Supporting Information

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SI Text

^{1}H NMR spectra were recorded on a Bruker DRX-600 spectrometer with a 5-mm QNP probe. Proton (^{1}H) chemical shifts, reported in parts per million (ppm), were indirectly referenced to external tetramethylsilane employing resonance as an internal reference. Deuterated mesitylene was obtained from Cambridge Isotope Laboratories, Inc.

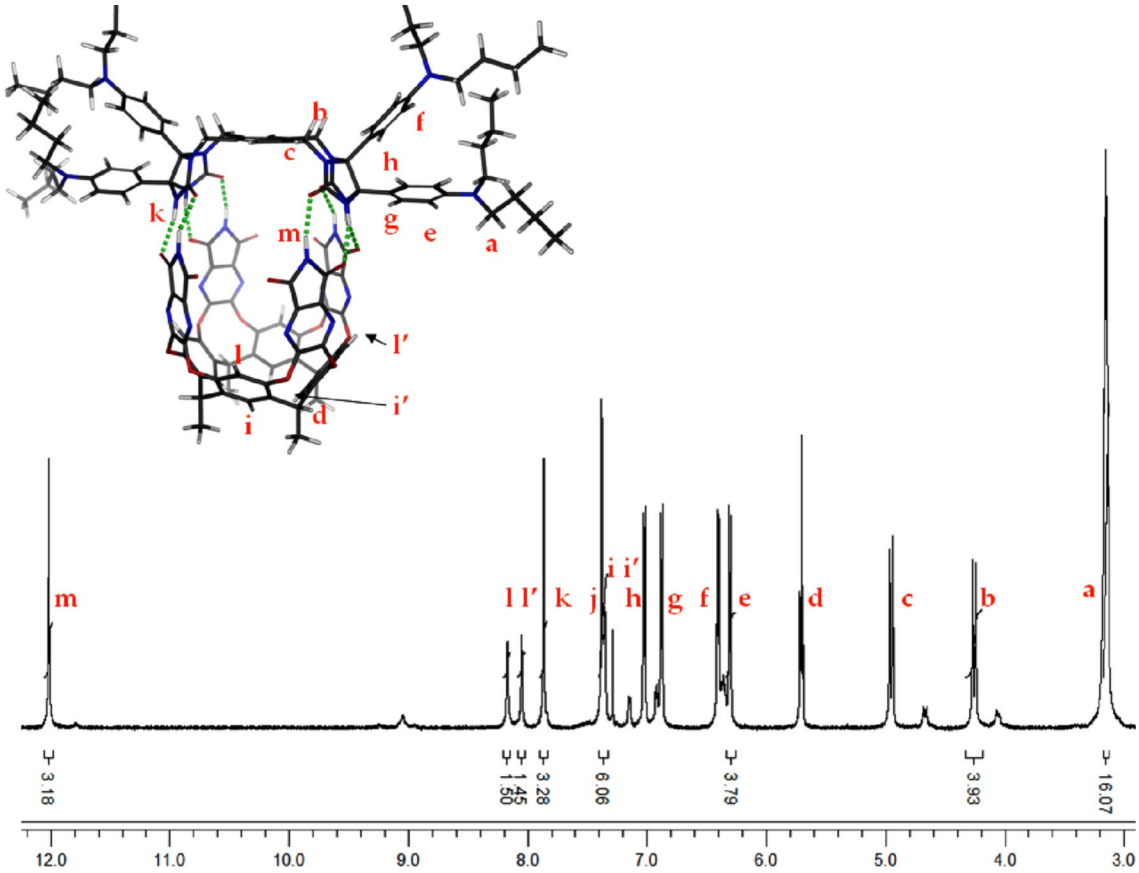

Fig. S1. ^{1}H NMR assignment of **2.3** in chloroform. ($CDCl_3$, 300 K.)

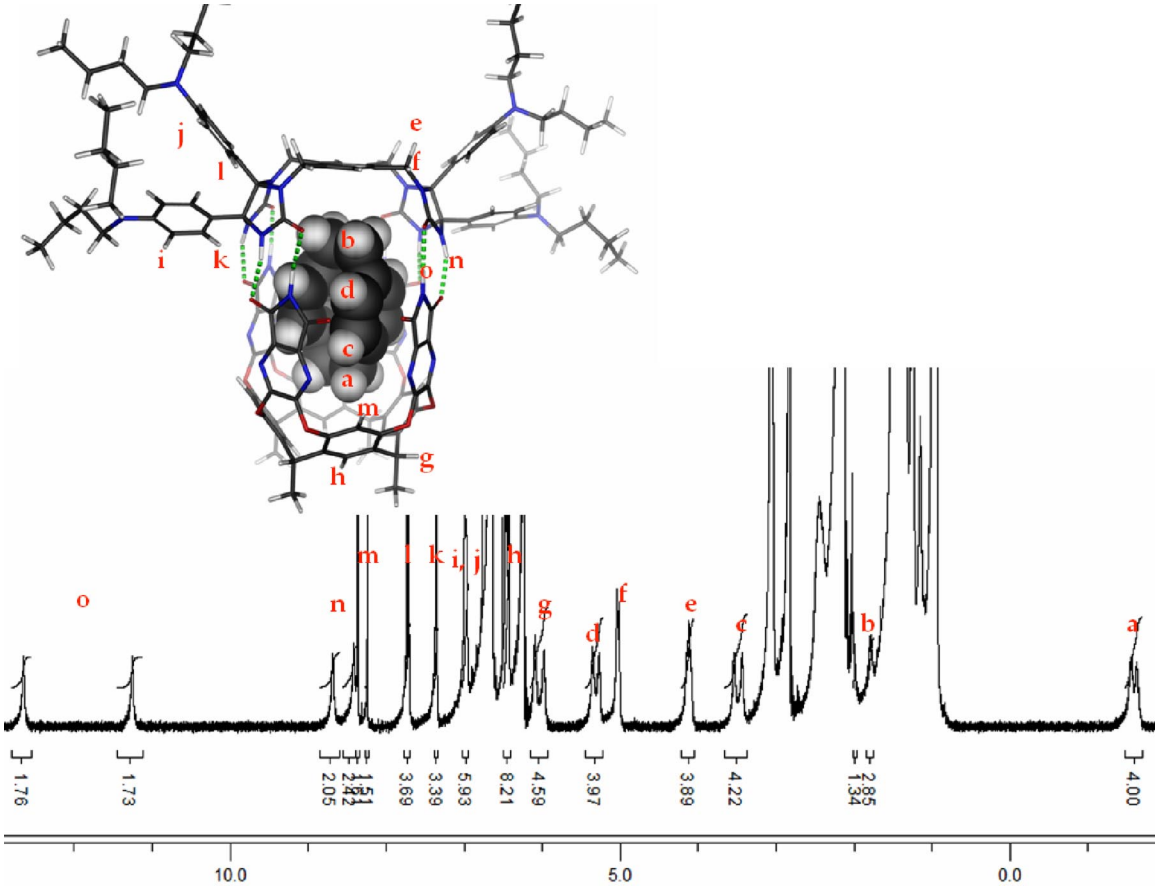

Fig. S2. ^{1}H NMR assignment of encapsulated paracyclophane in **2.3** (mesitylene-d_{12}, 300 K).

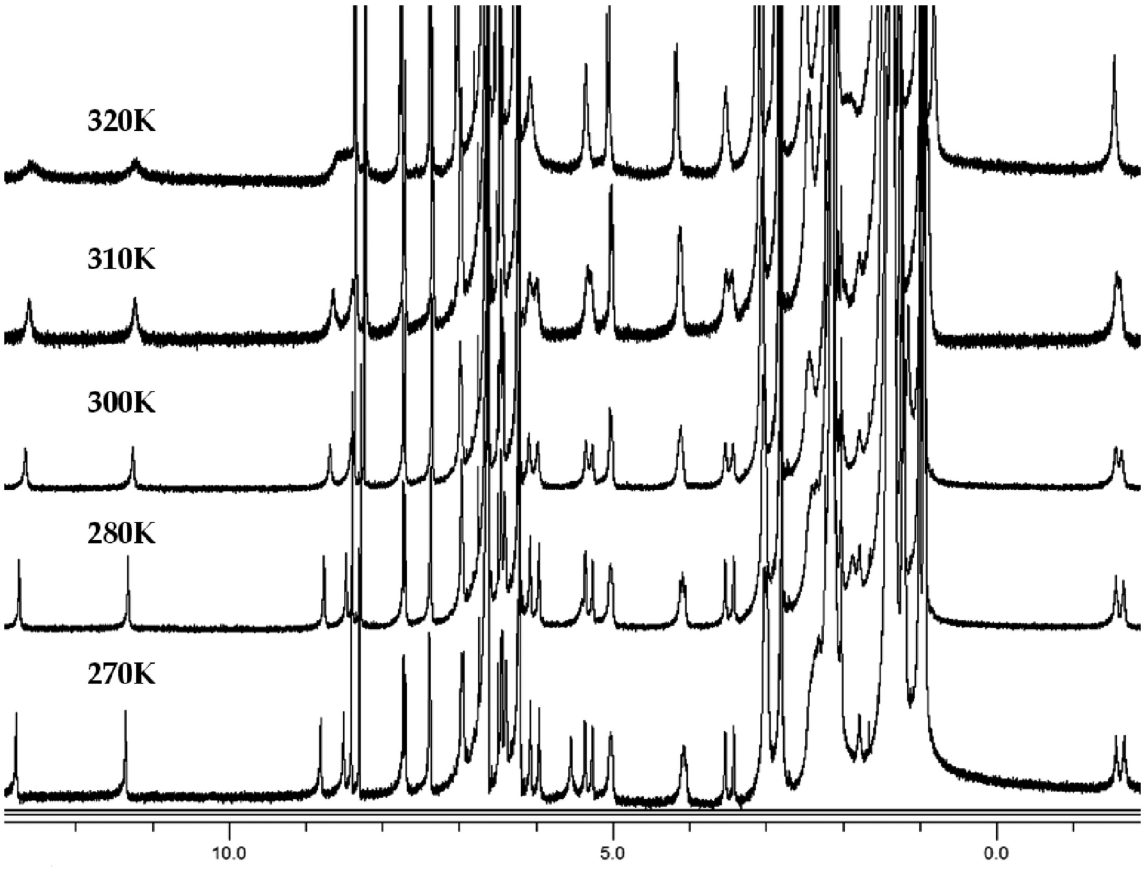

Fig. S3. ^{1}H NMR spectra (mesitylene-d_{12}, 300 K) of encapsulated paracyclophane in **2.3** at different temperature.

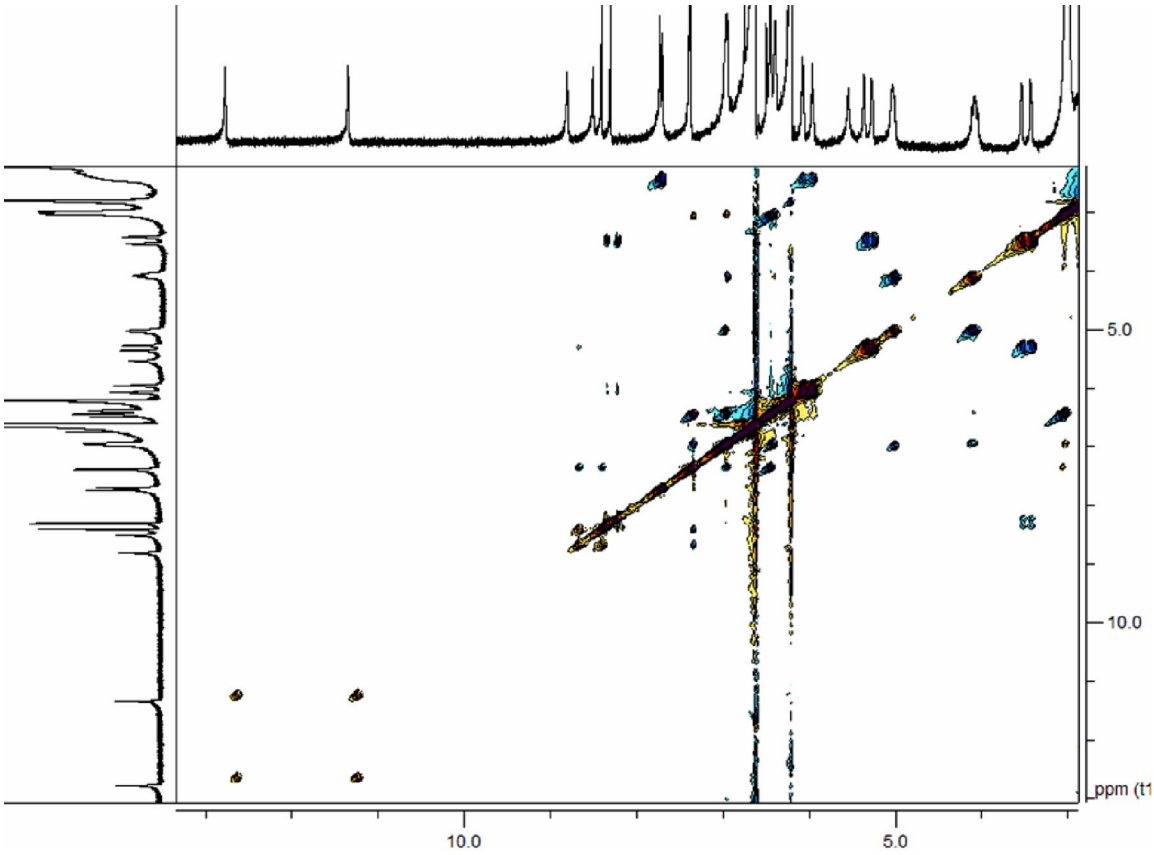

Fig. S4. Partial 2D ROESY spectrum (mesitylene-d_{12}, 300 K, mixing time = 0.3 s, D1 = 3 s) of encapsulated paracyclophane in **2.3**. The cross-peaks indicate exchange of 2 enantiomer on the NMR timescale.

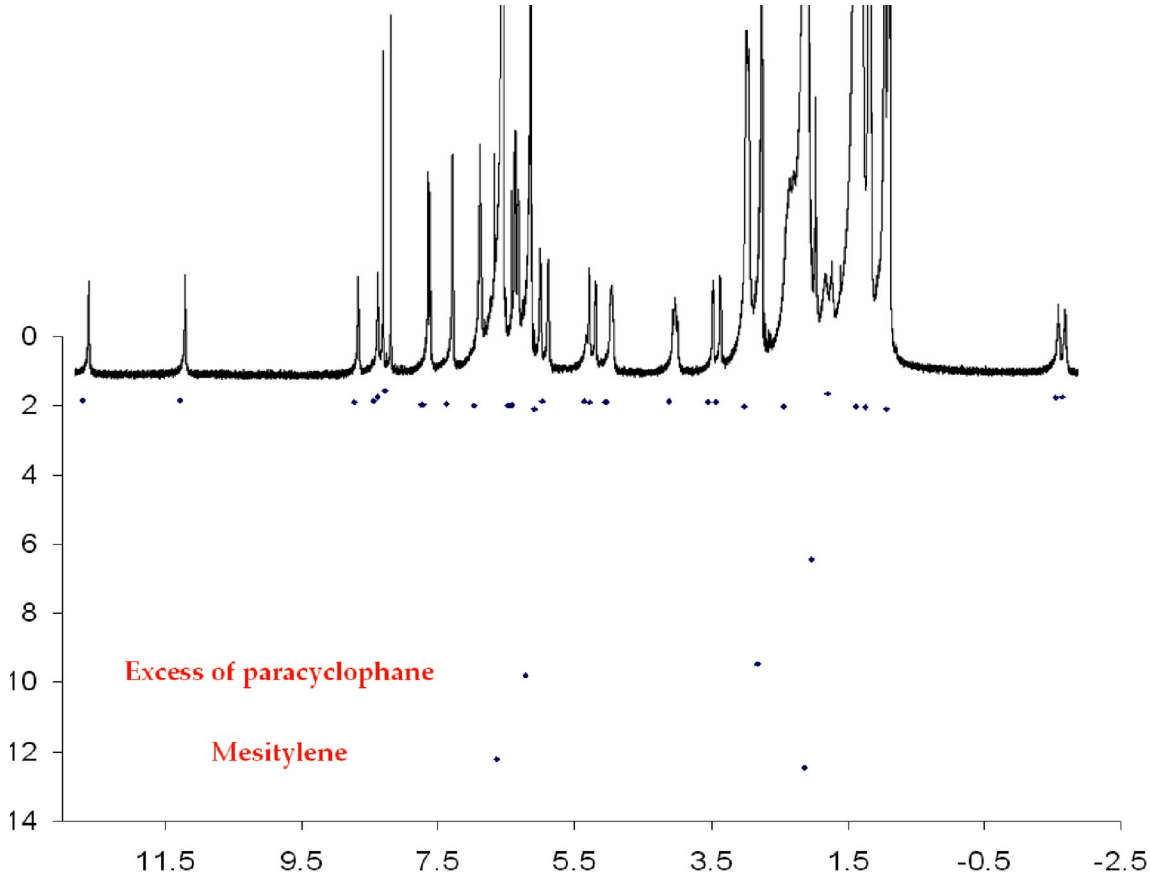

Fig. S5. DOSY spectrum (mesitylene-d_{12}, 290 K) of encapsulated paracyclophane in **2.3**. The cavitand **2** and half of tennis ball $\mathbf{3}_2$ and paracyclophane diffuse as a single species. The average diffusion coefficient for this complex is 1.87×10^{-10} m2·s^{-1}.

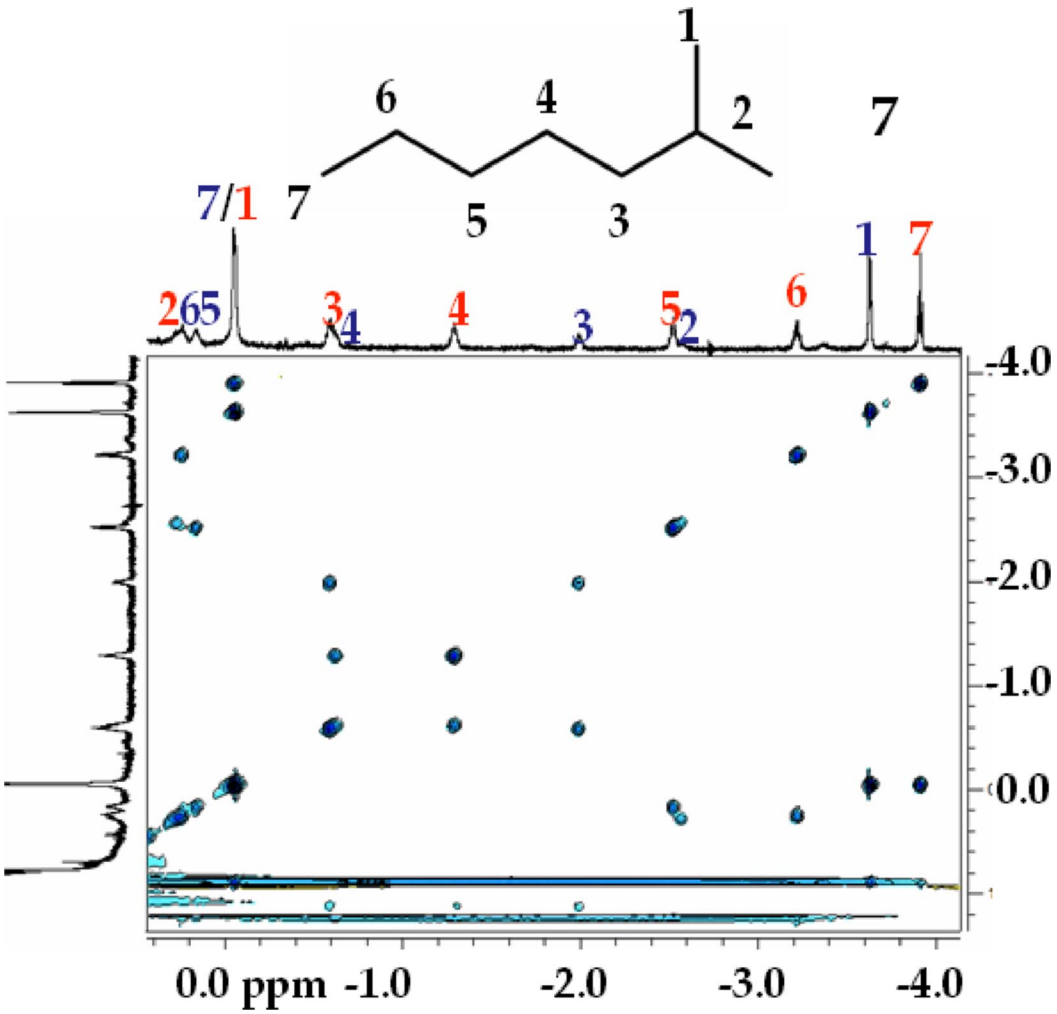

Fig. S6. Upfield regions of 2D ROESY spectrum (mesitylene-d_{12}, 300 K, mixing time = 0.3 s, D1 = 3 s) of encapsulated 2-dimethyl heptane **7** in **2.3**.

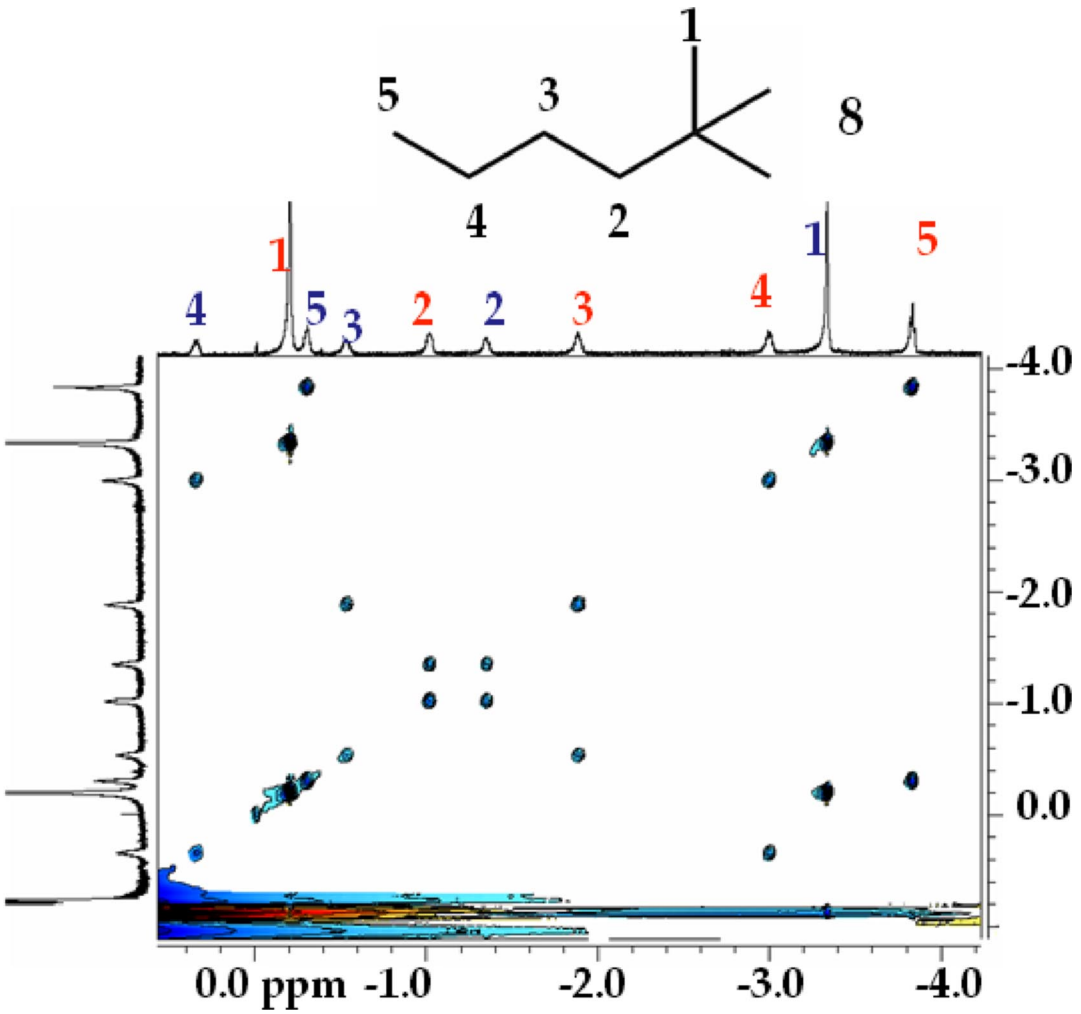

Fig. S7. Upfield regions of 2D ROESY spectrum (mesitylene-d_{12}, 300 K, mixing time = 0.3 s, D1 = 3 s) of encapsulated 2,2-dimethyl hexane **8** in 2.3.

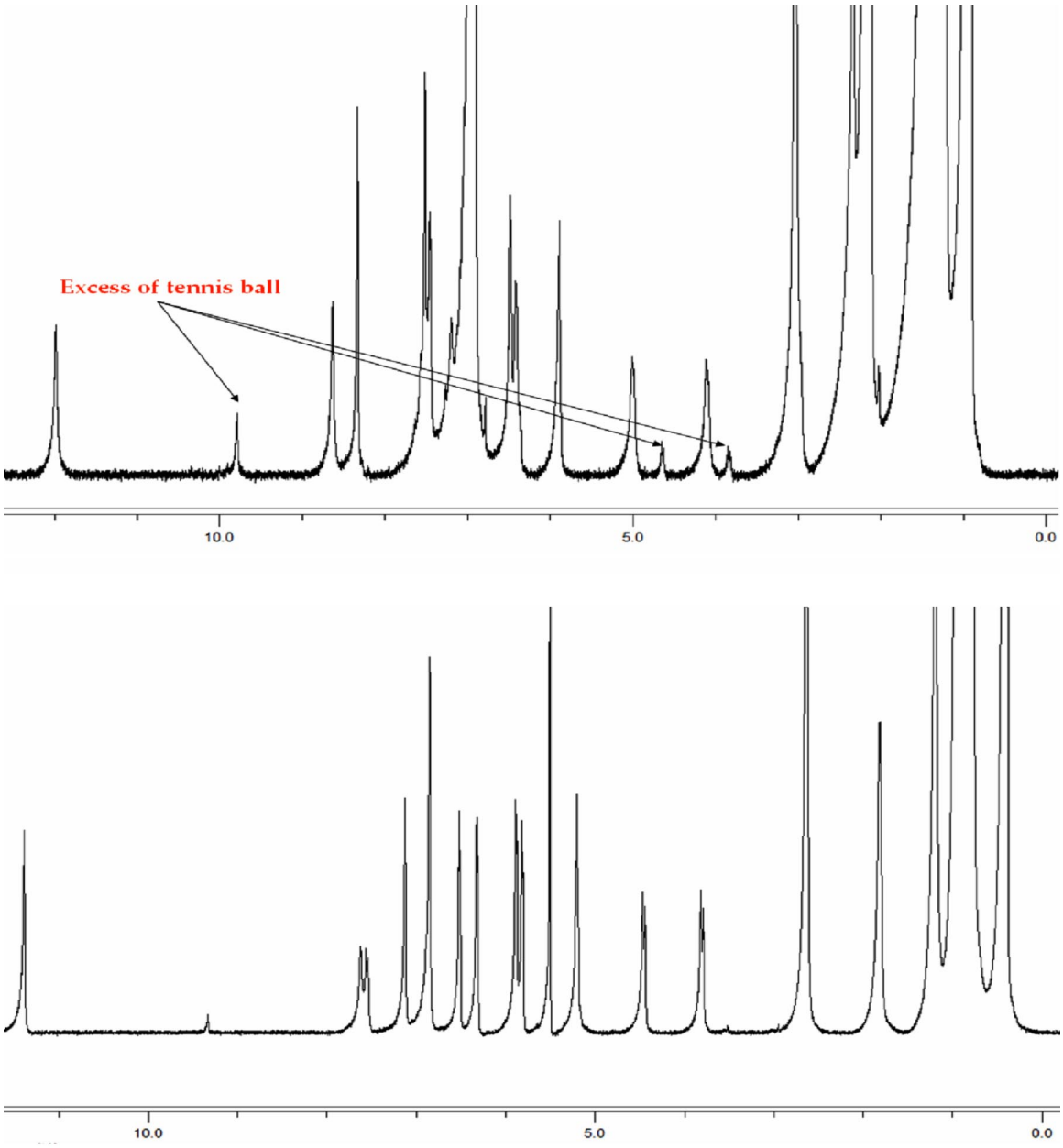

Fig. S8. ^{1}H NMR spectra of hybrid capsule **2.3** in paraxylene-d_{10}, 300 K (*Upper*) and tetrachloroethane-d_2, 300 K (*Lower*).

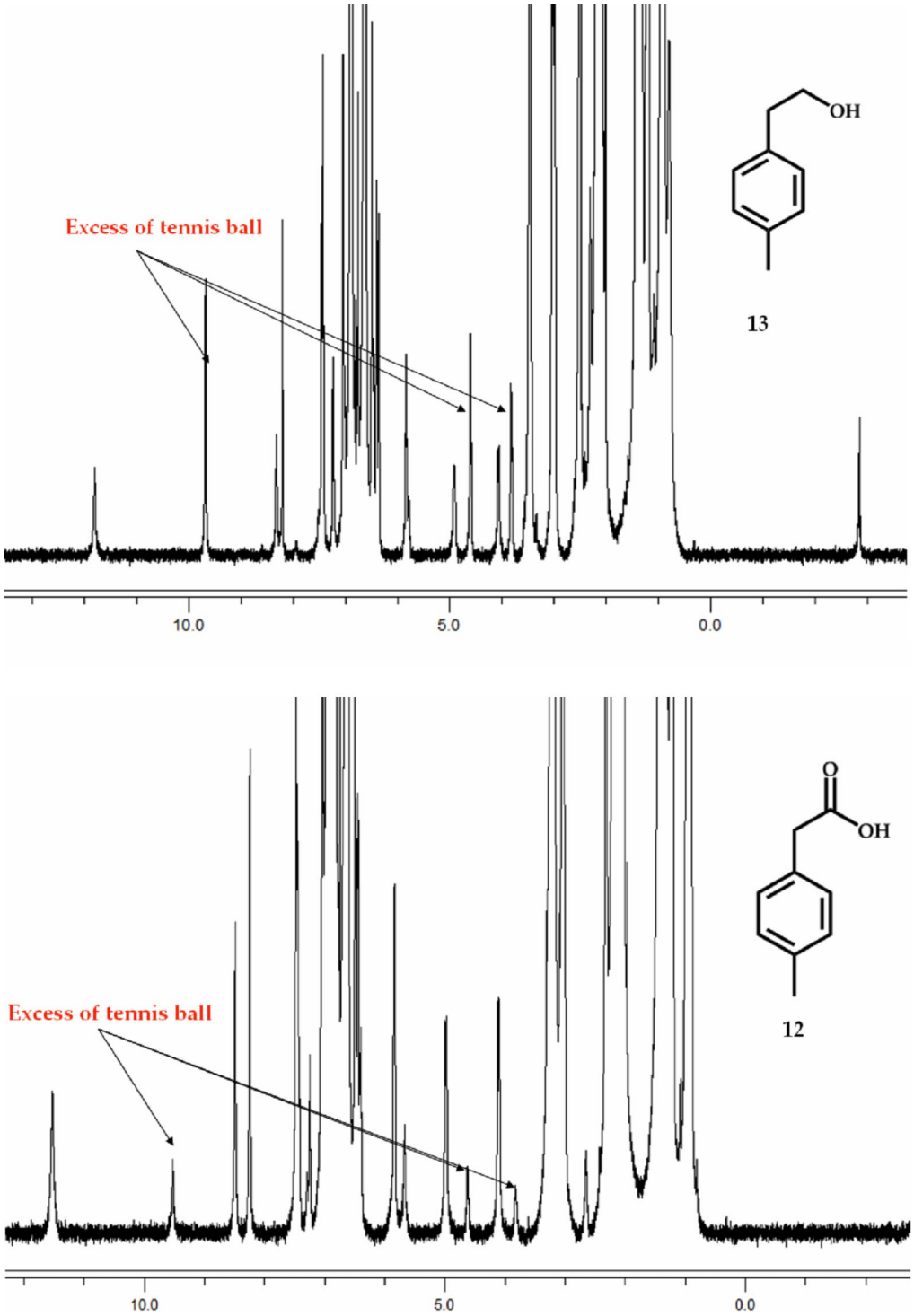

Fig. S9. ^{1}H NMR spectra (mesitylene-d_{12}, 300 K) of encapsulation of 4-methylphenethyl alcohol **12** in hybrid capsule **2.3** (*Upper*) and encapsulation of 4-methylphenyl acetic acid **13** in hybrid capsule **2.3** (*Lower*).

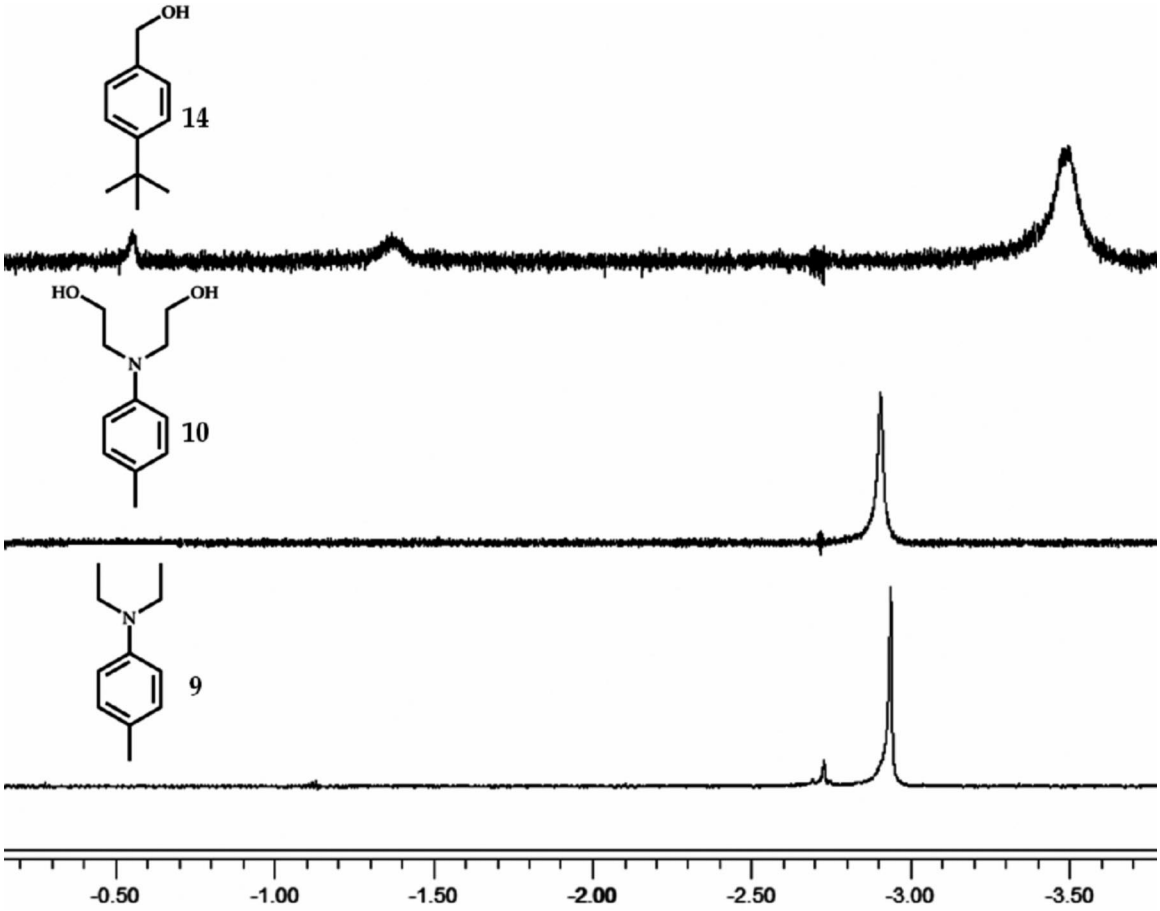

Fig. S10. Partial ^{1}H NMR spectra (mesitylene-d_{12}, 300 K) of hybrid capsule **2.3** complexes with *N*,*N*-diethyl-*p*-toluidine **9**, *p*-tolyldiethanol amine **10**, 4-tert-butylbenzyl alcohol **14**.

Table S1. Diffusion coefficient value for complex of paracyclophane in 1.2

Peak, ppm	Diffusion coefficient, 10^{-10} $m^2 \cdot s^{-1}$	Error, 10^{-5}
12.701	1.841	6.825
11.281	1.839	7.849
8.739	1.894	9.258
8.454	1.869	9.106
8.384	1.753	3.038
8.269	1.567	4.541
7.744	1.968	1.458
7.716	1.963	1.326
7.375	1.941	2.109
6.978	1.982	1.186
4.122	1.856	1.175
3.554	1.886	1.119
3.441	1.9	1.007
3.029	2.026	2.607
2.829	9.478	9.759
2.432	2.011	4.19
2.134	12.45	9.079
2.034	6.43	1.098
1.793	1.648	3.376
1.381	2.014	1.505
1.239	2.034	4.882
0.941	2.083	6.65
−1.545	1.761	7.342
−1.645	1.75	5.282