Electronic Supplementary Information

Isomorphous free-base, Ni(II)- and Cu(II)-5,10,15,20-tetra(4-hydroxyphenyl)porphyrin nitrobenzene hexasolvates with tetragonal 3D hydrogen-bonded network structures

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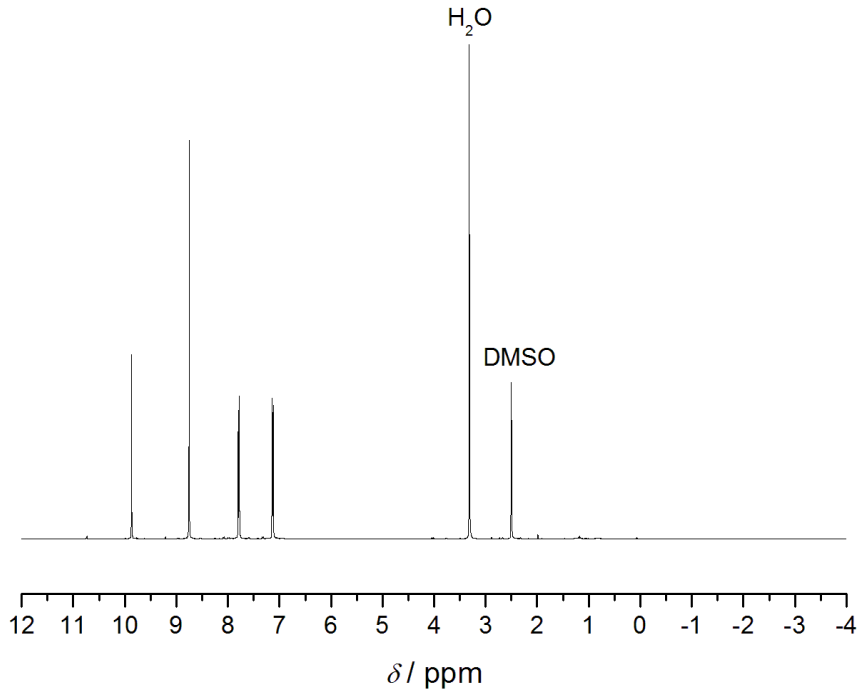


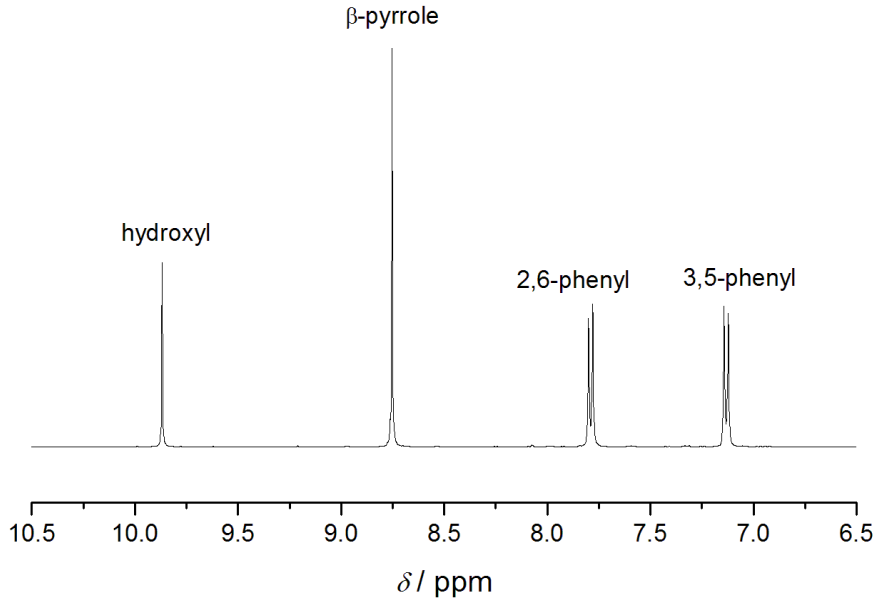


Figure S1 ^{1}H NMR spectrum of NiTOHPP in DMSO-*d*6 (top). The bottom picture shows the aromatic region.

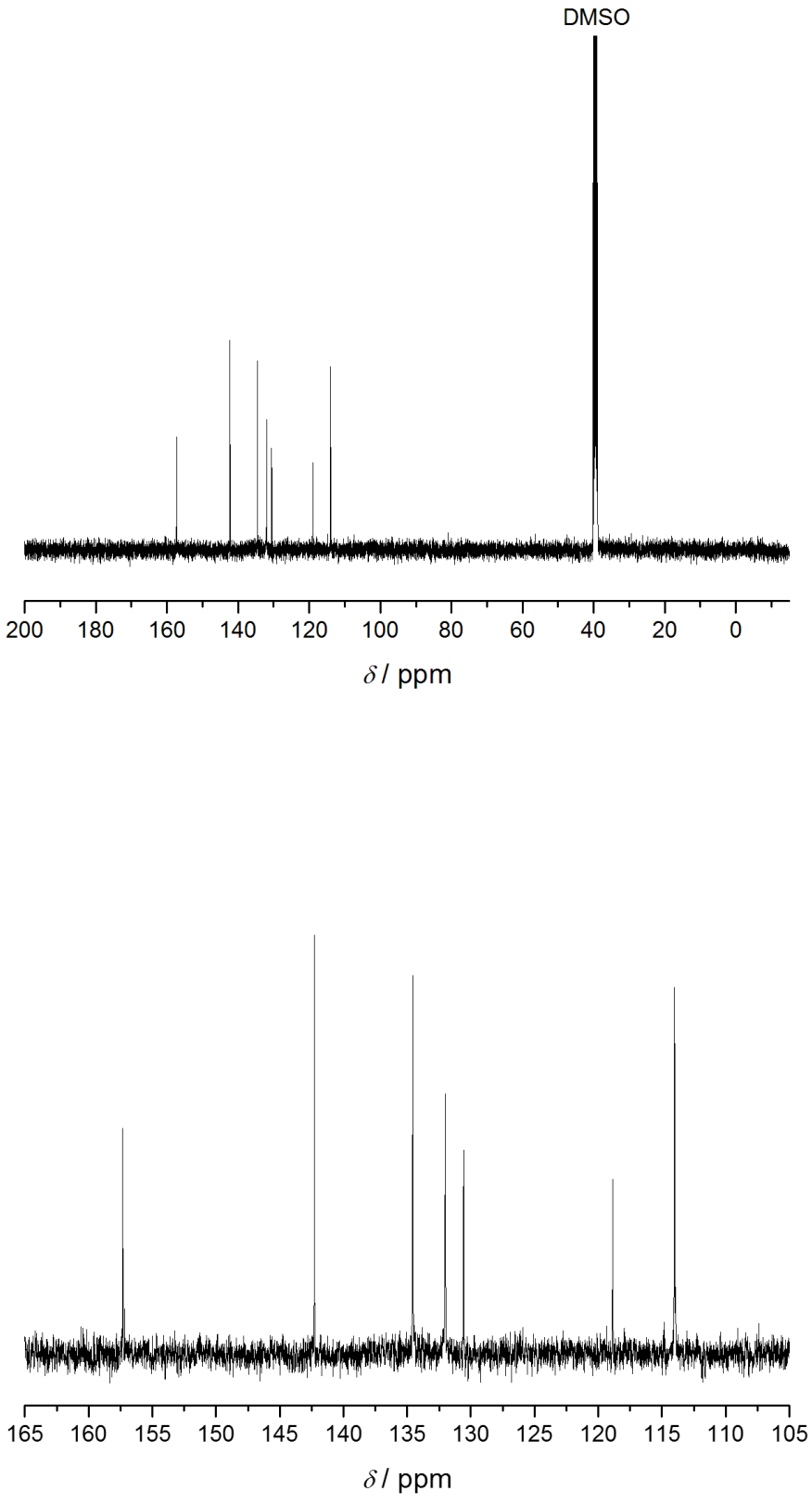


Figure S2 ^{13}C NMR spectrum of NiTOHPP in DMSO-*d*6 (top). The bottom picture shows the aromatic region.

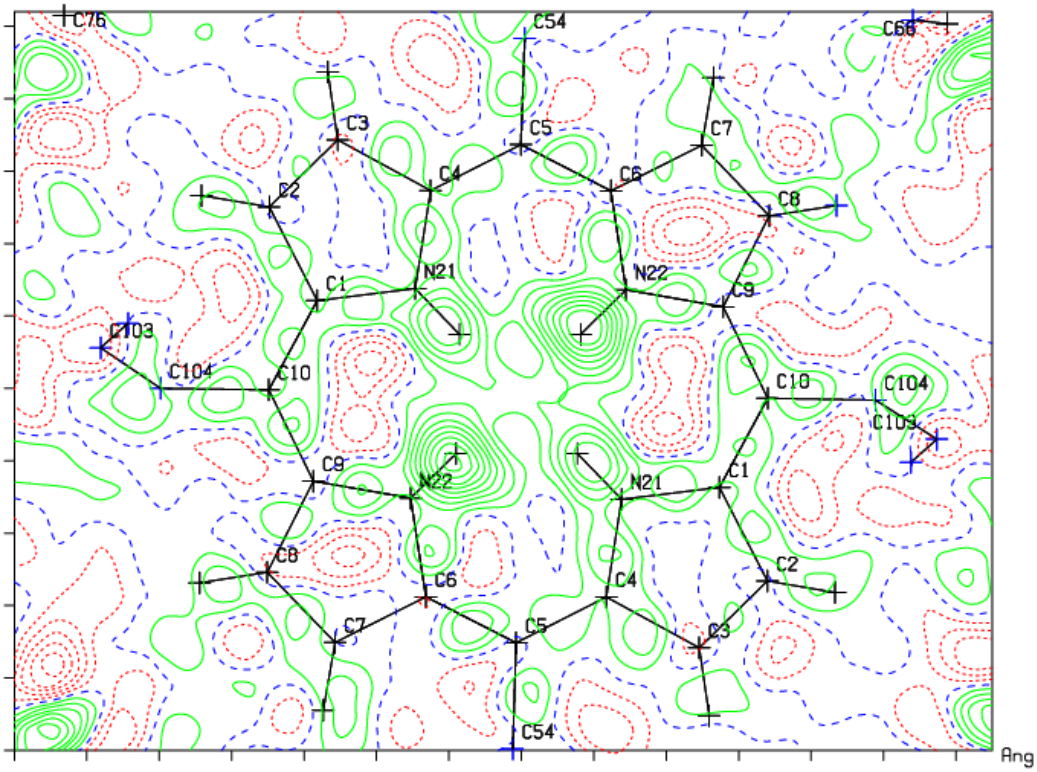
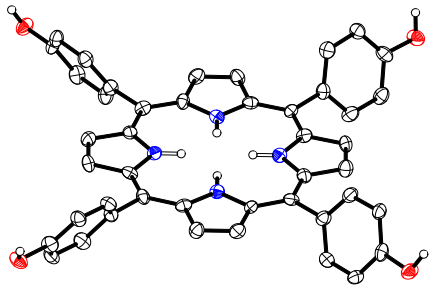
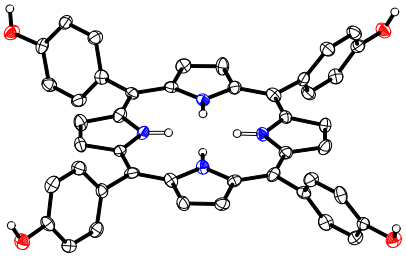


Figure S3 Contour plot of the difference Fourier map (F_o–F_c) in the porphyrin plane of H_2TOHPP in Wyckoff position 4c in **1** (0.94 Å resolution). Green lines and red dotted lines represent positive and negative electron density, respectively. Dashed blue lines show the zero line. Contours are drawn at 0.05 eÅ^{-3} intervals, starting at 0.50 eÅ^{-3}. The pyrrole NH atoms have been omitted from the structure factor calculation, but their geometrically calculated positions are shown for clarity.

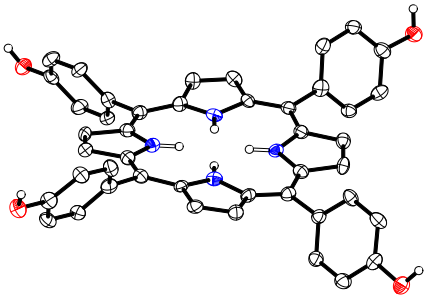
1



H_2TOHPP (2a)

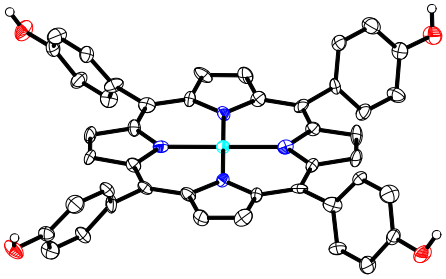


H_2TOHPP (2b)

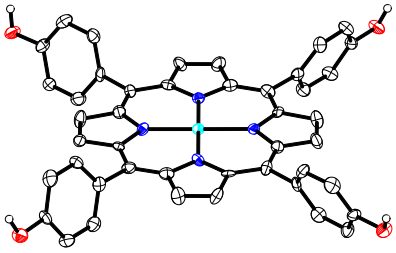


H_2TOHPP (4c)

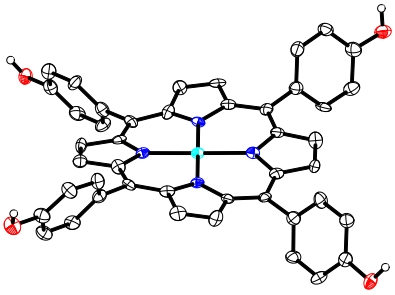
2



NiTOHPP (2a)

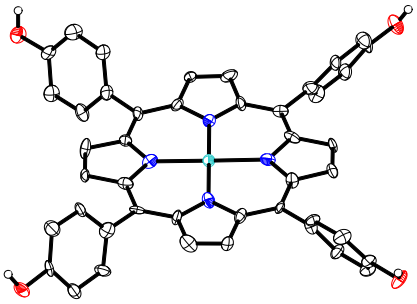


NiTOHPP (2b)

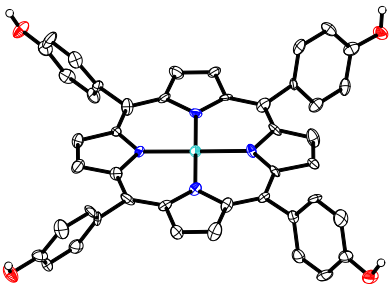


NiTOHPP (4c)

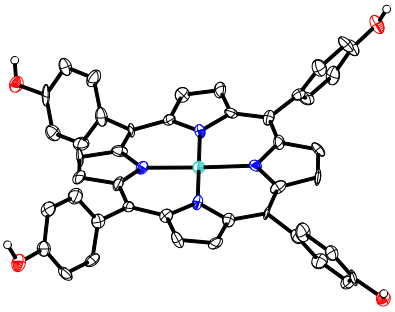
3



CuTOHPP (2a)



CuTOHPP (2b)



CuTOHPP (4c)

Figure S4 Displacement ellipsoid plots (50 % probability level) of the porphyrin building blocks in **1**–**3**. Hydrogen atoms are represented small spheres of arbitrary radii. Those attached to carbon have been omitted for clarity. The Wyckoff position in the crystal structure is given in parentheses in each case.