Normal Hydrocarbons Tumble Rapidly in a Deep, Water-Soluble Cavitand

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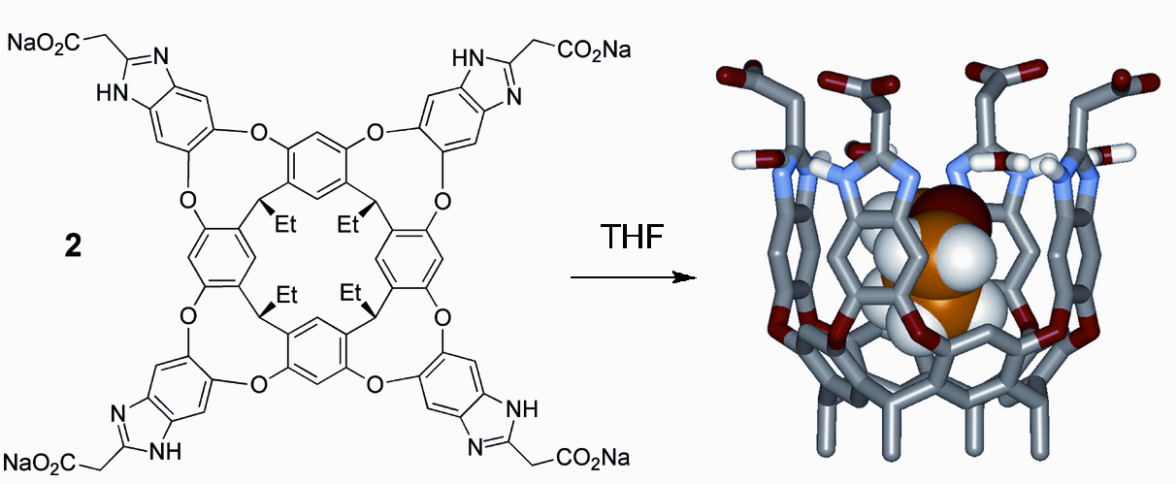
Supplementary Information

1. General Information

NMR spectra were recorded on a Bruker DRX-600 spectrometer. Proton (^{1}H) chemical shifts are reported in parts per million (δ) with respect to tetramethylsilane (TMS, δ=0), and referenced internally with respect to the protio solvent impurity. Deuterated NMR solvents were obtained from Cambridge Isotope Laboratories, Inc., Andover, MA, and used without further purification. *N*-alkanes (pentane-dodecane, >99%) were obtained from Aldrich Chemical Company, St. Louis, MO and were used as received. Molecular modeling (molecular mechanics calculations) was carried out using the AMBER force field with the solvation (dielectric) setting for water as implemented by Macromodel of Maestro (Schroedinger, Inc.) on a Silicon Graphics Octane workstation. Cavitand **2** was synthesized according to the procedure described in: Biros, S.M., Ullrich, E.C., Hof, F., Trembleau, L., Rebek, J., *J. Am. Chem. Soc.*, 2004, **126**, 2870.

2. Supplementary Figures.



Supplementary Figure 1. Structure of water-soluble cavitand (host) **2**.

3. Supplementary Tables.

Supplementary Table 1. Observed and predicted (calculated) chemical shifts for *n*-alkanes complexed with cavitand **2** in D_2O (2 mM, 600 MHz).

SDS observed δ's	*n*-alkane	Predicted δ's	Observed δ's
	HEXANE	Predicted	Observed
C_1: -3.95	$C_{1/6}$	-2.28	-2.17
C_2: -3.35	$C_{2/5}$	-2.33	-2.17
C_3: -2.95	$C_{3/4}$	-2.63	-2.67
C_4: -2.30			
C_5: -1.30	HEPTANE	Predicted	Observed
C_6: -0.20	$C_{1/7}$	-1.83	-1.80
C_7: 0.70	$C_{2.6}$	-1.78	-1.80
C_8: 1.10	$C_{3/5}$	-2.13	-2.10
C_9: 1.20	C_4	-2.40	-2.37
C_{10}: 1.20			
C_{11}: 1.20	OCTANE	Predicted	Observed
	$C_{1/8}$	-1.63	-1.59
	$C_{2/7}$	-1.33	-1.35
	$C_{3/6}$	-1.58	-1.59
	$C_{4/5}$	-1.80	-1.83
	NONANE	Predicted	Observed
	$C_{1/9}$	-1.58	-1.50
	$C_{2/8}$	-1.13	-1.11
	$C_{3/7}$	-1.13	-1.11
	$C_{4/6}$	-1.25	-1.25
	C_5	-1.40	-1.50
	DECANE	Predicted	Observed
	$C_{1/10}$	-1.58	-1.48
	$C_{2/9}$	-1.08	-1.00
	$C_{3/8}$	-0.93	-0.91
	$C_{4/7}$	-0.80	-0.82
	$C_{5/6}$	-0.75	-0.75
	UNDECANE	Predicted	Observed
	$C_{1/11}$	-1.58	-1.49
	$C_{2/10}$	-1.08	-0.99
	$C_{3/9}$	-0.88	-0.83
	$C_{4/8}$	-0.60	-0.60

	$C_{5/7}$	-0.30	-0.33
	C_6	-0.30	-0.23