

Electronic supplementary information

Encapsulation of Hexaaza Macrocyclic Nickel(II) Complex in zeolite Y: An Experimental and Theoretical investigations

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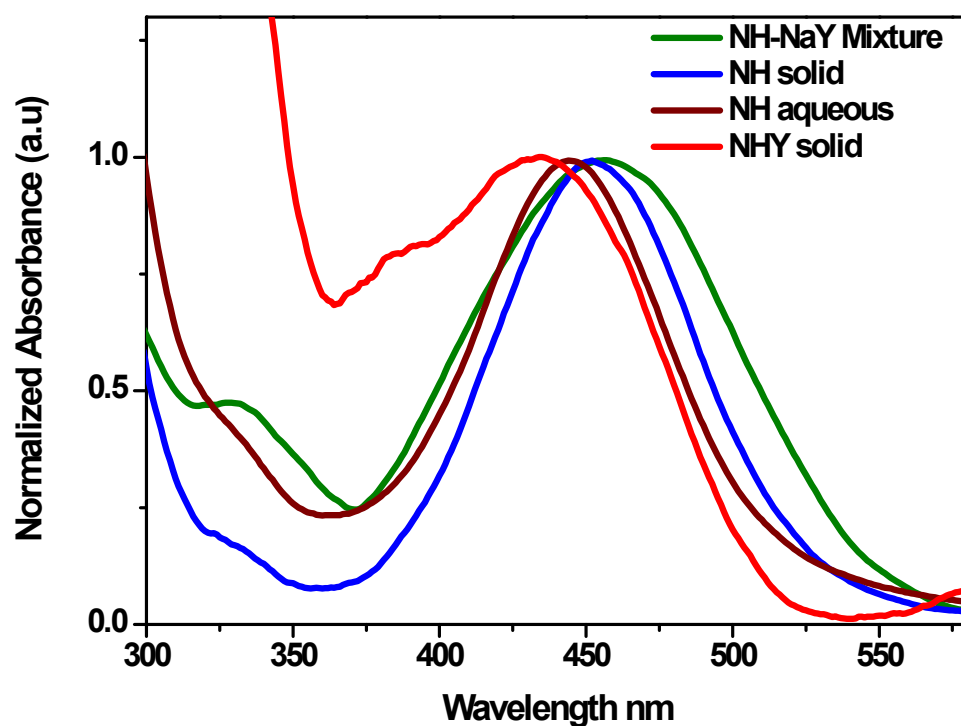


Figure S1. DRS UV-Visible spectra of the Physical mixture of Ni(II)hexaaza complex (NH) and zeolite Y (Na Y), Ni(II)hexaaza complex (NH), Ni(II)hexaaza complex in Y (NHY) and UV-Visible spectra of Ni(II)hexaaza complex (NH) in aqueous medium.

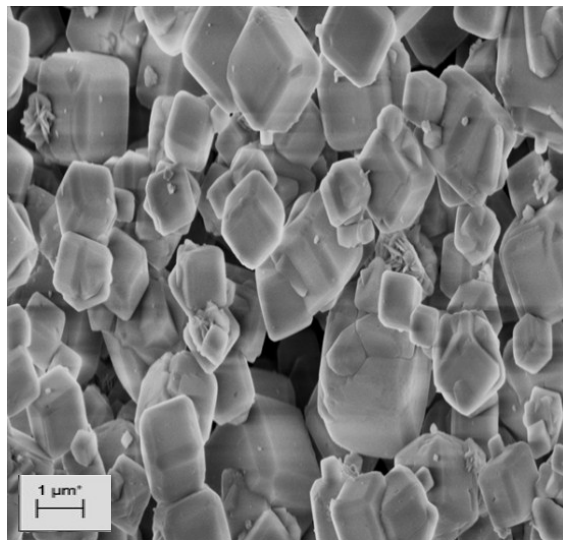


Figure S2. FESEM micrograph of Zeolite Na Y

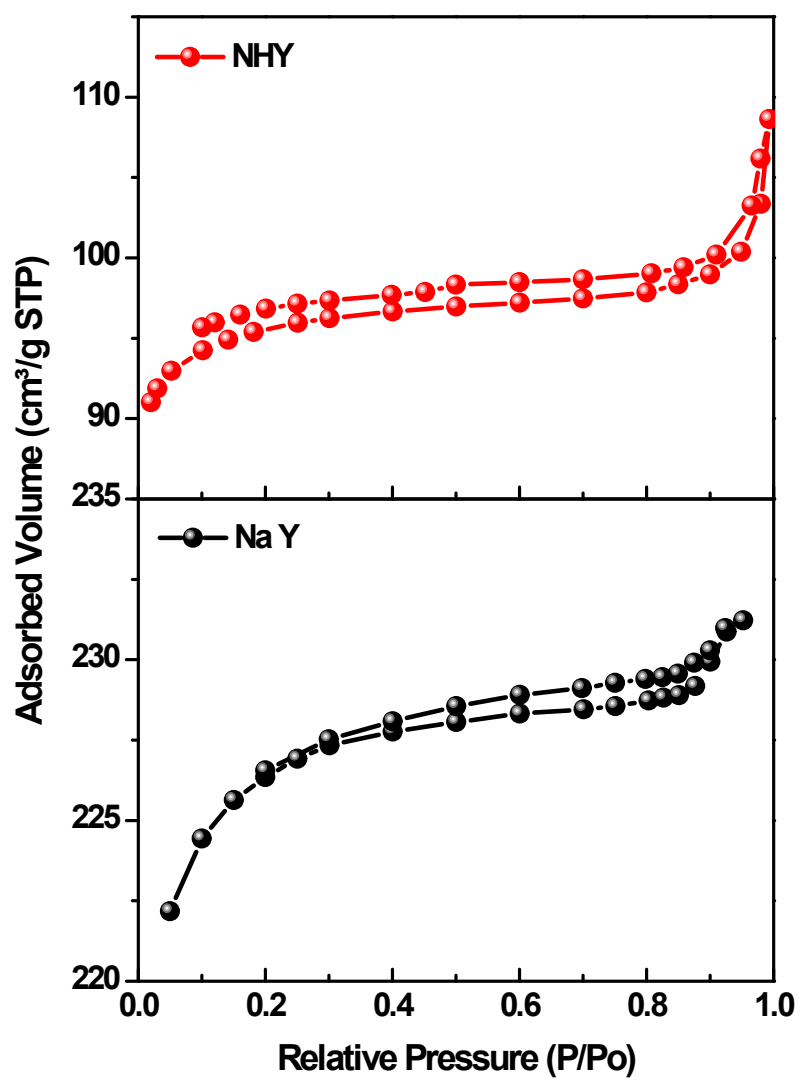


Figure S3. N₂ adsorption and desorption isotherms of Na Y and NHY

Table S4. Selected bond parameters of the neat complex and zeolite encapsulated complex computed at BP86/TZP.

Bonds	Neat Complex	Zeolite encapsulated Complex
Ni -N2	1.9753	2.0099
Ni -N7	1.9756	2.0078
Ni -N23	1.9753	2.0099
Ni -N28	1.9756	2.0078
N2-H6	1.0415	0.9697
N7-H11	1.0416	0.9122
N23-H27	1.0415	0.9697
N28-H32	1.0416	0.9122

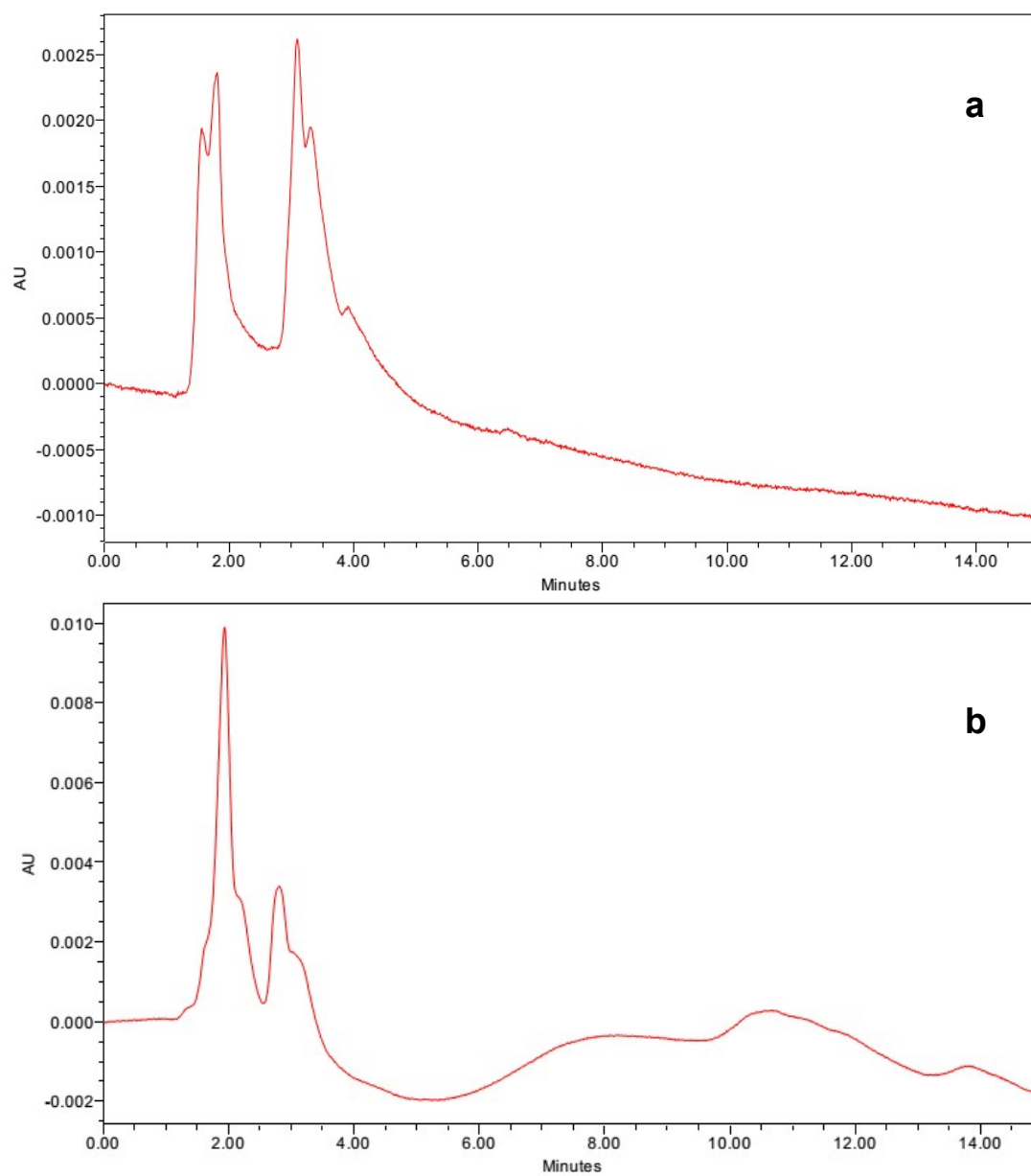


Figure S5. HPLC chromatograms of Methylene Blue (a) before and (b) after photocatalytic degradation.

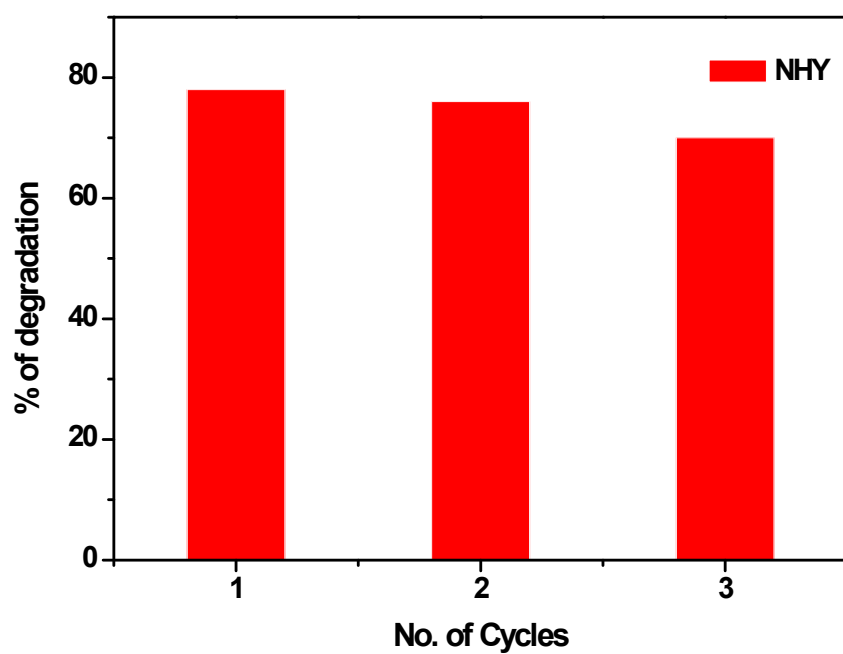


Figure S6. Re-usability test of NHY catalyst on degradation of methylene blue.