

Preparation, Characterizations and Theoretical Calculations of a Mg(II) Porphyrin Complex with Axial O-bonded 4-Pyrrolidinopyridine

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Section 1. IR Spectroscopy

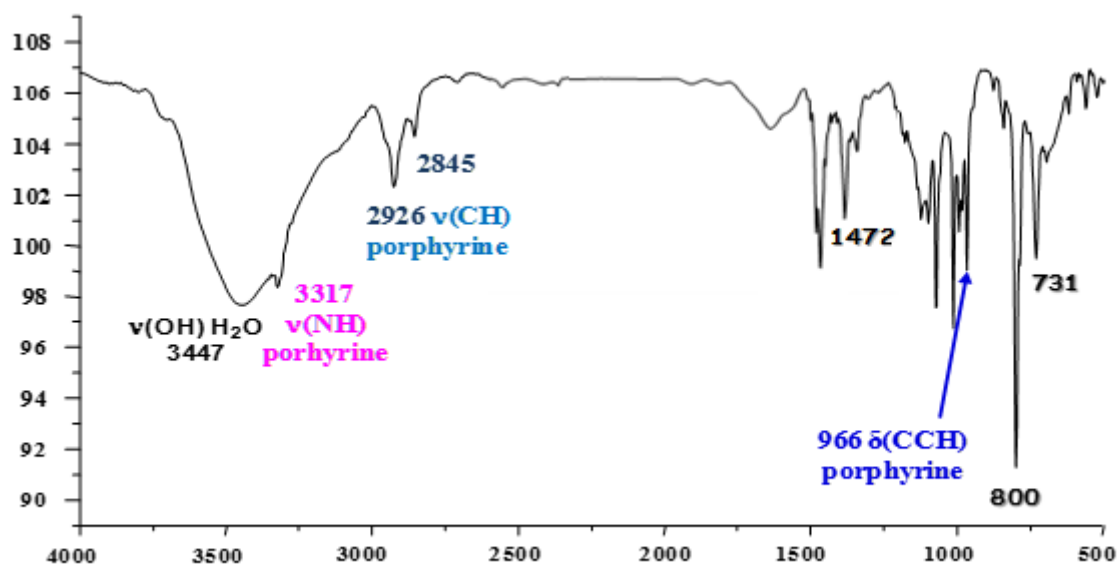


Fig. S1. IR spectrum of the H_2TBrPP free base porphyrin.

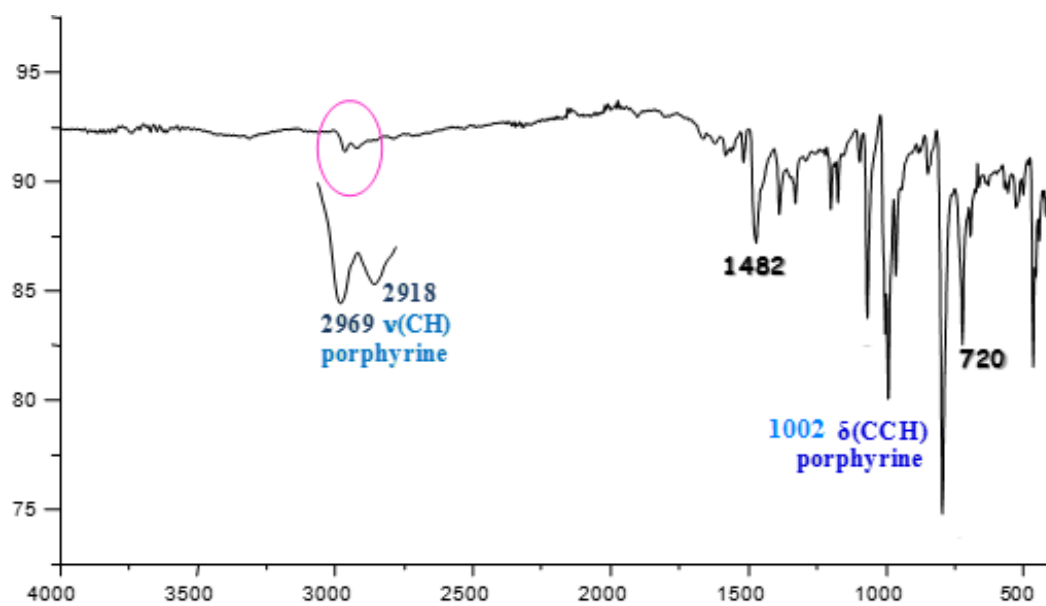
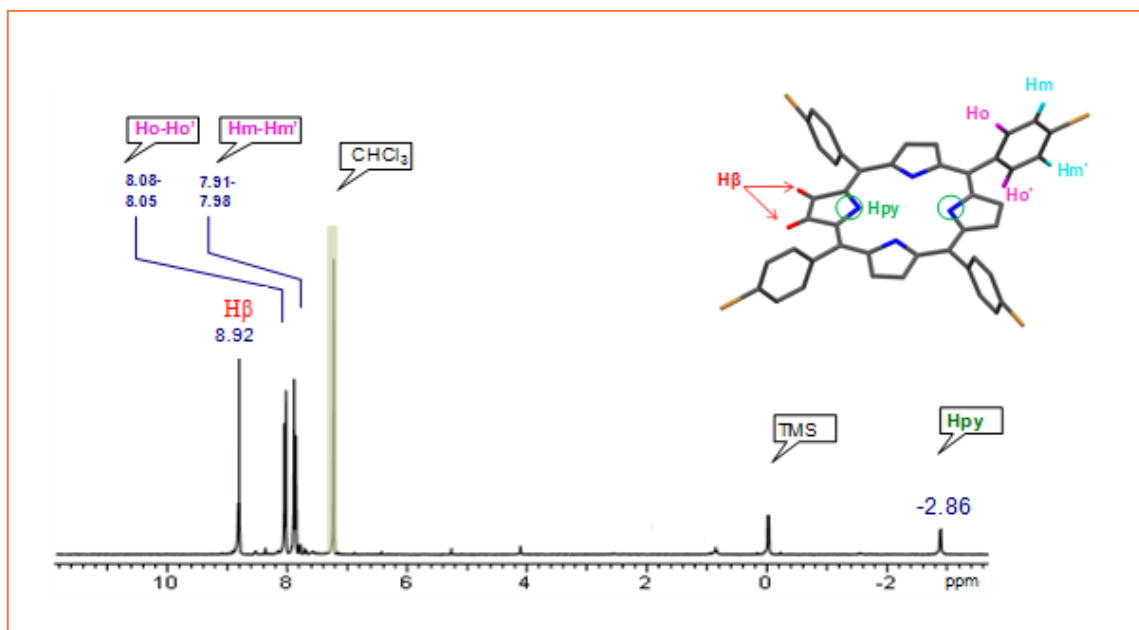


Fig. S2. Neat IR spectrum of $[\text{Mg}(\text{TBrPP})]$



Section 2. ^1H NMR Spectroscopy

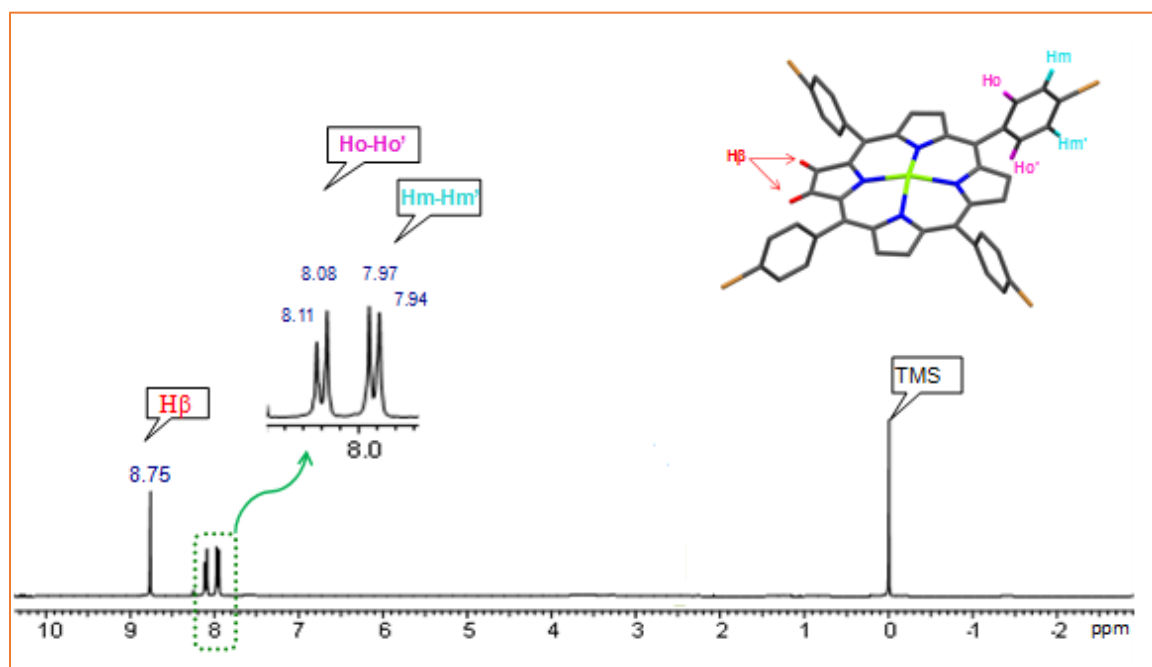


Fig. S3. ^1H NMR spectrum of the H_2TBrPP free base porphyrin recorded in CDCl_3 at room temperature with concentration $C \sim 10^{-3}$ M.

Fig. S4. ^1H NMR spectrum of the $[\text{Mg}(\text{TBrPP})]$ recorded in CDCl_3 at room temperature with concentration $C \sim 10^{-3}$ M.

Section 3: UV/Vis spectroscopy

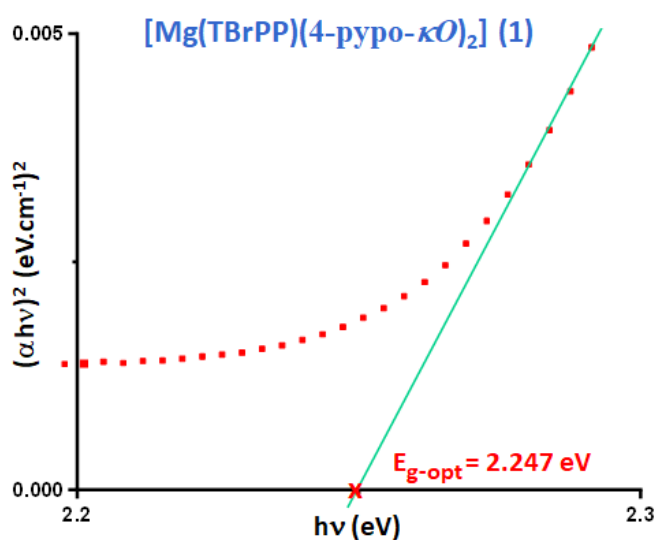


Figure S5. Plots of $(\alpha h\nu)^2$ versus the photon energy ($h\nu$) complex **1**. $h\nu$ is the incident photon energy and α is the absorption coefficient.

Section 4: Crystallography

Table S1. π - π interactions (\AA , $^\circ$) in the crystal structure of complex **1**.

$Cg(I)$	$Cg(J)$	$Cg\dots Cg$	α	CgI_Perp	CgJ_Per	<i>Slippage</i>
Cg3	Cg4	3.998(4)	23.1	25.9	3.598(3)	3.873(2)
Cg4	Cg3	3.998(4)	23.1	14.4	3.872(2)	3.598(3)

$Cg...Cg$ = distance between ring centroids, α = dihedral planes I and J , CgI_Per = perpendicular distance of CgI on ring J , CgJ_Perp = perpendicular distance of CgJ on ring I .

$Cg3$ = centroid of the five membered ring $N3/C23-C24-C25-C26$ of 4-pipo- κO axial ligand.

$Cg4$ = centroid of the pyridyl ring $N4/C29-C28-C27-C31-C32$ of a 4-pipo- κO axial ligand

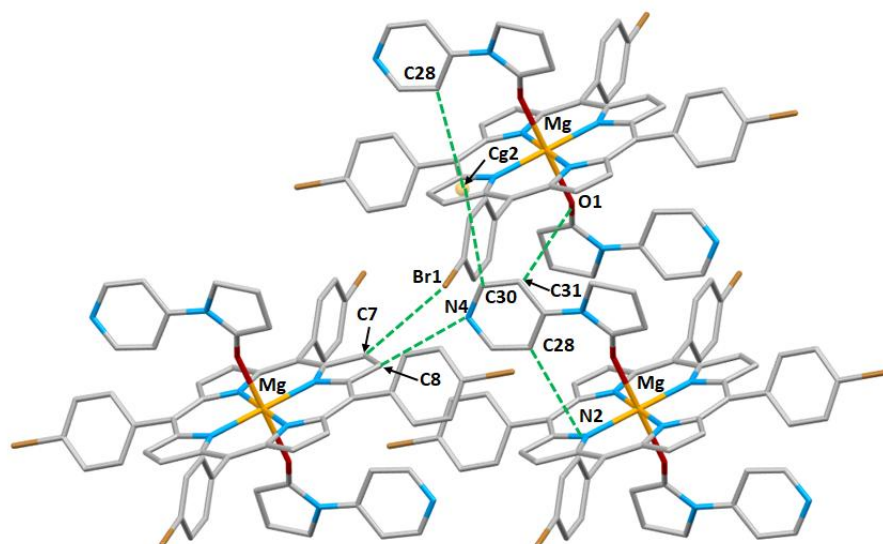


Figure S6. Drawing illustrating the C–H \cdots N, C–H \cdots O and C–H \cdots Br intermolecular interactions in complex **1**.

Table-S2. Selected intermolecular interactions for complex **1**.

D–H \cdots A ^a	Symmetry of A	D \cdots A (Å)	D–H \cdots A (°)
C28–H28 \cdots N2	-x,-y+2,-z+2	3.674(5)	169
C31–H31 \cdots O1	-x+1,-y+2,-z+2	3.447(6)	132
C31–H31 \cdots N2	-x+1,-y+2,-z+2	3.687(8)	130
C7–H7 \cdots Br1	-x+1,-y+1,-z+1	3.752(5)	142
C8–H8 \cdots N4	x,+y,+z-1	3.479(6)	151
C28–H28 \cdots Cg2	-x,2-y,2-z	3.568(8)	151
C30–H30 \cdots Cg2	1-x,2-y,2-z	3.574(8)	140

^a: D = donor atom and A = acceptor atom.

Cg2: is the centroid of the pyrrole ring N2/C6-C9

Section 5: Hirshfeld surface analysis

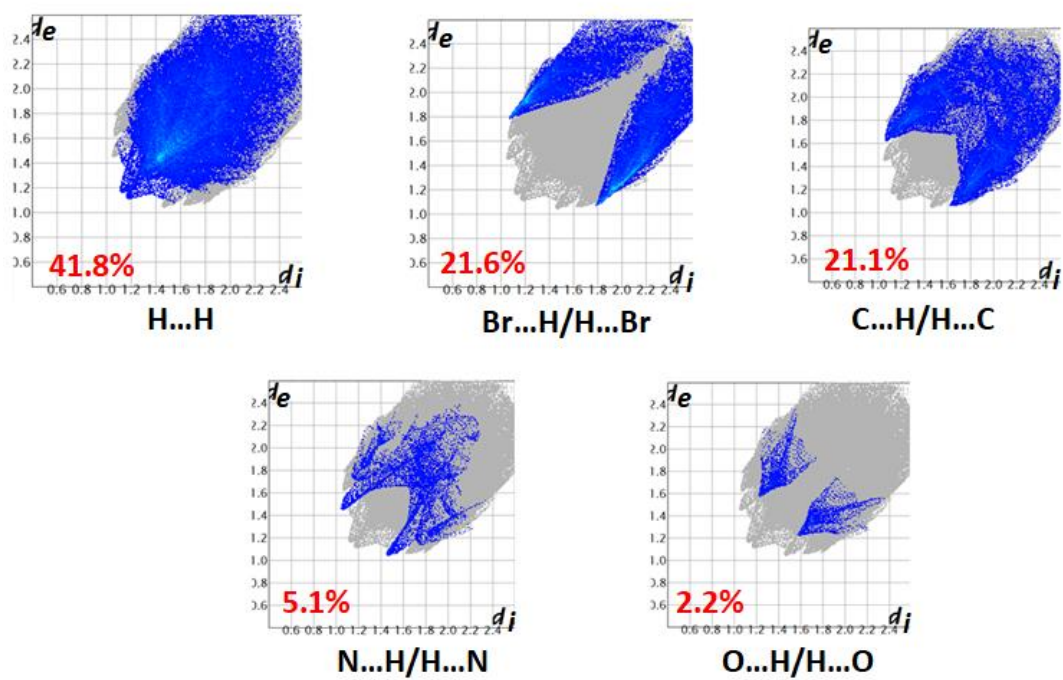


Figure S7. Decomposed fingerprint plots for the dominant interactions in complex 1 .