

Supporting Information for

Synthesis and structure of mono-bridged resorcinarene host: Ditopic receptor for ammonium guests

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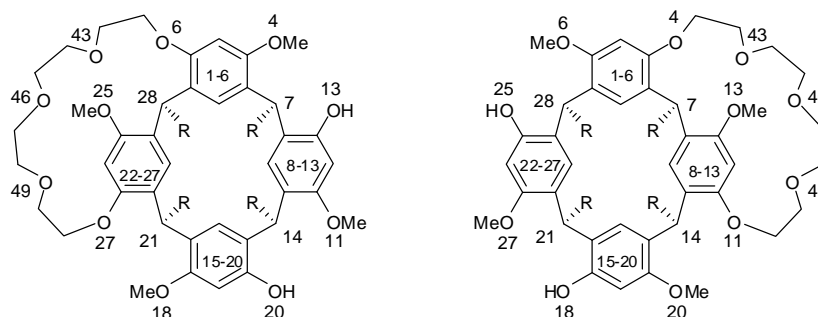
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1. Crystallographic details and data



Scheme 1. Crystallographic numbering (left- and right-handed) of **1**.

Table 1. Conformational properties of **1**.

	I	II	III	average
angle ^a (°)	26.2 / 158.1	36.3 / 145.2	33.6 / 153.1	32.0 / 152.1
distance ^a (Å)	5.58 / 7.96	5.78 / 7.91	5.87 / 7.85	5.74 / 7.91
Crown pocket diameter (Å)	6.13	6.36	6.28	6.26
Contact angle (°)	125.7	119.5	135.5	-
Pair distance (Å)	4.03	4.69	7.34	-

^a Between the opposite aromatic ring centroids

2. NMR titration data and Job plot

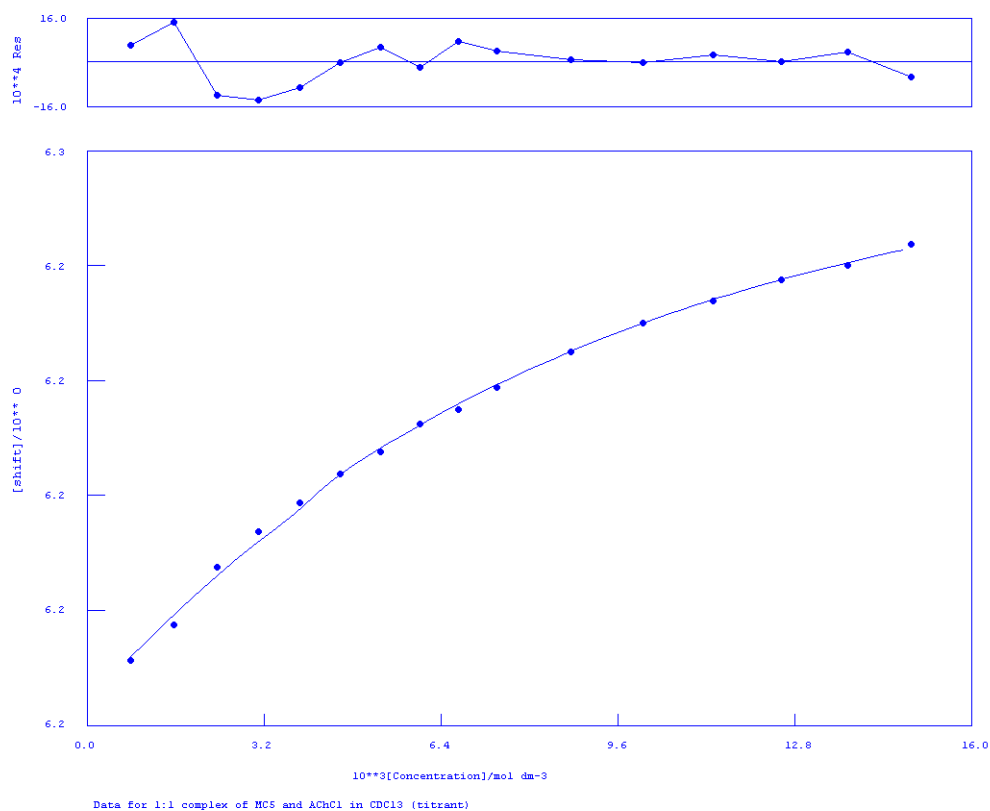


Figure 1. FitPlot of **1** and AChCl in CDCl₃.

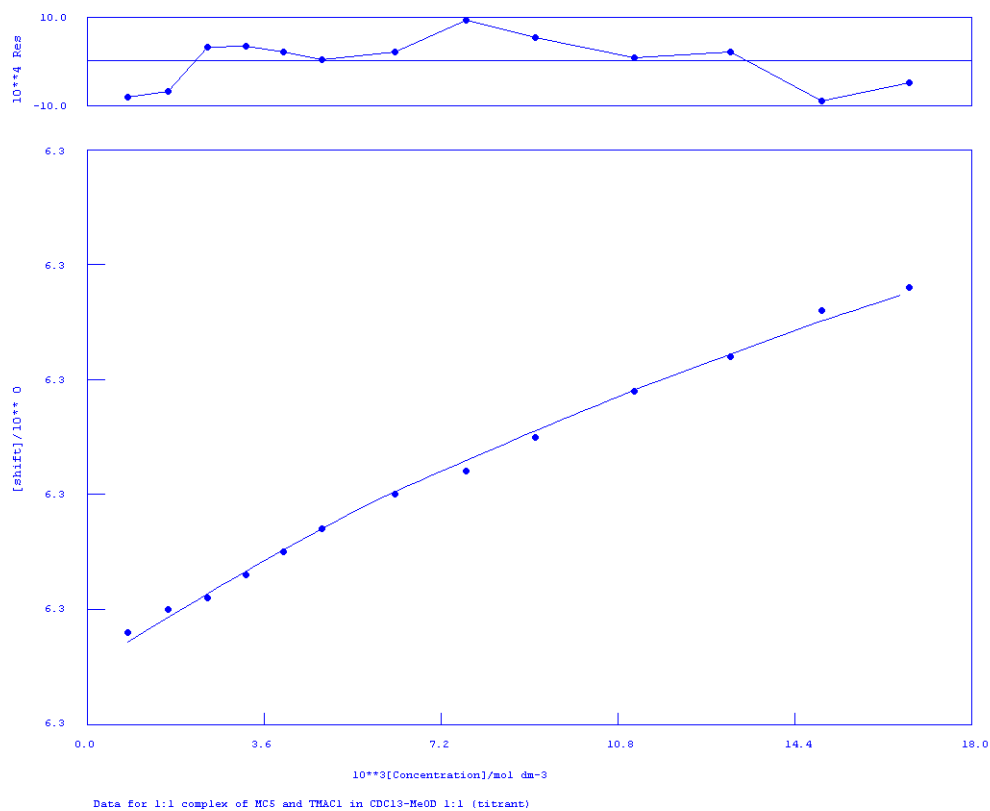


Figure 2. FitPlot of **1** and TMAcI in MeOD-CDCl₃ (1:1).

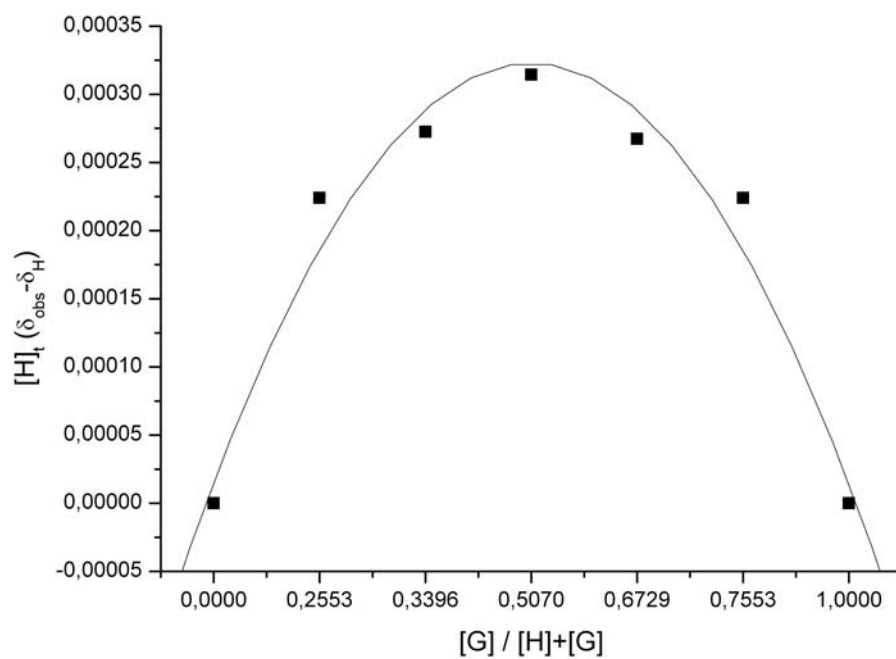


Figure 3. Job plot of **1** and AChCl in CDCl_3 .

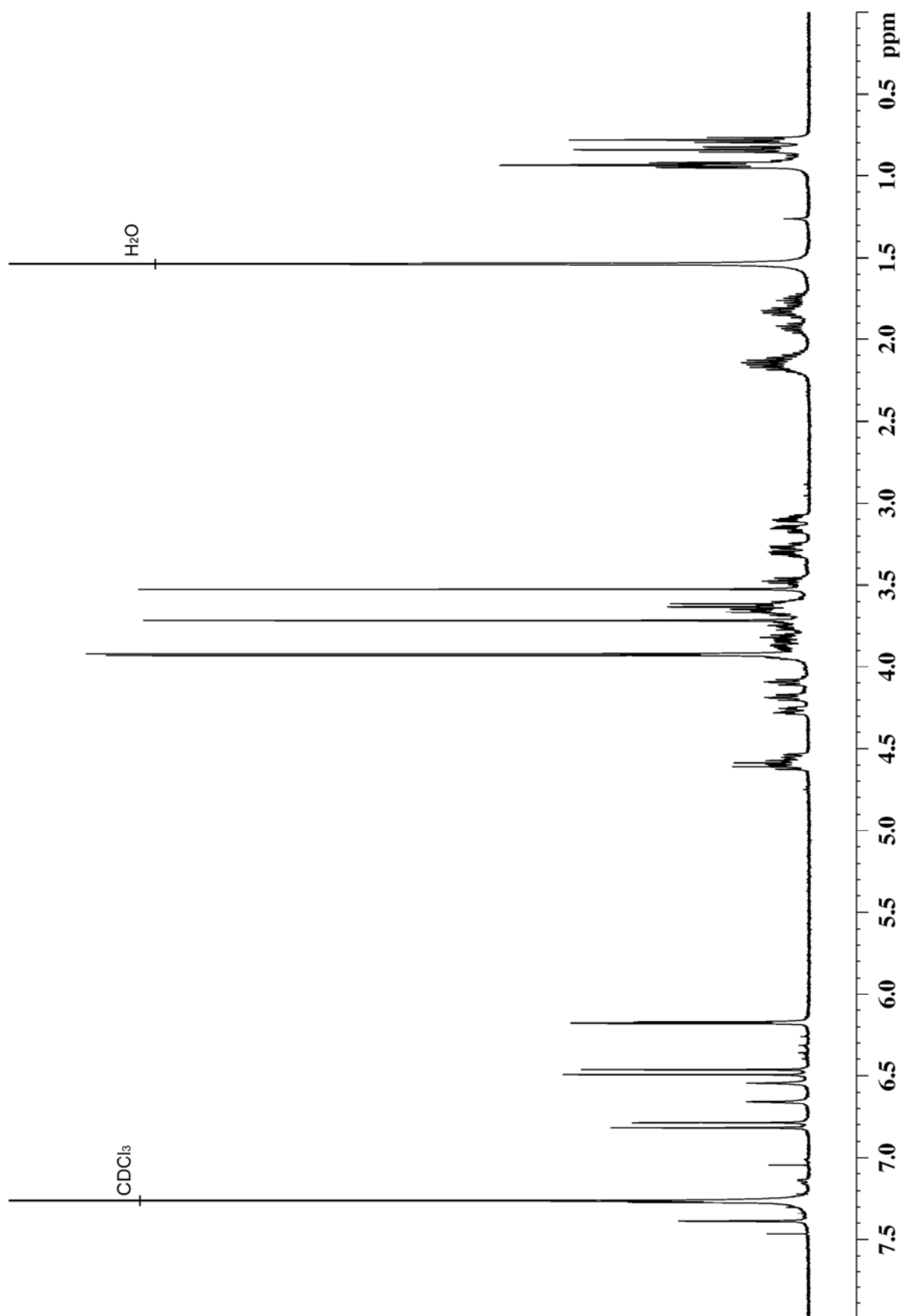


Figure 4. ^1H NMR spectrum of **1** in CDCl_3 .

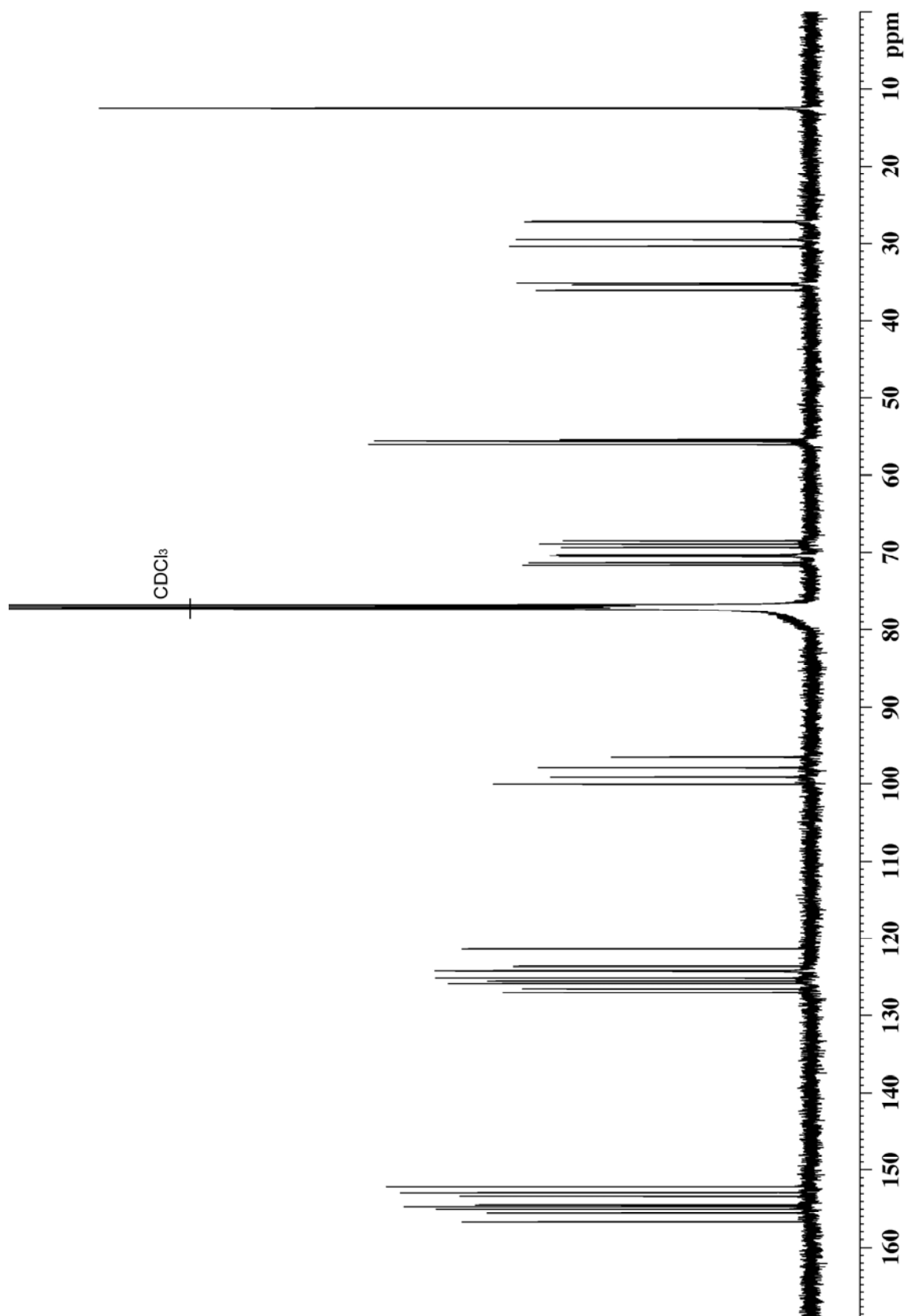


Figure 5. ^{13}C NMR spectrum of **1** in CDCl_3 .