Electronic Supplementary Information for Dalton Transactions

The Cu(II) complex of a C-lipophilized 13aneN4 macrocycle with a further protonable amine as micellar anion receptor

Franck Denat,[a] Yuri Antonio Diaz-Fernandez[b] Piersandro Pallavicini,[b] Luca Pasotti,[b] Yoann Rousselin,[a] and Nicolas Sok[a]

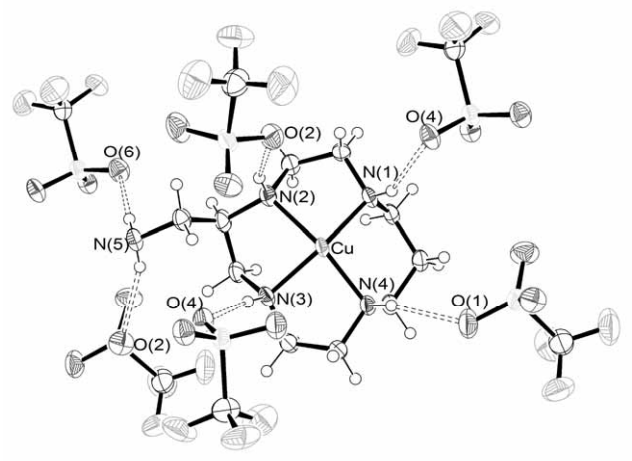
Table S1

Selected bond lengths [Å] and angles [°] in [Cu(**MA13**)]$^{2+}$

Cu-N(1)	2.025(5)	N(1)-Cu-N(2)	86.5(2)
Cu-N(2)	2.035(5)	N(2)-Cu-N(3)	83.5(2)
Cu-N(3)	2.039(5)	N(3)-Cu-N(4)	85.3(2)
Cu-N(4)	2.065(6)	N(4)-Cu-N(1)	94.2(2)
Cu-N(5)#1	2.199(5)	N(1)-Cu-N(5)#1	101.2(2)
		N(2)-Cu-N(5)#1	102.4(2)
		N(3)-Cu-N(5)#1	108.8(2)
		N(4)-Cu-N(5)#1	98.3(2)

Symmetry transformations used to generate equivalent atoms: #1 -x,y+1/2,-z-1/2

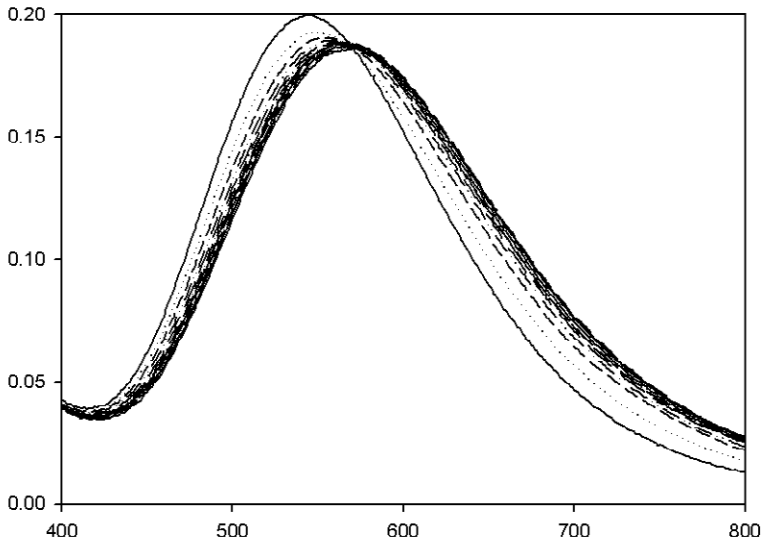
Figure S1



ORTEP view of [**Cu(MA13)**]$^{2+}$ with their counter-anions, showing thermal ellipsoids at the 50% probability level. Hydrogen bonds are indicated by dashed lines. The conformation of this macrocycle is also imposed by the intermolecular hydrogen bonds between the oxygen atoms of triflate anions and the nitrogen atoms of the macrocycle as testify the N-H...N distances between N(1)-O(4) (3.091(7) Å), N(2)-O(2) (3.210(8) Å), N(3)-O(4) (2.966(7) Å), N(4)-O(1) (2.935(7) Å), N(5)-O(6) (3.092(8) Å), N(5)-O(2) (3.092(8) Å).

Figure S2

a) Series of spectra relative to the titration of [Cu(C10MA13]2+ with $H_2P_3O_{10}^{3-}$ at pH 5.8



b) profiles of titration (blue diamonds) and fit with calculated profile (red line) based on the determined intaraction constants