Synthesis, X-ray Crystallography, Spectroscopic Characterizations, Density Functional Theory, and Hirshfeld Surface Analyses of a Novel (carbonato) picket fence iron(III) complex

Mondher Dhifet[a,b], Bouzid Gassoumi[c], Maxim Lutoshkin[d] , Anna S Kazachenko[e], S. KAZACHENKO[f] Omar M. Al-Dossary[g], Noureddine ISSAOUI[h]* and Habib Nasri[a]

[a] University of Monastir, Laboratory of Physical Chemistry of Materials (LR01ES19), Faculty of Sciences of Monastir, Avenue of the Environment, 5019 Monastir, Tunisia.
[b] University of Gafsa, Faculty of Sciences of Gafsa.
[c] Laboratory of Advanced Materials and Interfaces (LIMA), University of Monastir, Faculty of Science of Monastir, Avenue of Environnment, 5000 Monastir, Tunisia.
[d] Institute of Chemistry and Chemical Technology SB RAS, FRC KSC SB RAS,Russian Federation, 660036, Krasnoyarsk, Akademgorodokst., 50/24
[e] Siberian Federal University, Russian Federation, 660041, Russian Federation, Krasnoyarsk, pr. Svobodny, 79
[f] Institute of Chemistry and Chemical Technology SB RAS, Federal Research Center, Krasnoyarsk Science Center SB RAS", Akademgorodok, 50/24, Krasnoyarsk, 660036, Russia
[g] Department of Physics and Astronomy, College of Science, King Saud University, PO Box 2455, Riyadh 11451, Saudi Arabia.
[h] Laboratory of Quantum and Statistical Physics LR18ES18, Faculty of Sciences of Monastir, Avenue of the Environment, Monastir, 5079, Tunisia.
* E-mail: issaoui_noureddine@yahoo.fr

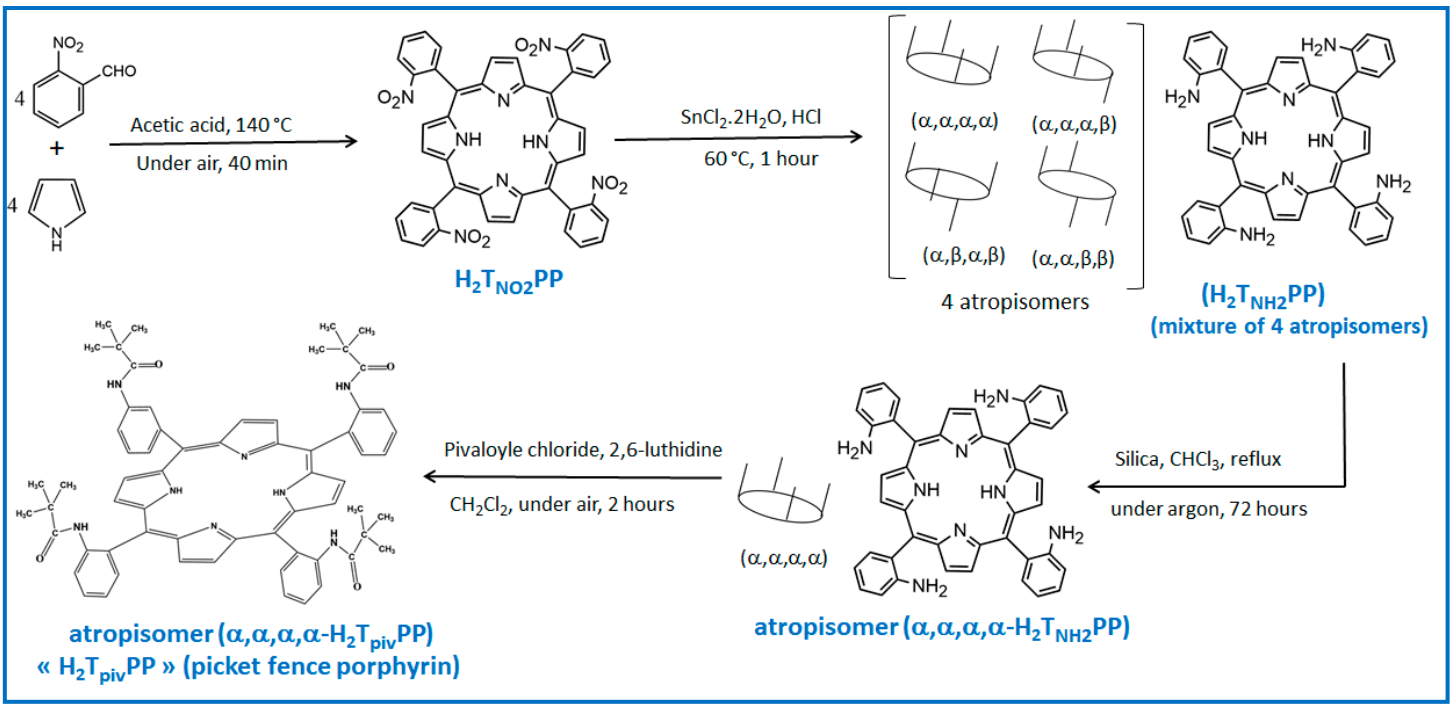
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1. Synthesis of the picket fence porphyrin (H_2TpivPP)



Scheme S1. Scheme of the preparation of the picket fence porphyrin (H_2TpivPP).

2. UV/Vis spectroscopy

Table S1. Electronic absorption data for complex **I** and a selection of *meso*-arylporphyrin compounds.

Complex	λmax (nm)					Solvents[e]	Ref.
	Soret region		β, α region				
Meso-arylporphyrins							
H_2TpivPP	**416**	514	548	590	646	CH_2Cl_2	t.w.
H_2TPP [a]	**418**	515	549	591	647	CH_2Cl_2	[1]
H_2TBrPP [b]	**419**	515	549	590	648	CH_2Cl_2	[2]
H_2TPBP [c]	**419**	514	551	590	646	CH_2Cl_2	[3]
H_2TClPP [d]	**418**	515	550	549	647	CH_2Cl_2	[4]
Iron(III) porphyrins							
$[Fe^{III}(TpivPP)Cl]$	**417**	506	575	603		C_6H_5Cl	t.w.
$[Fe^{III}(TpivPP)(CO_3)]^-$	**424**	510	567	607		C_6H_5Cl	t.w.
$[Fe^{III}(TpivPP)(OAc)]$	**414**	505	574	-		C_6H_5Cl	[5]
$[Fe^{III}(TpivPP)(NCS)]$	**417**	513	586	-		C_6H_5Cl	[6]
$[Fe^{III}(TpivPP)(NCO)]$	**414**	508	576	-		C_6H_5Cl	[7]
$[Fe^{III}(TpivPP)(NO_2)_2]^-$	**426**	553	-	-		C_6H_5Cl	[8]
$[Fe^{III}(TpivPP)(NO_2)(py)]$	**420**	546	-	-		C_6H_5Cl	[9]

[a] H_2TPP = *meso* –tetraphenylporphyrin; [b] H_2TBrPP = 4-bromophenylporphyrin, [c] H_2TPBP = 4-(benzoyloxy)phenyl] porphinato; [d] H_2TClPP = meso-tetrakis(4-chlorophenyl)porphyrin; ; [e]: C_6H_5Cl is chlorobenzene and CH_2Cl_2 is dichlorometane ; t.w: this work.

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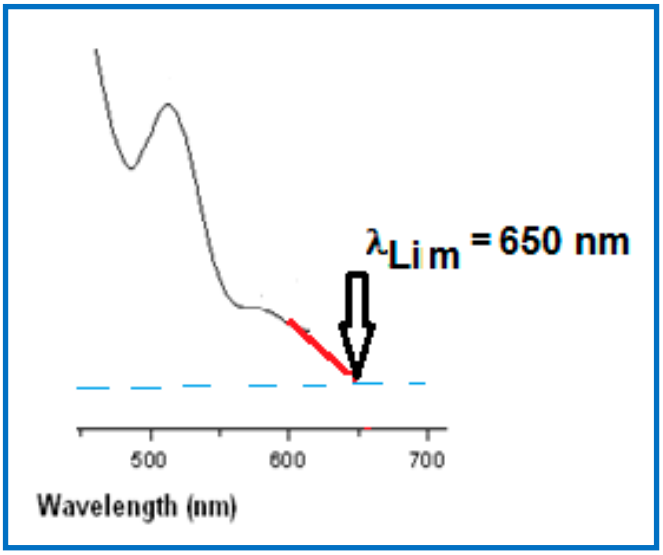


Fig. S1. Region of Q bands of complex **I**. Determination of the λ_{Lim}.

3. X-ray molecular structure of complex I

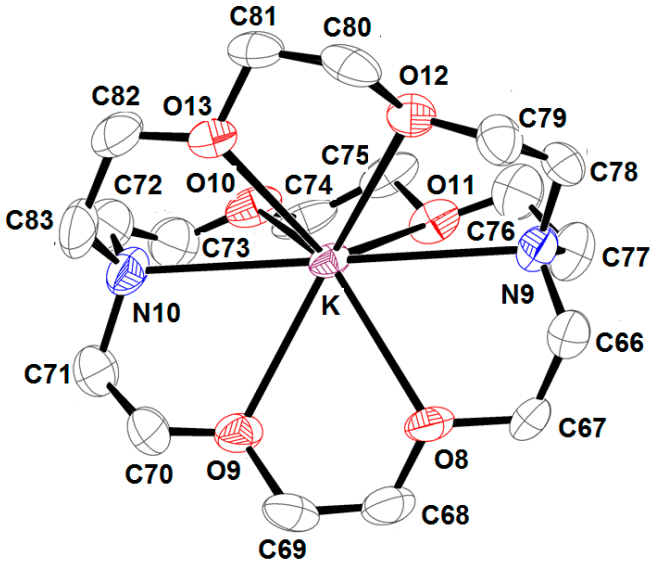


Fig. S2. ORTEP view of $[K(crypt\text{-}222)]^+$ counterion, the thermal ellipsoids are drawn at the 30% probability level. Hydrogen atoms have been omitted for clarity.