Supplementary Material (ESI) for New Journal of Chemistry

Linear Recognition of Dicarboxylates by Ditopic Macrocyclic Complexes

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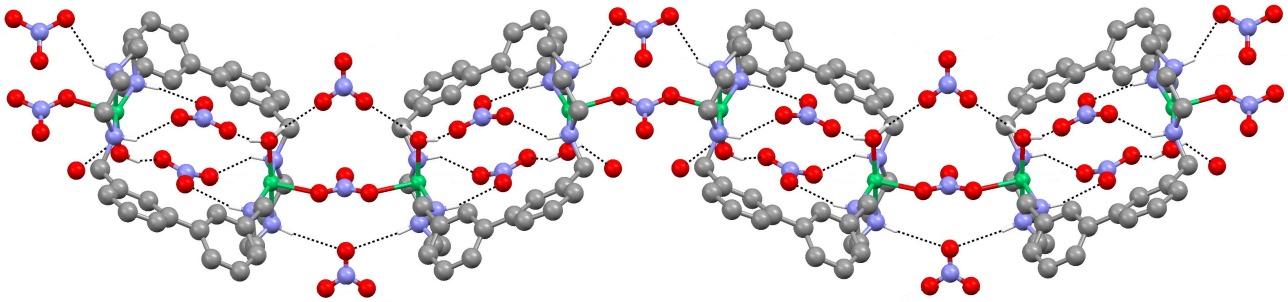

Fig.1S A simplified sketch of the infinite molecular chains that form along the *a* axis in the crystal (Et_2O solvent molecules have been omitted for clarity, only amine and water protons are show). The $[Cu_2(\mathbf{L})(H_2O)_2]^{4+}$ cationic complexes are related by crystallographic mirror planes normal to the projection plane and passing through the nitrogen of the intermediate NO_3^- anions. H-bond motif is shown as dashed lines.

Table 1S. Selected bond distances (Å) and bond angles (°) for the metal centers in the $[Cu_2(\mathbf{1})(NO_3)_4(H_2O)_2]\cdot Et_2O\cdot 1.5(H_2O)$ crystal.

Cu(1)-N(1)	2.037(6)	Cu(2)-N(4)	2.007(5)
Cu(1)-N(2)	2.011(6)	Cu(2)-N(5)	1.978(5)
Cu(1)-N(3)	2.033(5)	Cu(2)-N(6)	2.024(5)
Cu(1)-O(1w)	2.000(5)	Cu(2)-O(2w)	1.980(5)
Cu(1)-O(3)	2.253(5)	Cu(2)-O(5)	2.310(5)
N(1)-Cu(1)-N(2)	84.3(2)	N(4)-Cu(2)-N(5)	85.3(2)
N(1)-Cu(1)-N(3)	156.4(2)	N(4)-Cu(2)-N(6)	155.8(2)
N(1)-Cu(1)-O(1w)	93.1(2)	N(4)-Cu(2)-O(2w)	91.2(2)
N(1)-Cu(1)-O(3)	113.4(2)	N(4)-Cu(2)-O(5)	113.9(2)
N(2)-Cu(1)-N(3)	84.7(2)	N(5)-Cu(2)-N(6)	85.4(2)
N(2)-Cu(1)-O(1w)	176.6(3)	N(5)-Cu(2)-O(2w)	175.7(2)
N(2)-Cu(1)-O(3)	93.0(3)	N(5)-Cu(2)-O(5)	88.8(2)
N(3)-Cu(1)-O(1w)	97.0(2)	N(6)-Cu(2)-O(2w)	96.8(2)
N(3)-Cu(1)-O(3)	87.9(2)	N(6)-Cu(2)-O(5)	88.23(19)
O(1w)-Cu(1)-O(3)	90.0(3)	O(2w)-Cu(2)-O(5)	94.9(2)

Table 2S. Features of the H-bond interactions in the $[Cu_2(\mathbf{1})(NO_3)_4(H_2O)_2]\cdot Et_2O\cdot 1.5(H_2O)$ crystal

Donor group	D···A / Å	H···A / Å	D-H···A / °	Acceptor atom
N(1)-H(1)	2.92(1)	2.28	126	O(11)
N(2)-H(2)	3.36(1)	2.49	160	O(13)
N(3)-H(3)	3.07(1)	2.21	158	O(12)
N(4)-H(4)	2.95(1)	2.27	131	O(7)
N(5)-H(5)	3.02(1)	2.23	145	O(15)
N(6)-H(6)	3.08(1)	2.21	161	O(8)
O(1w)-H(1wA)	2.78(1)	1.95(6)	152(4)	O(9)
O(2w)-H(2wA)	2.78(1)	2.02(5)	140(4)	O(10)

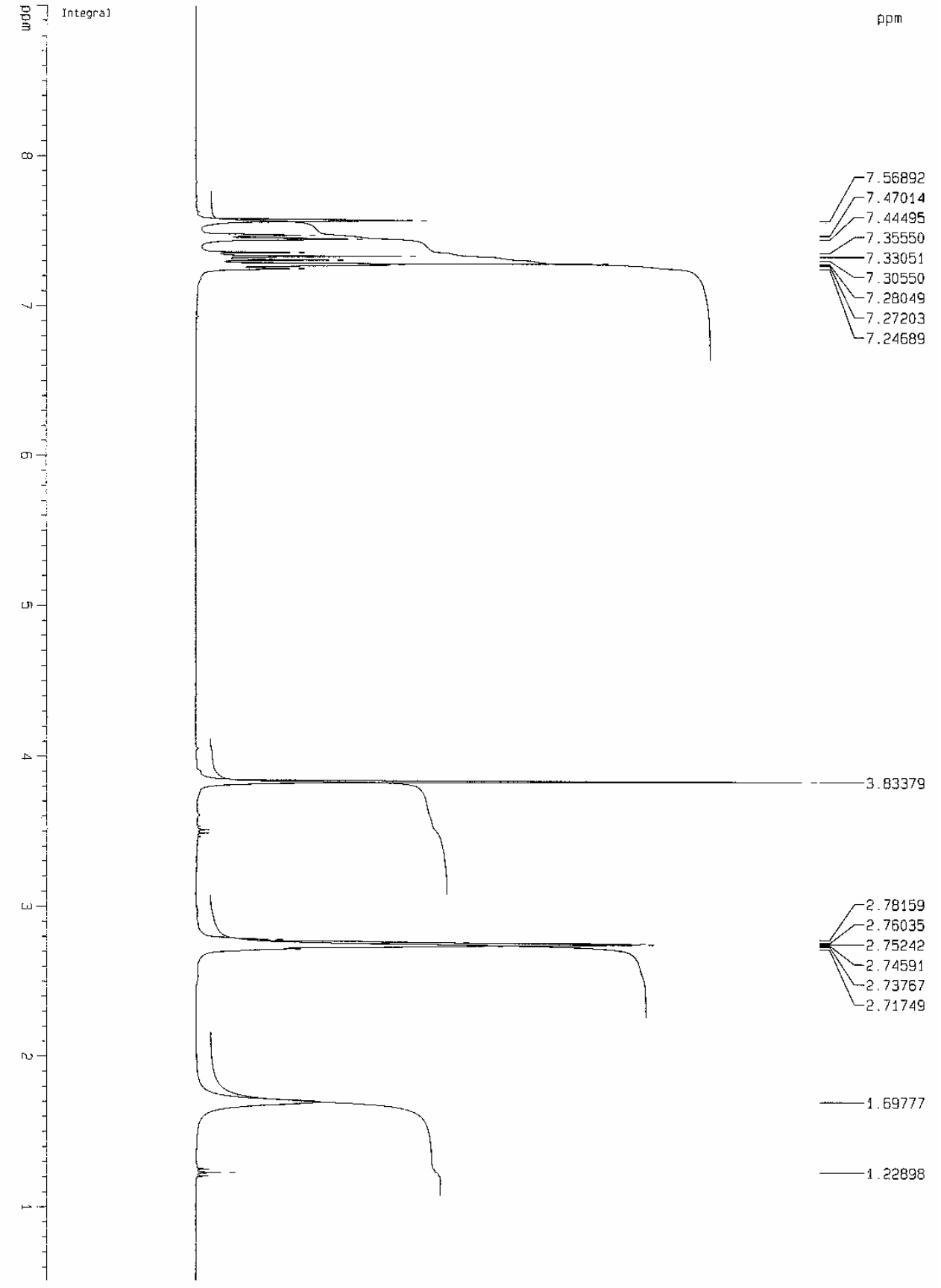

Figure 2S. ^{1}H-NMR spectra of **1** ($CDCl_3$, 300 MHz, 25ºC).

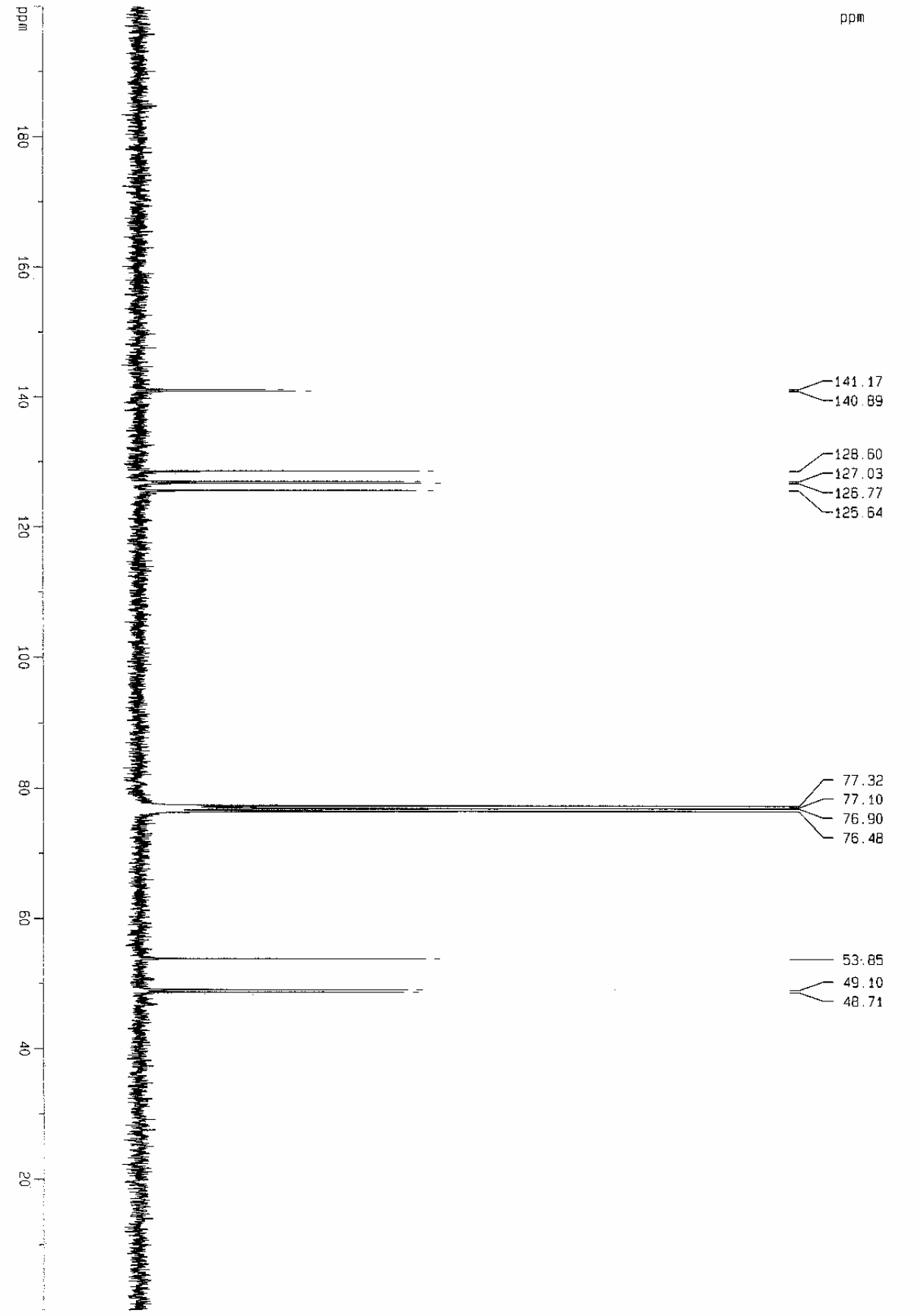

Figure 3S. ^{13}C-NMR spectra of **1** ($CDCl_3$, 75 MHz, 25ºC).

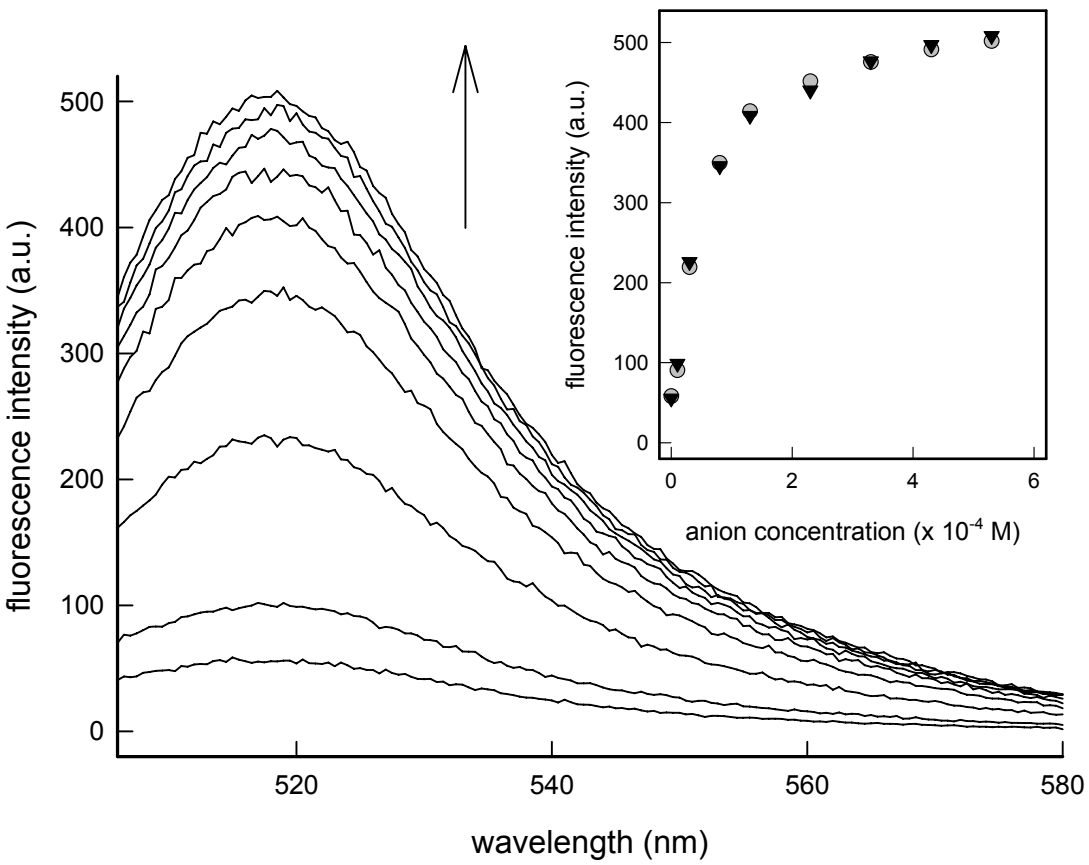

Figure 4S Selected emission spectra obtained during the titration with malonate of a solution containing the receptor complex $[Cu_2(\mathbf{1})]^{4+}$ (5 x 10^{-6} M) and indicator 3 (10^{-6} M). Inset: titration profile at 518.5 nm (black triangles) and data obtained from the fit (grey circles). Fitting of data was obtained with Hyperquad package, using 20 selected wavelength. Data were fitted according to a competition model: for data processing details see: N. Marcotte, A. Taglietti, *Supramol. Chem.*, 2003, **15**, 617 and references therein.