Supplementary Material (ESI) for New Journal of Chemistry

Towards sensory Langmuir monolayers consisting of macrocyclic pentaaminoanthraquinone

Elena Ranyuk,[a] Elizaveta V. Ermakova,[b,c] Laura Bovigny,[a,d] Michel Meyer,*[a] Alla Bessmertnykh-Lemeune,[a] Roger Guilard,[a] Yoann Rousselin,[a] Aslan Yu. Tsivadze[b] and Vladimir V. Arslanov*[b]

[a] *Institut de Chimie Moléculaire de l'Université de Bourgogne (ICMUB), UMR CNRS 6302, 9 avenue A. Savary, 21078 Dijon Cedex, France. E-mail: michel.meyer@u-bourgogne.fr; Fax: +33 3 80 39 61 17; Tel: 33 3 80 39 37 16*
[b] *Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Leninsky Pr., 31 GSP-1, Moscow, 119071, Russia. E-mail: pcss_lab@mail.ru*
[c] *On leave from Higher Chemical College, Russian Academy of Sciences, Moscow, Russia*
[d] *Erasmus fellow on leave from the Ecole d'Ingénieurs et d'Architectes de Fribourg, boulevard de Pérolles 80, 1705 Fribourg, Switzerland*

Table of Contents

1. Hydrogen bond distances and angles

Table S1. Hydrogen bonds for [(PENTAQ)H]CF_3SO_3•H_2O

D	H	A	*d*(D–H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(D–H···A) (°)
O10	H10A	O6B[a]	1.00(2)	1.80(3)	2.77(2)	163(5)
O10	H10A	O6A[a]	1.00(2)	1.99(9)	2.94(9)	157(5)
O10	H10B	O6B[b]	0.997(19)	1.96(4)	2.91(1)	160(7)
O10	H10B	O4A[b]	0.997(19)	1.91(9)	2.75(7)	141(6)
N1	H1	O1	0.77(5)	2.02(5)	2.631(4)	136(4)
N5	H5	O1	0.80(5)	2.07(5)	2.630(4)	127(4)
N5	H5	N4	0.80(5)	2.35(4)	2.765(6)	113(4)
N3	H3A	O10	0.99	1.85	2.829(7)	169.0
N3	H3B	O2[c]	0.99	2.34	3.054(5)	128.4

Symmetry transformations used to generate equivalent atoms: (*a*) –*x*, 1 – *y*, 1 – *z*; (*b*) *x*, *y*, 1 + *z*. (*c*) 1 – *x*, 1 – *y*, 1 – *z*.

Table S2. Hydrogen bonds for [(PENTAQ)H_2](CF_3SO_3)$_2$

D	H	A	*d*(D–H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠(D–H···A) (°)
N1	H1	O1	0.82(2)	1.92(2)	2.582(2)	137(2)
N2	H2C	O3[a]	0.87(3)	1.99(3)	2.853(3)	174(2)
N2	H2D	O7[b]	0.91(2)	2.00(2)	2.844(3)	152(2)
N3	H3	O8[b]	0.86(2)	2.32(2)	3.085(3)	147(2)
N4	H4C	O4	0.92(2)	2.36(2)	2.886(2)	115.8(16)
N4	H4C	O5[a]	0.92(2)	2.03(2)	2.802(2)	139.9(18)
N4	H4D	O6[b]	0.90(2)	2.11(2)	2.877(2)	143(2)
N5	H5	O1	0.81(2)	1.94(2)	2.590(2)	137(2)
N5	H5	O5[a]	0.81(2)	2.59(2)	3.216(2)	135(2)

Symmetry transformations used to generate equivalent atoms: (*a*) 2 – *x*, 1 – *y*, 1 – *z*; (*b*) 1 – *x*, 1 – *y*, 1 – *z*.

2. Spectrophotometric protonation studies

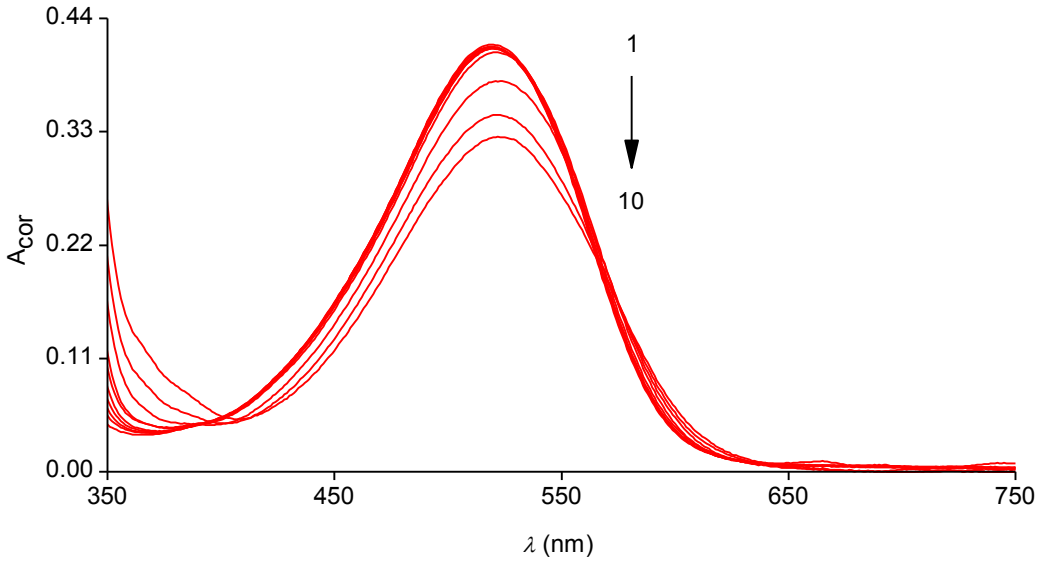
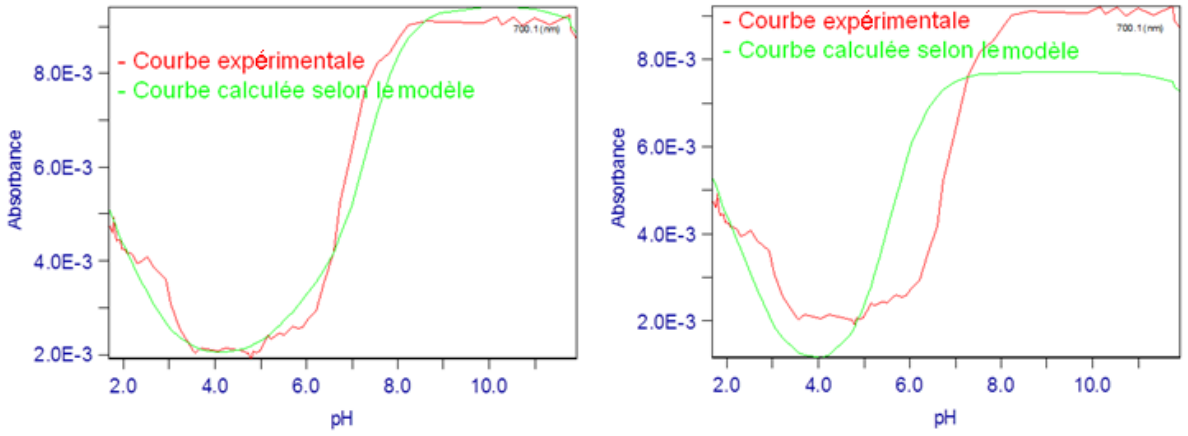
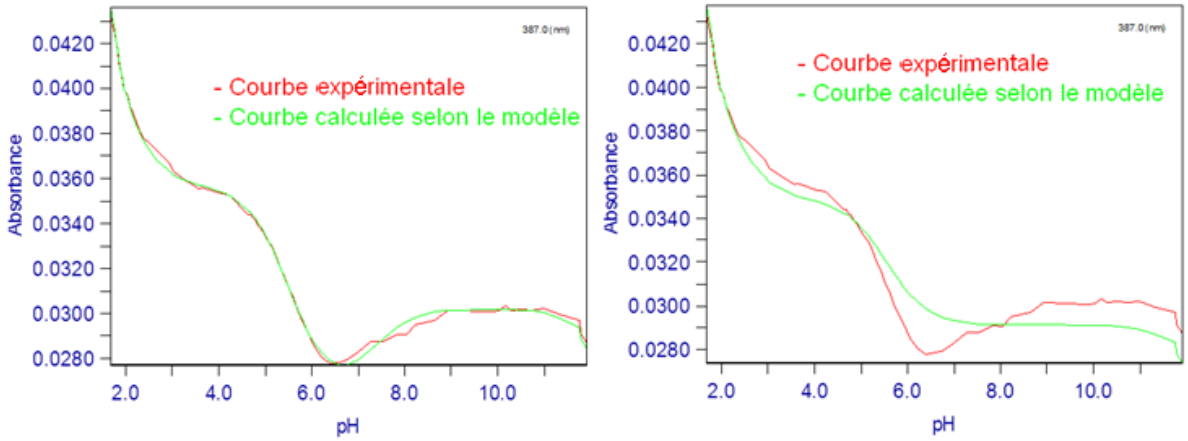


Fig. S1 Spectrophotometric batch titration of PENTAQ (L) at high acidities in CH_3OH/H_2O 80:20 v/v. $[L]_{tot}$ = 47 μM, $[N(CH_3)_4NO_3]_0$ = 0.1 M (the total ionic strength increased with each added aliquot of HNO_3), V_0 = 2 mL; T = 298.2(2) K, l = 1 cm, spectra 1–10 (corrected for dilution effects): p[H] = –log $[HNO_3]_{tot}$ = 1.67, 1.17, 0.94, 0.72, 0.51, 0.30, 0.07, –0.2, –0.4, –0.6.



(a)



(b)

Fig. S2 Absorbance *vs*. p[H] titration profiles at (a) 700 and (b) 387 nm of PENTAQ (L) in CH_3OH/H_2O 80:20 v/v. The red curves correspond to the experimental data and the green ones to the best fit obtained with a chemical model comprising either 3 (L, LH^+, LH_2^{2+}; right graph) or 4 absorbing species (L, LH^+, LH_2^{2+}, LH_3^{3+}; left graph). $[L]_{tot}$ = 47 µM, $[N(CH_3)_4OH]$ = 0.1040 M, V_0 = 30 mL, I = 0.1 M $N(CH_3)_4NO_3$, T = 298.2(2) K, l = 1 cm.

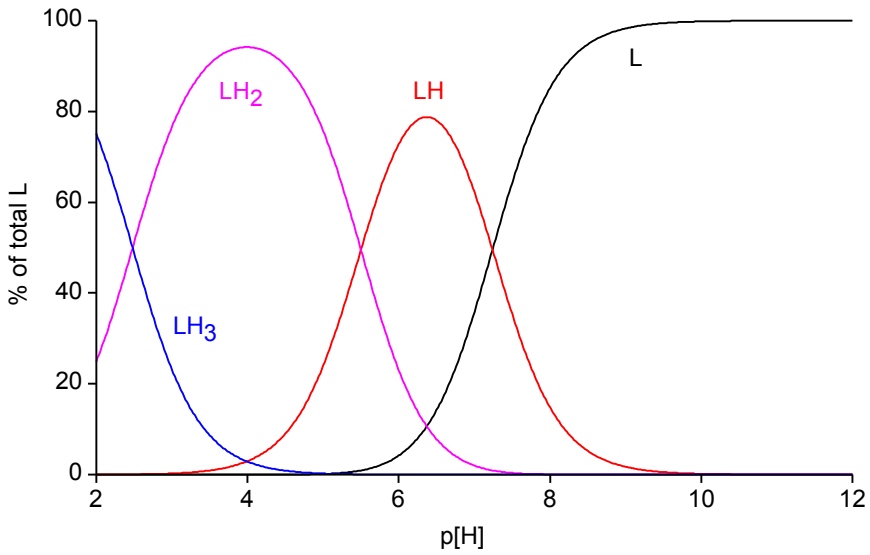


Fig. S3 Species distribution diagram for PENTAQ (L) in CH_3OH/H_2O 80:20 v/v. I = 0.1 M $N(CH_3)_4NO_3$, T = 298.2(2) K.

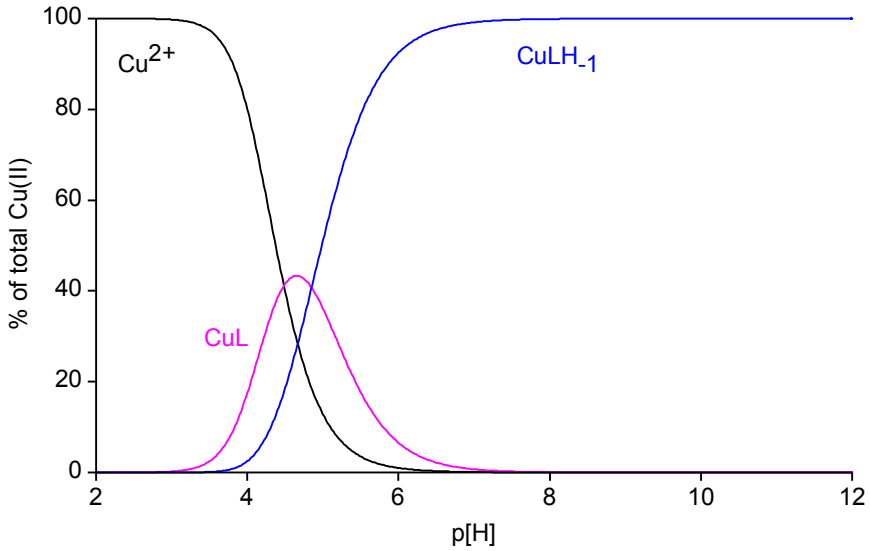


Fig. S4 Species distribution diagram for the Cu^{2+}/PENTAQ (L) system in CH_3OH/H_2O 80:20 v/v. $[L]_{tot}$ = $[Cu]_{tot}$ = 42.9 μM, I = 0.1 M $N(CH_3)_4NO_3$, T = 298.2(2) K.

3. XPS studies of Cu^{2+} uptake by Langmuir-Blodgett monolayers of PENTAQ

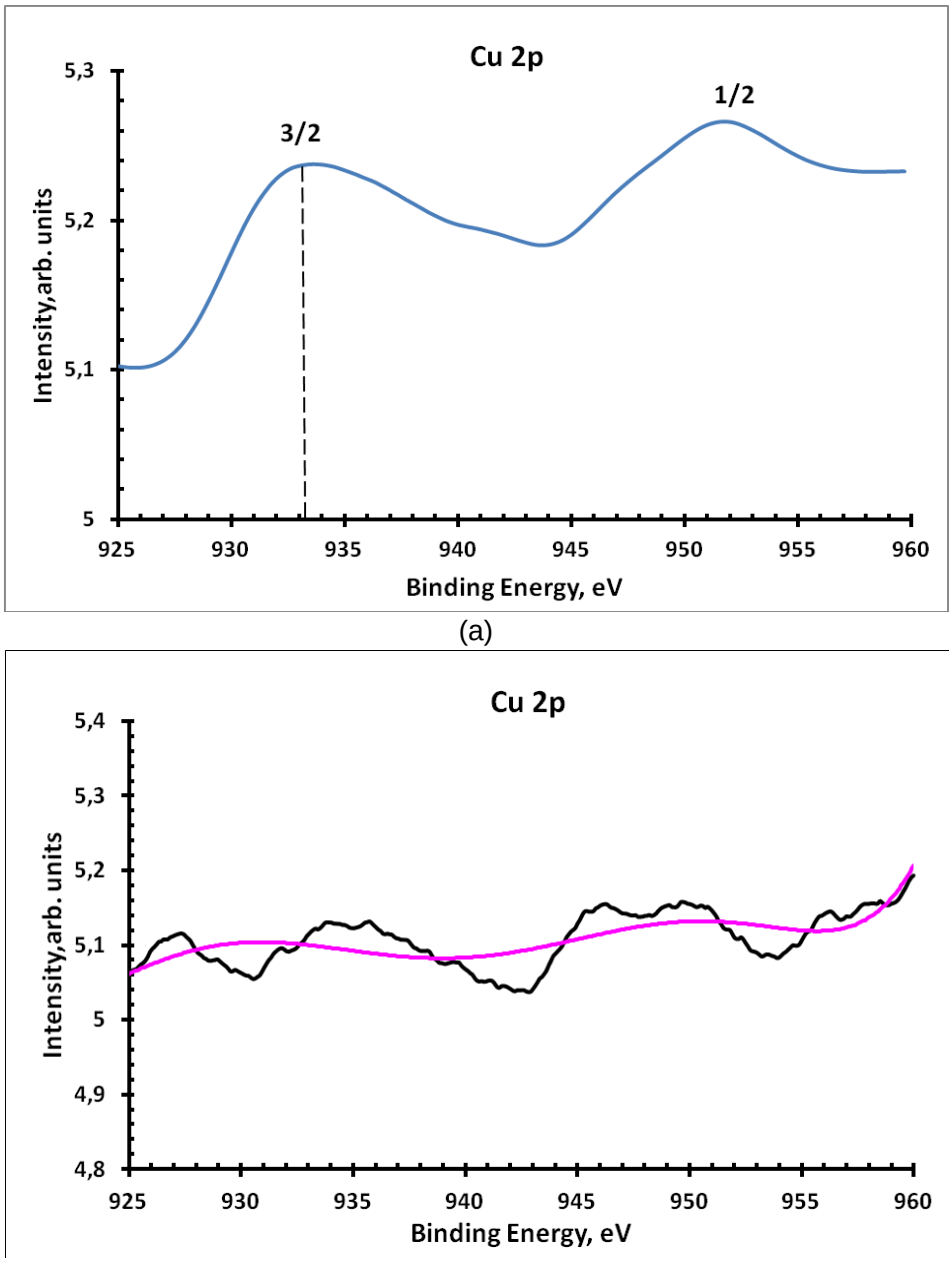


Fig. S5 XPS spectra in the Cu 2*p* region of PENTAQ Langmuir-Blodgett films transferred from a water subphase (pH = 9.8) to a quartz slide. (a) Sample A was air-dried directly after deposition and analyzed. (b) Sample B was rinsed with deionized water for 30 s after deposition, then air-dried and analyzed. The magenta line corresponds to the smoothed spectrum.