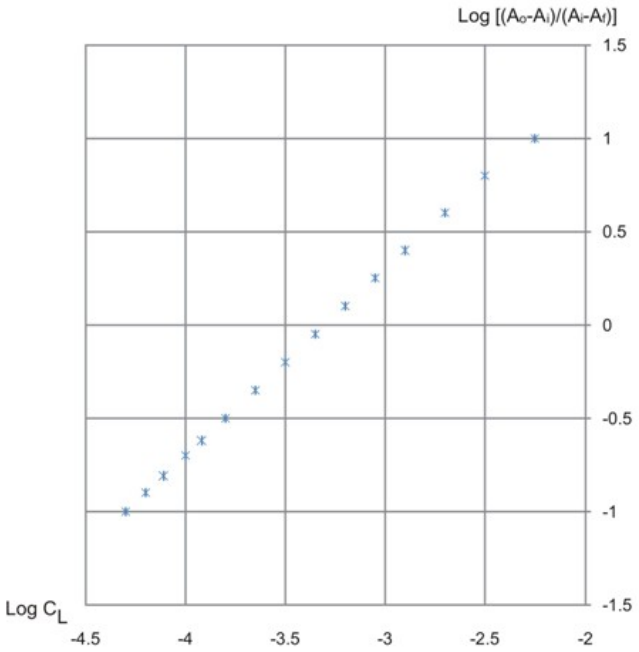
SUPPORTING INFORMATION

Cation assisted complexation of octacarbazolylphenyl substituted Zn(II)-tetraphenylporphyrin with [2,2,2]cryptand

Galina M. Mamardashvili[a], Olga V. Maltseva[a], Nugzar Zh. Mamardashvili[*, a], Nguyen Tran Nguyen[b], Wim Dehaen [*, b]

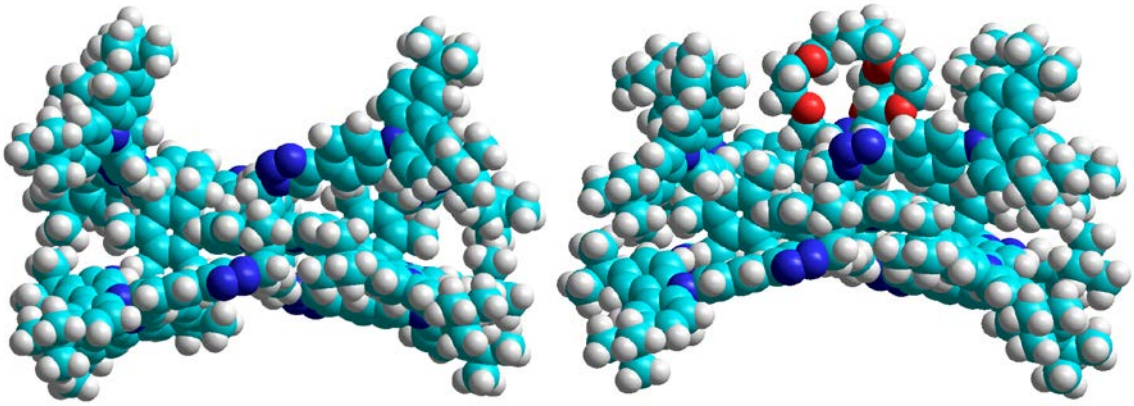
[a] *Coordination Chemistry of Macrocyclic Compounds, G.A. Krestov Institute of Solution Chemistry of Russian Academy of Sciences, Akademicheskaya St.1, 153045 Ivanovo, Russia*

[b] *Molecular Design and Synthesis, Department of Chemistry, KU Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium. Fax: (+32) 16 327990; Tel:+32 16 3 27439; E-mail: wim.dehaen@chem.kuleuven.be*



C_L is the ligand concentration, A_0 is the initial optical density at the wavelength λ, A_f is the final optical density at the wavelength λ, and A_i is the current optical density at the wavelength λ at the given concentration.

Figure 1._SI. The logarithmic dependence of the optical density of the reaction system **ZnTPP-L** ($\log[(A_0-A_i)/(A_i-A_f)]$) in function of the ligand concentration ($\log C_{ligand}$).



ZnD **ZnD-L**

Figure 2._SI. The structure of **ZnD** and its complex with **L** obtained by computer simulation.

L **L-K^+**

Figure 3._SI. The structure of **L** and its complex with potassium **L-K^+** obtained by computer simulation.

Table_SI. Geometric parameters of the [2,2,2]cryptand and its complex with potassium obtained by computer simulation, DFT/B3LYP/6-31G**.

	[2,2,2]cryptand	K^+[2,2,2]cryptat
N_1-N_{10}	5.995	6.466
O_4-O_{13}	4.789	3.853
O_4-O_{21}	4.633	4.309
O_{21}-O_{13}	5.373	4.231
O_7-O_{16}	5.096	4.220
O_7-O_{24}	3.780	4.456
O_{16}-O_{24}	4.523	3.863
C_{11}-N_1-C_{19}	118.168	113.522
C_{19}-N_1-C_2	117.308	114.418
C_2-N_1-C_{11}	114.355	112.800
C_9-N_{10}-C_{18}	117.337	114.026
C_9-N_{10}-C_{26}	118.774	112.731
C_{18}-N_{10}-C_{26}	112.450	113.101
O_{13}-C_{14}-C_{15}-O_{16}	64.849	63.103
O_4-C_5-C_6-O_7	76.678	67.065
O_{21}-C_{22}-C_{23}-O_{24}	-69.011	-67.402

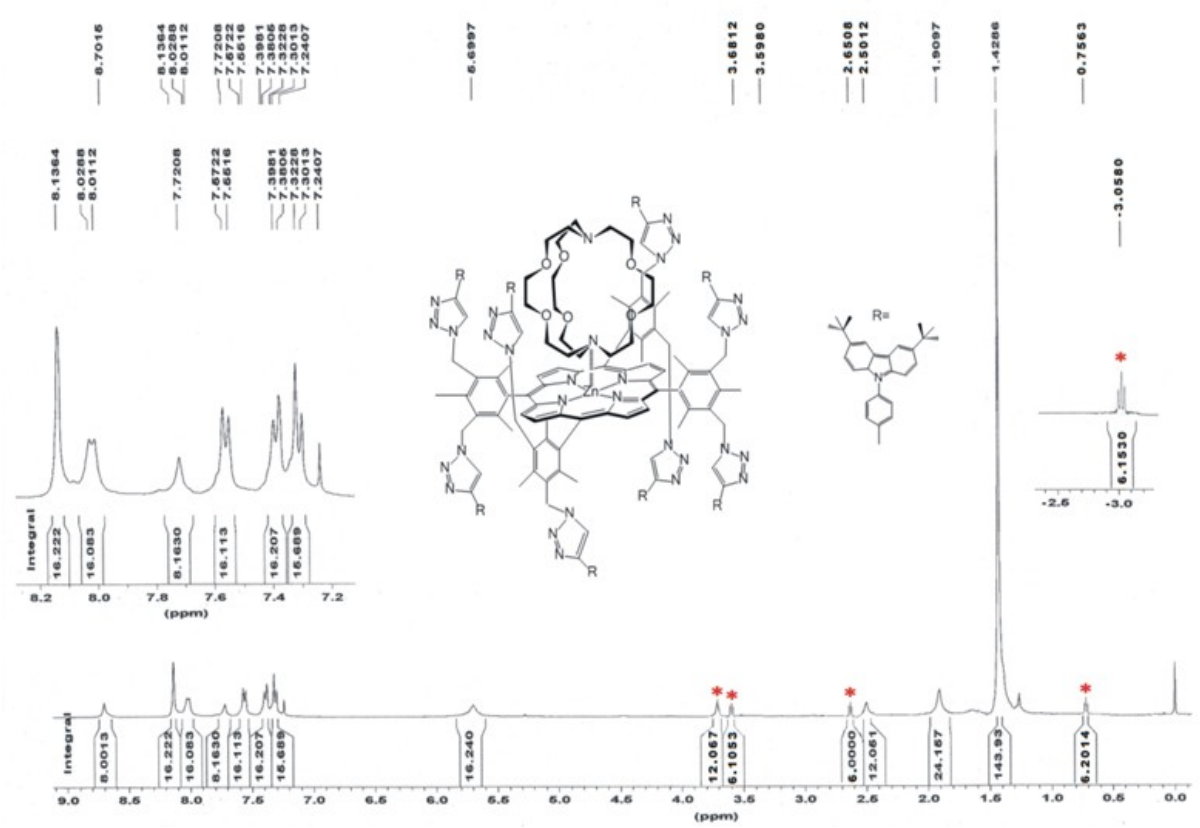


Figure 4._SI. ^{1}H NMR spectrum of the complex **ZnD-L** in $CDCl_3$ at 25^0C; $C_{\mathbf{ZnD\text{-}L}} = 6.0\times10^{-6}$ M. (Red signs in the ^{1}H NMR spectrum of the complex label the protons of the ligand).