Electronic Supplementary Information (ESI)

Endo/exo binding of alkyl and aryl diammonium ions by cyclopentanocucurbit[6]uril

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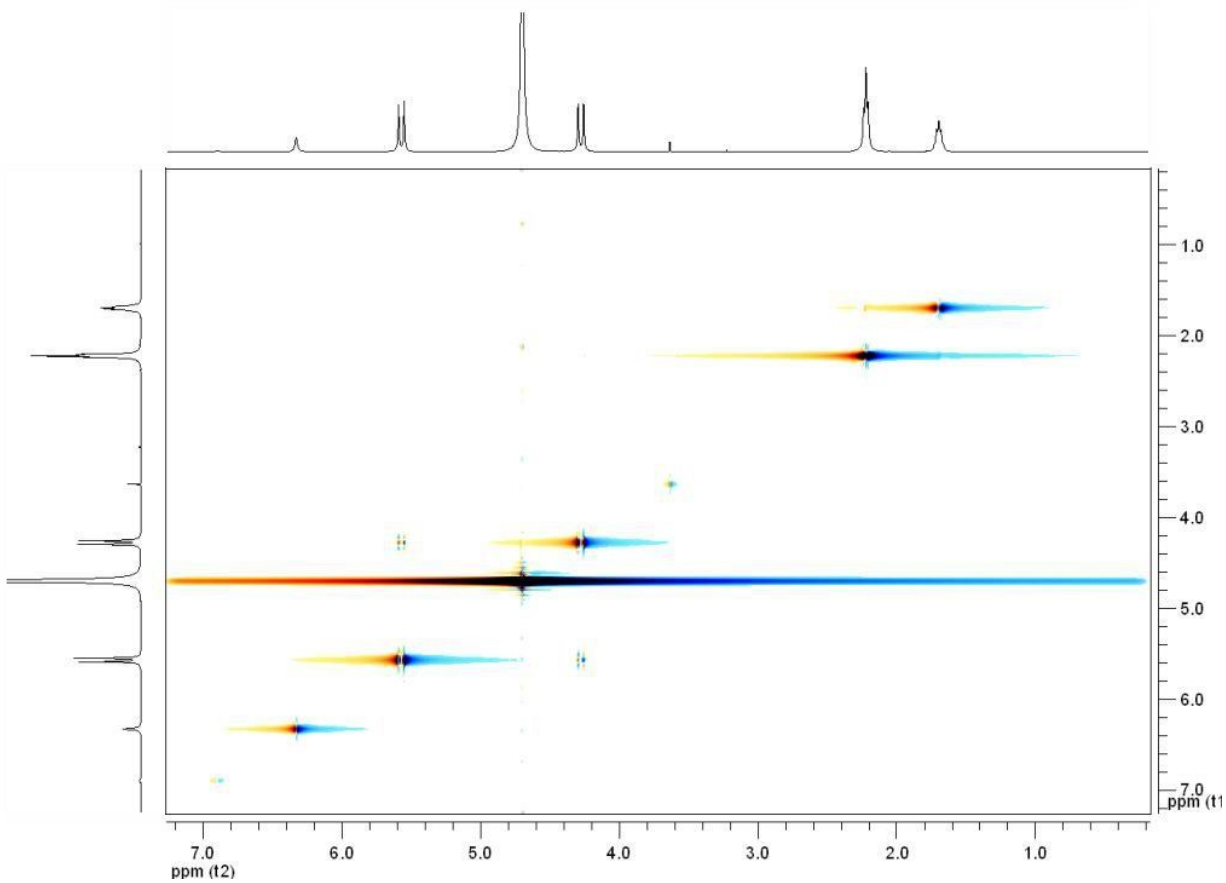
S1. Crystallographic Information:

CCDC 1511433, 1534795, 1511619, 1511458 and 1554031 contain the supplementary crystallographic data for this paper. The data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif (or from The Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336 033; e-mail: deposit@ccdc.cam.ac.uk).

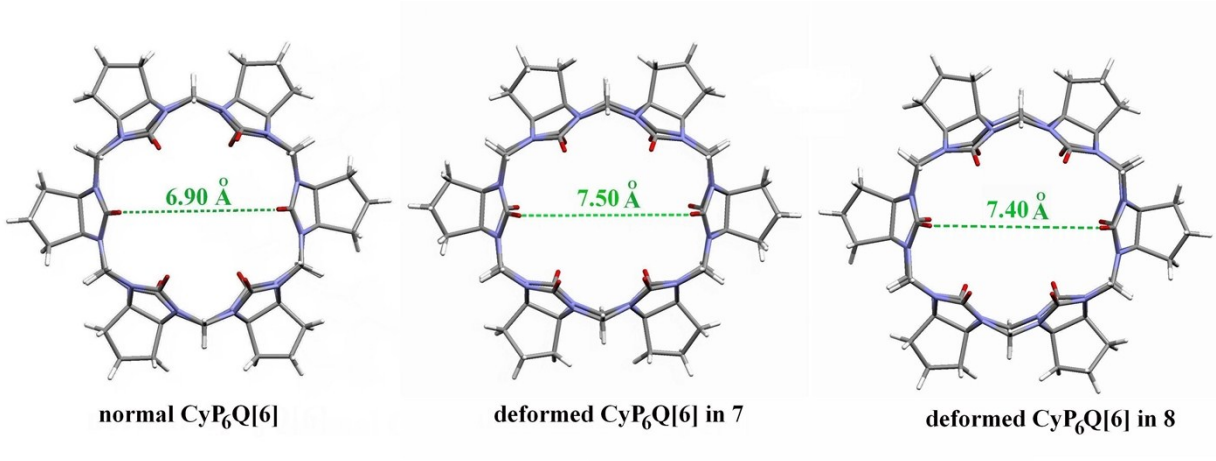
Table 1. The Crystallographic data for compounds **2**, **3**, **4** and **7**.

compound	**2**	**3**	**4**	**7**	**8**
Formula	$C_{58}H_{94}N_{26}O_{22}Zn_2Cl_8$	$C_{60}H_{112}N_{26}O_{28}Zn_2Cl_8$	$C_{62}H_{106}N_{26}O_{24}Zn_2Cl_8$	$C_{60}H_{90}N_{26}O_{22}Zn_2Cl_8$	$C_{62}H_{108}N_{26}O_{28}Zn_2Cl_{10}$
M_r	1921.93	2131.00	2014.07	1941.92	2150.98
crystal system	Triclinic	Triclinic	Monoclinic	Monoclinic	Triclinic
space group	*P*-1	*P*-1	*C*2/*c*	*C*2/*c*	*P*-1
a (Å)	12.2894(18)	12.298(3)	29.3492(15)	27.520(3)	12.315(4)
b (Å)	12.4667(17)	12.903(3)	12.5025(6)	17.250(3)	12.875(4)
c (Å)	14.986(2)	15.662(3)	25.3876(13)	18.358(3)	15.525(6)
α (deg)	73.289(4)	75.259(3)	90	90	75.131(11)
β (deg)	84.747(4)	70.211(3)	113.650(3)	94.006(7)	70.361(11)
γ (deg)	62.451(4)	76.684(3)	90	90	77.820(10)
V (Å^3)	1947.3(5)	2233.0(8)	8533.3(7)	8694(2)	2219.6(14)
Z	1	1	4	4	1
*D*c (g·cm^{-3})	1.639	1.585	1.568	1.484	1.609
μ (mm^{-1})	0.981	0.926	0.901	0.879	0.933
Data/params	6969 / 478	8767 / 505	6530 / 505	7894 / 497	7854 / 550
θ (deg)	1.42 - 25.27	1.41 - 26.00	1.75 - 25.00	1.39 - 25.59	1.42 - 25.10
GOF	1.003	1.007	1.006	1.009	1.003
Final *R* indices [*I*>2*(I)*]	R_1 = 0.0529 wR_2 = 0.1427	R_1 = 0.0576 wR_2 = 0.1827	R_1 = 0.0743 wR_2 = 0.2376	R_1 = 0.0685 wR_2 = 0.1991	R_1 = 0.0836 wR_2 = 0.2457
R indices (all data)	R_1 = 0.0758 wR_2 = 0.1547	R_1 = 0.0667 wR_2 = 0.1918	R_1 = 0.0863 wR_2 = 0.2487	R_1 = 0.1061 wR_2 =0.2199	R_1 = 0.1104 wR_2 =0.2745

S2. 2D NOESY NMR of the guests 7 complexed with $CyP_6Q[6]$.



S3. Structural comparion of normal and deformed $CyP_6Q[6]$ in compounds 7 and 8.



normal $CyP_6Q[6]$ deformed $CyP_6Q[6]$ in 7 deformed $CyP_6Q[6]$ in 8