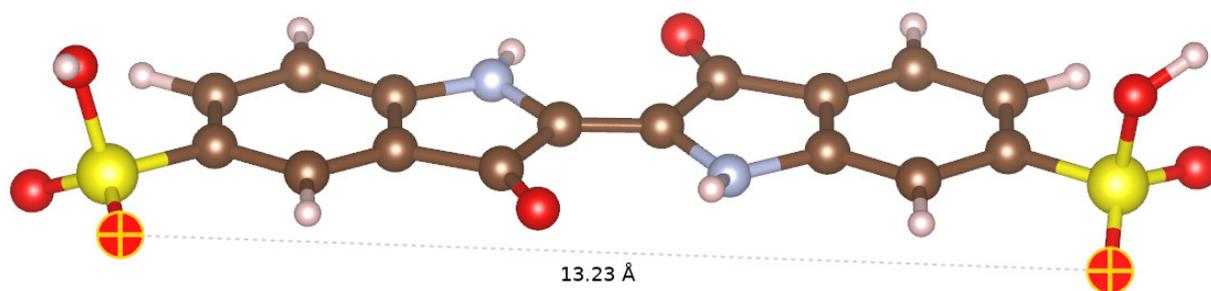


Figure S2. X-ray diffractograms in Bragg-Brentano configuration (left) and the same diffraction pattern using d-spacing instead of diffraction angles (right).

The optimized geometry of indigo carmine (IC) is shown in Figure S3. In order to estimate the diameter of the indigo carmine (IC) molecule an AM1 geometry optimization was performed with GAMESS 2021 R2 Patch 2 [41].



**Figure S3.** Optimized molecular structure of IC molecule visualized by VESTA [42].

The distance between the two S atoms is about 13.48 Å, while the distance between the two O atoms is about 13.23 Å (Figure S2).

## References

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