Recognition of C₆₀ by Tetra- and Tri-Quinoxaline Cavitands

Francesco P. Ballistreri,^{*,a} Giovanna Brancatelli,^b Nicola Demitri,^c Silvano Geremia,^b Dirk M. Guldi,^d Michele Melchionna,^b Andrea Pappalardo,^{a,e} Maurizio Prato,^b Gaetano A. Tomaselli,^a Giuseppe Trusso Sfrazzetto^{*,a}

^a *Dipartimento di Scienze Chimiche, Università di Catania, Viale Andrea Doria 6, 95125 Catania, Italy*

^b *Dipartimento di Scienze Chimiche e Farmaceutiche, Centro di Eccellenza in Biocristallografia, Università di Trieste, Via L. Giorgieri 1, Trieste, Italy*

^c *Elettra - Sincrotrone Trieste, S. S. 14 Km 163.5 in Area Science Park, Basovizza, Trieste, Italy*

^d *Department of Chemistry and Pharmacy and Interdisciplinary Center for Molecular Materials, Frierich-Alexander Universität Erlangen-Nürnberg, 91058, Erlangen, Germany*

^e *I.N.S.T.M. UdR of Catania, Viale A. Doria 6, 95125 Catania, Italy*

Supplementary Material

^1H NMR spectrum of **Octol** in acetone- d_6 (500 MHz, 27° C)

ESI-MS spectrum of **Octol**

^1H NMR spectrum of **2** in CDCl_3 (500 MHz, 27°C)

ESI-MS spectrum of **2**

Room temperature absorption spectra of cavitand **1** (2.14×10^{-5} M) in toluene as solvent upon adding variable concentration of C_{60} ($0.21 \times 10^{-5} - 3.21 \times 10^{-5}$ M).

Room temperature absorption spectra of cavitand **2** (2.61×10^{-5} M) in toluene as solvent upon adding variable concentration of C_{60} ($0.26 \times 10^{-5} - 5.22 \times 10^{-5}$ M).

^1H NMR stack plot of the signal decay (toluene- d_8 , 1 mM, 298 K) as a function of the gradient strength (D) for the cavitand **1**.

Fitting for the diffusion constant derived from the signal decays for the cavitand **1** (toluene- d_8 , 1 mM, 298 K).

^1H NMR stack plot of the signal decay (toluene- d_8 , 1 mM, 298 K) as a function of the gradient strength (D) for the supramolecular complex 1:1 between **1** and C_{60} .

Fitting for the diffusion constant derived from the signal decays for the supramolecular complex 1:1 between **1** and C_{60} (toluene- d_8 , 1 mM, 298 K).

EI-MS spectrum of the supramolecular complex 1:1 between **1** and C₆₀

Fluorescence titration between cavitand 1 and C₆₀

HypSpec output file:

Converged in 4 iterations with sigma = 0,078816

Log beta value stand. dev.

AB 5.2387 0.1422

Fluorescence titration between cavitand 2 and C₆₀

HypSpec output file:

Converged in 4 iterations with sigma = 0,095619

Log beta value stand. dev.

AB 4.9518 0.1424