

Study on the Synthesis, Physicochemical, Electrochemical Properties, Molecular Structure and Antifungal Activities of the 4-Pyrrolidinopyridine Mg(II) Meso-tetratolylPorphyrin Complex

*Souhir Jabli^a, Soukaina Hrichi^a, Raja Chaabane-Banaoues^b, Florian Molton^c,
Frédérique Loiseau^c, Thierry Roisnel^d, Ilona Turowska-Tyrk^e, Hamouda Babba^b
Habib Nasri^{a,*}*

^a: University of Monastir, Laboratory of Physical Chemistry of Materials (LR01ES19), Faculty of Sciences of Monastir, Avenue de l'environnement, 5019 Monastir, Tunisia.

^b: University of Monastir, Faculty of Pharmacy, Laboratory of Medical and Molecular Parasitology-Mycology (LP3M), LR12ES08, 5000 Monastir, Tunisia.

^c: Département de Chimie Moléculaire, 301 rue de la Chimie, Université Grenoble Alpes, CS 40700, 38058 Grenoble, Cedex 9, France

^d: Institute of Chemical Sciences of Rennes, UMR 6226, University of Rennes 1, Beaulieu Campus, 35042 Rennes, France

^e: Faculty of Chemistry, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland.

Contents

1. ¹ H NMR Spectroscopy	2
2. Infrared Spectroscopy.....	3
3. Mass spectroscopy.....	3
4. X-ray Molecular structure	4

1. ^1H NMR Spectroscopy:

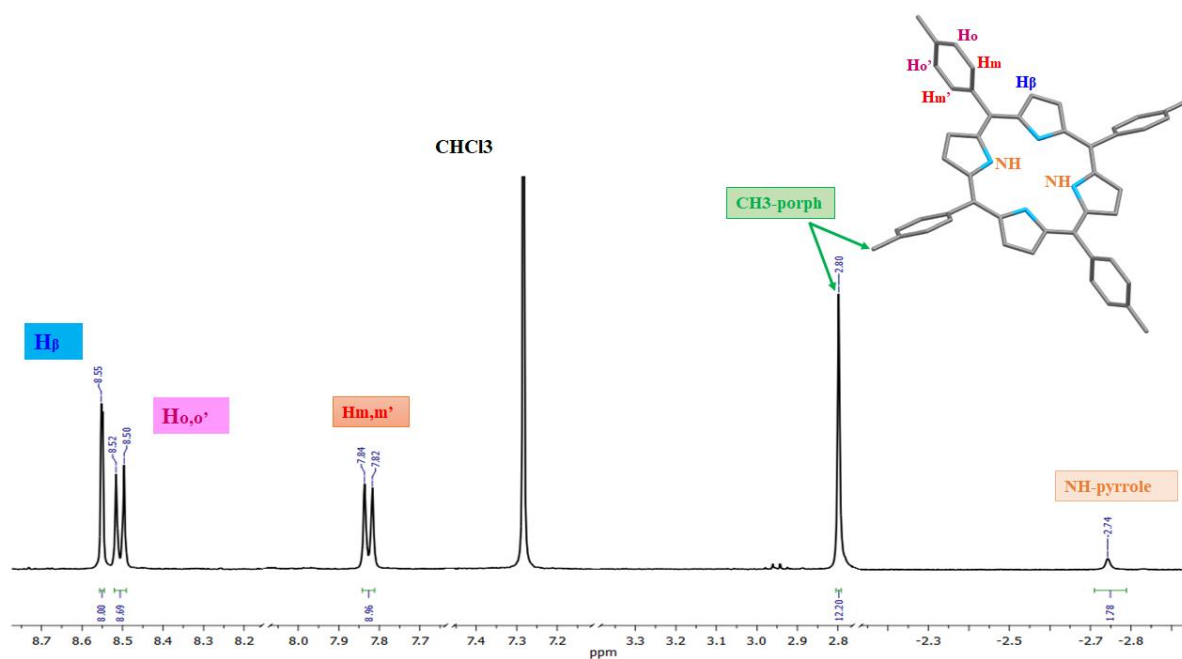


Fig. S1. ^1H NMR spectrum of the H_2TTP free base porphyrin recorded in CHCl_3 at room temperature with concentration $C \sim 10^{-3}$ M.

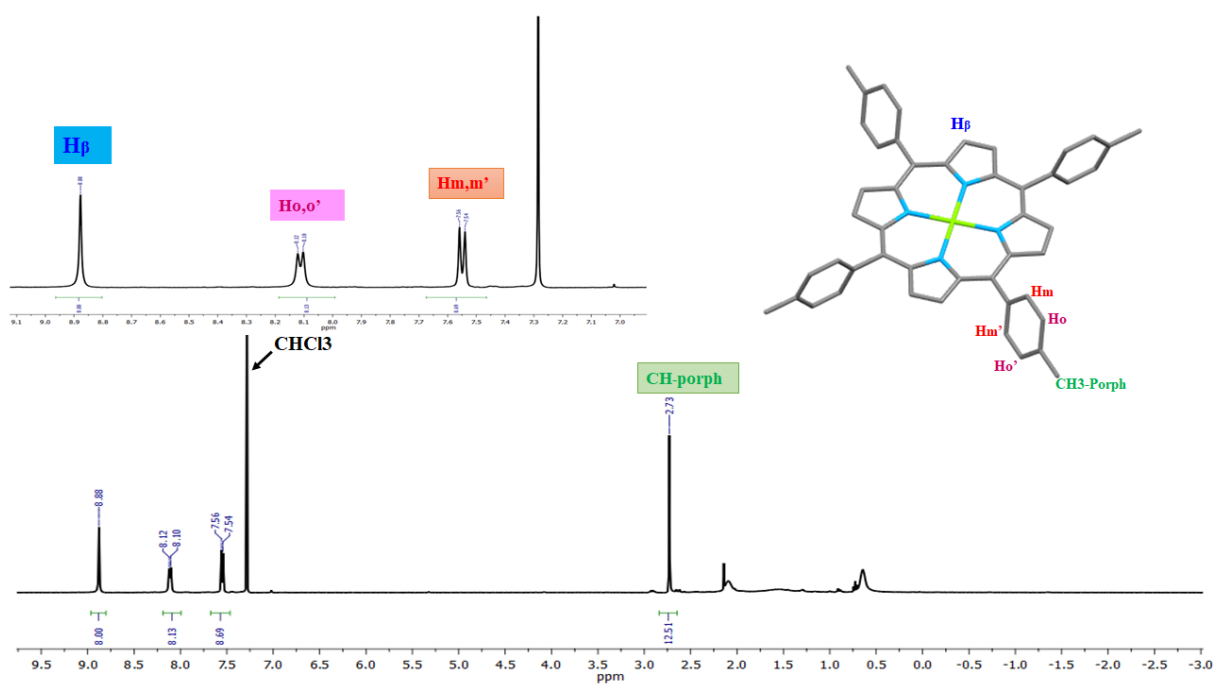


Fig. S2. ^1H NMR spectrum of the $[\text{Mg}(\text{TTP})]$ porphyrin recorded in CHCl_3 at room temperature with concentration $C \sim 10^{-3}$ M.

2. Infrared Spectroscopy:

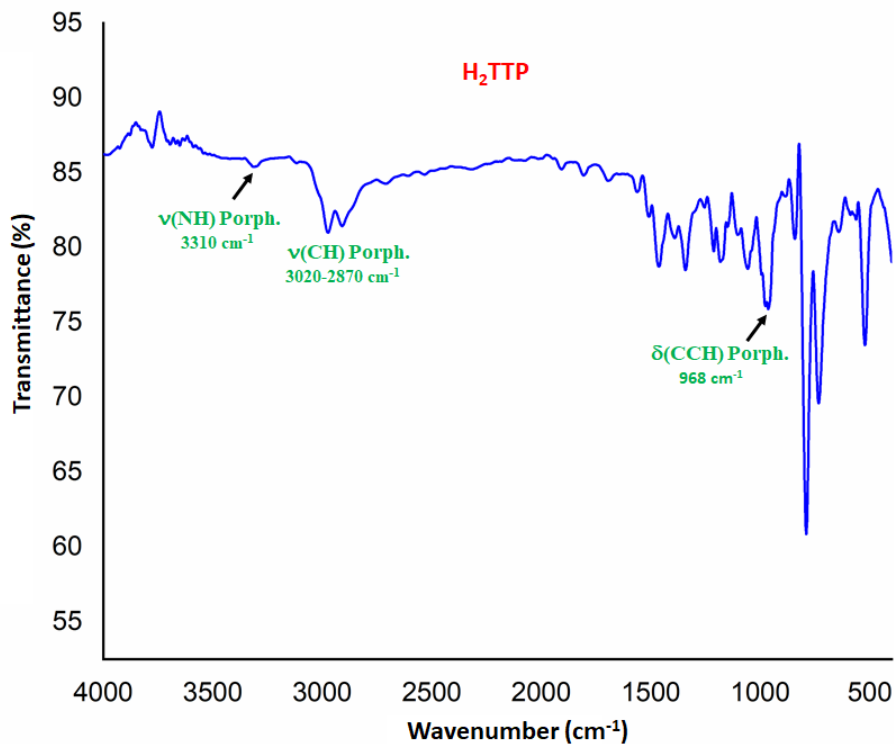


Fig. S3. Neat IR spectrum of the H₂TTP free base porphyrin.

3. ESI-HRMS mass study on [Mg(TTP)(4-pypo)₂]⁺·2CH₂Cl₂ (I) :

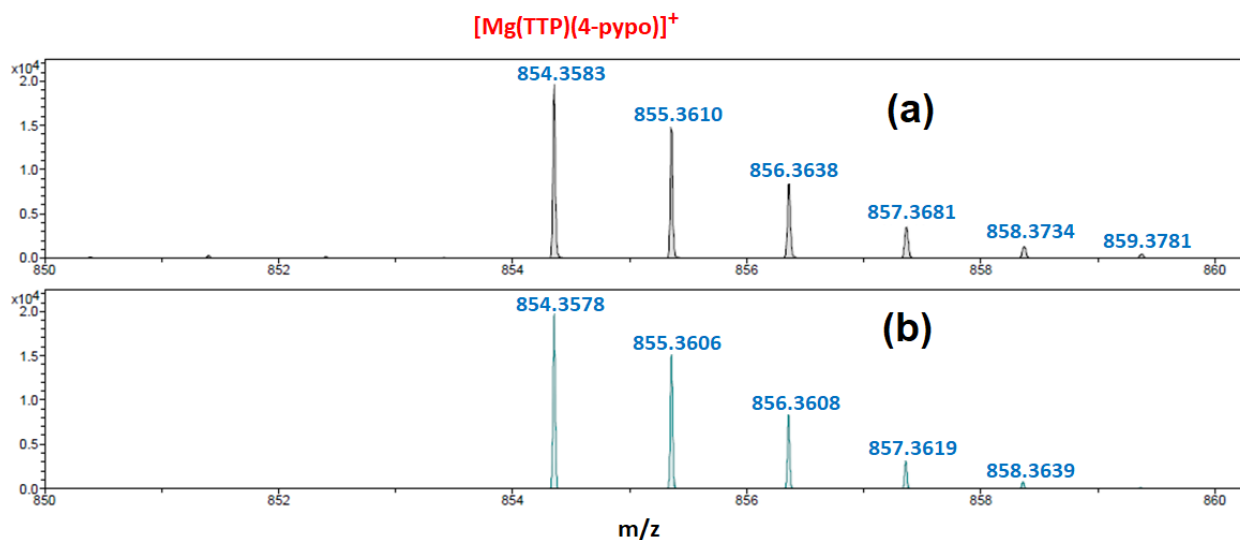


Fig.S4. ESI-HRMS spectrum of complex **I** showing the isotopic ratio. (a): experimental spectrum, (b): simulated spectrum.

4. X-ray Molecular structure:

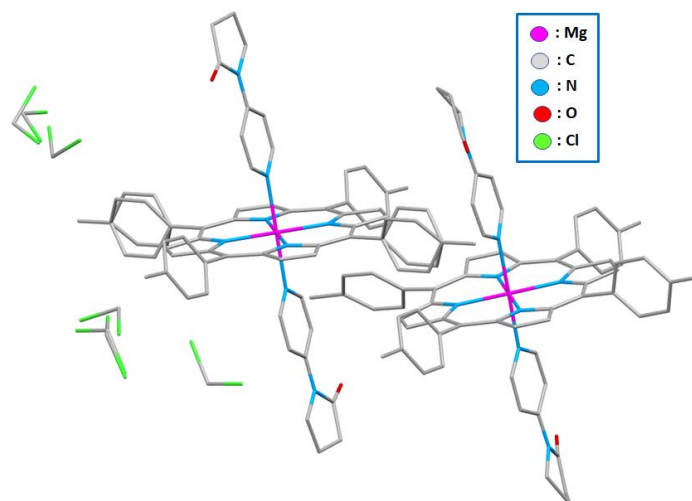


Fig.S5. Drawing showing the asymmetric unit of $[\text{Mg}(\text{TTP})(4\text{-pypo})_2]\cdot\text{CH}_2\text{Cl}_2$ (**I**).

Table-S1. Selected intermolecular interactions for complex **I**.

D-H \cdots A ^a	Symmetry of A	D \cdots A (Å)	D-H \cdots A (°)
C56-H56B-Cg17	1-x,1-y,2-z	3.762 (6)	153
C65-H65A-Cg19	2-x,-y,1-z	3.553 (6)	153
C103-H10G-Cg3	x,y,z	3.66 (5)	130
C105-H10L-Cg12	-x,1-y,1-z	3.47 (2)	120
PARST			
C54-H54B-O2	-x+1,-y+1,-z+1	3.555 (9)	128
C96-H96A-O1	-x,-y+2,-z+1	3.417 (9)	143
C100-H10A-O1	-x,-y+2,-z+1	3.231 (6)	159
C102-H10C-O2	-x+1,-y+1,-z+1	3.118 (9)	142
C101-H10C-O2	-x+1,-y+1,-z+1	3.401 (4)	163
C106-H10J-O3	x,y-1,z	3.463 (9)	120
C104-H10J-O3	x,y-1,z	3.445 (9)	113

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

Cg17 is the centroid of the N5/C49-C53 pyrrole ring.

Cg19 is the centroid of the N11/C91-C95 pyridyl ring of the 4-pipo axial ligand.

Cg12 is the centroid of the C35-C36-C37-C38-C39-C40 phenyl ring.
Cg3 is the centroid of the C77-C78A-C79A-C80-C81A-C82A phenyl ring.

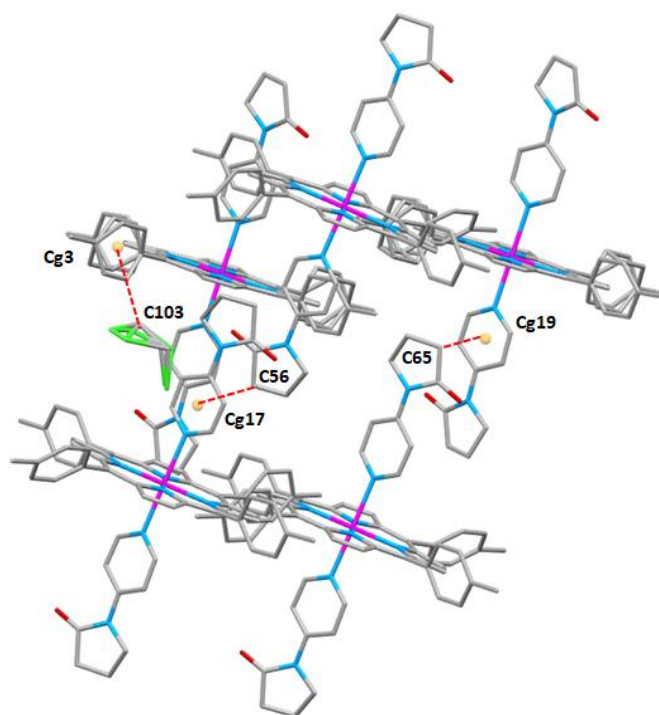


Fig. S6. Drawing showing the C-H...Cg (Cg is the centroid of a phenyl ring the TTP porphyrinate) intermolecular interactions in the structure of **I**.

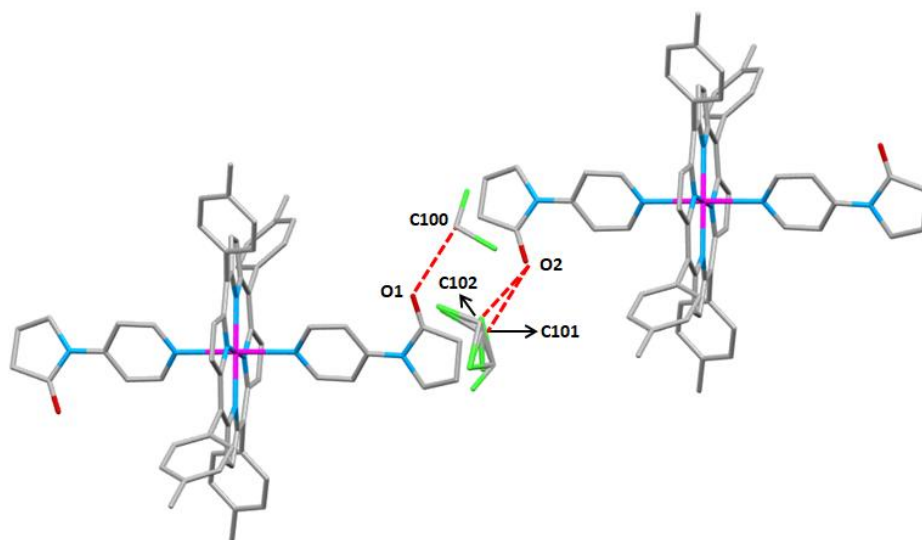


Fig. S7. Drawing showing the C-H...O intermolecular interactions in the structure of **I**.