Electronic Supplementary Information for Dalton Transactions

P,N-Containing Cyclophanes with Large Helical Hydrophobic Cavities: Prospective Precursors for the Design of a Molecular Reactor

Andrey A. Karasik, Dmitrii V. Kulikov, Anna S. Balueva, Svetlana N. Ignat'eva, Olga N. Kataeva, Peter Lönnecke, Artem V. Kozlov, Shamil K. Latypov, Evamarie Hey-Hawkins, Oleg G. Sinyashin

Electronic Supplementary Information

1) 1D ^{1}H ROESY spectra of 1

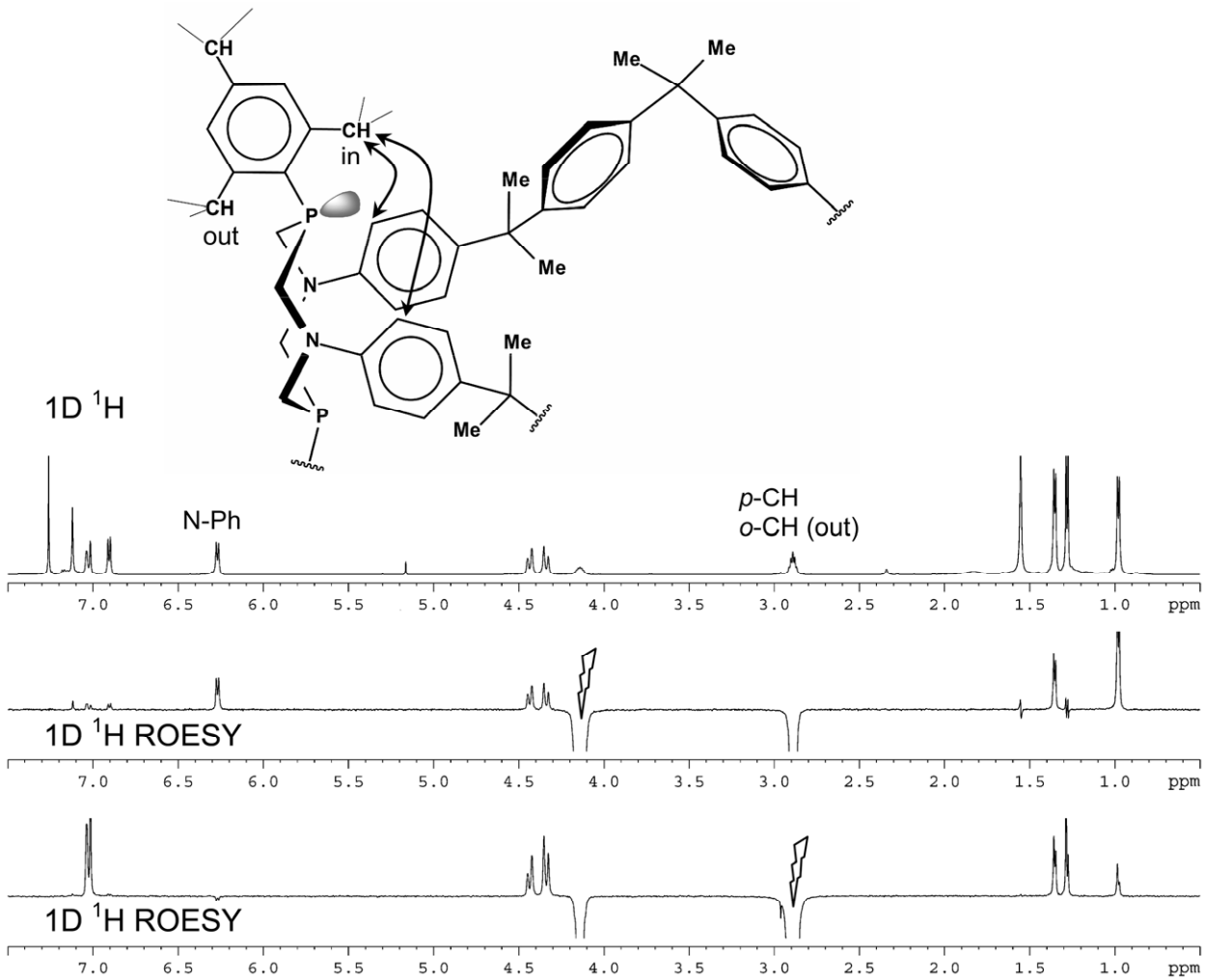

Fig. S1 1D ^{1}H ROESY spectra of **1** in $CDCl_3$ at T=288K and fragment of the molecule with observed nOes.

2) The binding constants measurement (30 °C, $CDCl_3$).

The binding constants values K_a were calculated from single host and guest concentrations according to eqs 1 and 2, because the large excess of the guest was used.

$$K_a = \frac{P}{(1 - P) \cdot C_{guest}} \quad (1)$$

$$P = \frac{\Delta\delta_{observed}}{\Delta\delta_{max}} \quad (2)$$

Table 1 "Single-point" binding constants K_a of hosts **1** and **2** and aromatic guests in $CDCl_3$

Host	Guest	C_{host}, 10^{-3} M	C_{guest}, 10^{-2} M	Δδ, ppm[e]	K_a, M^{-1}
1[a]	C_6D_6	6.73	6.73	-0.020	0.65
1[a]	C_6D_6	6.57	13	-0.039	0.68
1[a]	C_6D_6	2	4	-0.012	0.64
2[b]	C_6D_6	2	4	-0.012	0.56
1[c]	$C_6D_5CD_3$	2	4	-0.055	2.75
2[d]	$C_6D_5CD_3$	2	4	-0.016	0.66

[a] $\Delta\delta_{max}$ = -0.48 ppm; [b] $\Delta\delta_{max}$ = -0.55 ppm; [c] $\Delta\delta_{max}$ = -0.55 ppm; [d] $\Delta\delta_{max}$ = -0.61 ppm ; [e] for the signal of the central phenylene group