Supplementary Material (ESI) for Organic and Biomolecular Chemistry

Supplementary Data

Reasons for the exclusive formation of heterodimeric capsules between tetra-tolyl and tetra-tosylurea calix[4]arenes

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Contents

Table S1 Average energetic and geometric parameters of the monomers **1a** and **1b**.

	1a	**1b**
steric energy (kcal/mol)	-404.4 ± 10.1	-531.7 ± 9.4
number of hydrogen bonds	1.5	2.6
$NH_{\alpha}\cdots O$ distance [Å]	2.57 (0.54)	2.30 (0.28) / 2.28 (0.28)
$NH_{\beta}\cdots O$ distance [Å]	1.97 (0.43)	2.20 (0.27) / 2.21 (0.28)

F**ig. S1** Compounds used for the calculation of RESP charges and the corresponding RESP derived charges for the constituting fragments of the tetra-tolyl- and tetra-tosylurea calix[4]arenes **1a** and **1b**. Also given are the corresponding atom types used for the AMBER 7 calculations.

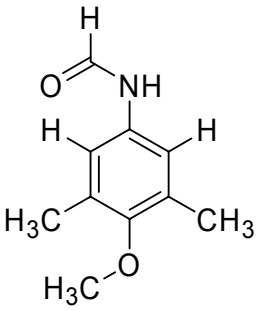
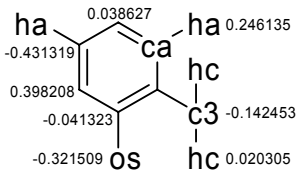
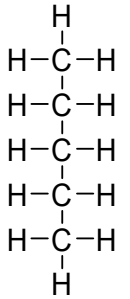
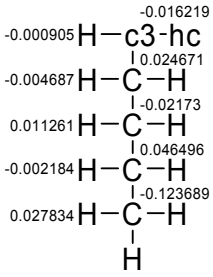
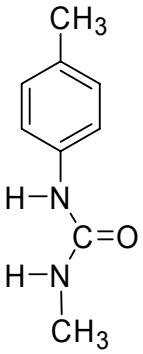
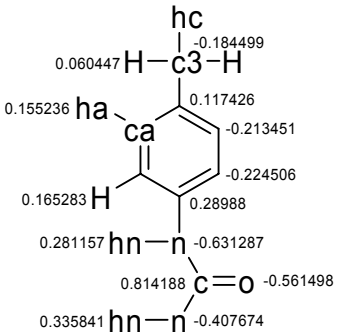
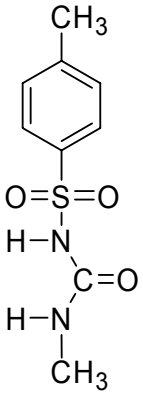
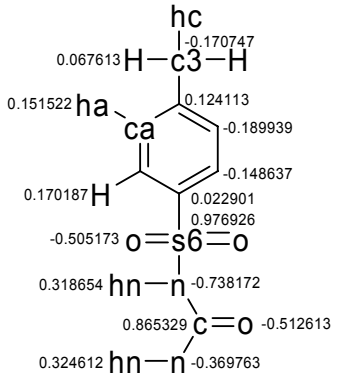
Molecule for the RESP calculation	Fragment in **1a** and **1b**
	
	
	
	

Figure S2. Histogram of the C–S–N–C dihedral angles of acyclic sulfonyl ureas (S–N–C(O)–N angle restricted to 180 ± 20°) in the Cambridge Structural Database (2006 release). The total number of hits was 42, multiple crystal structures were omitted from the data set.

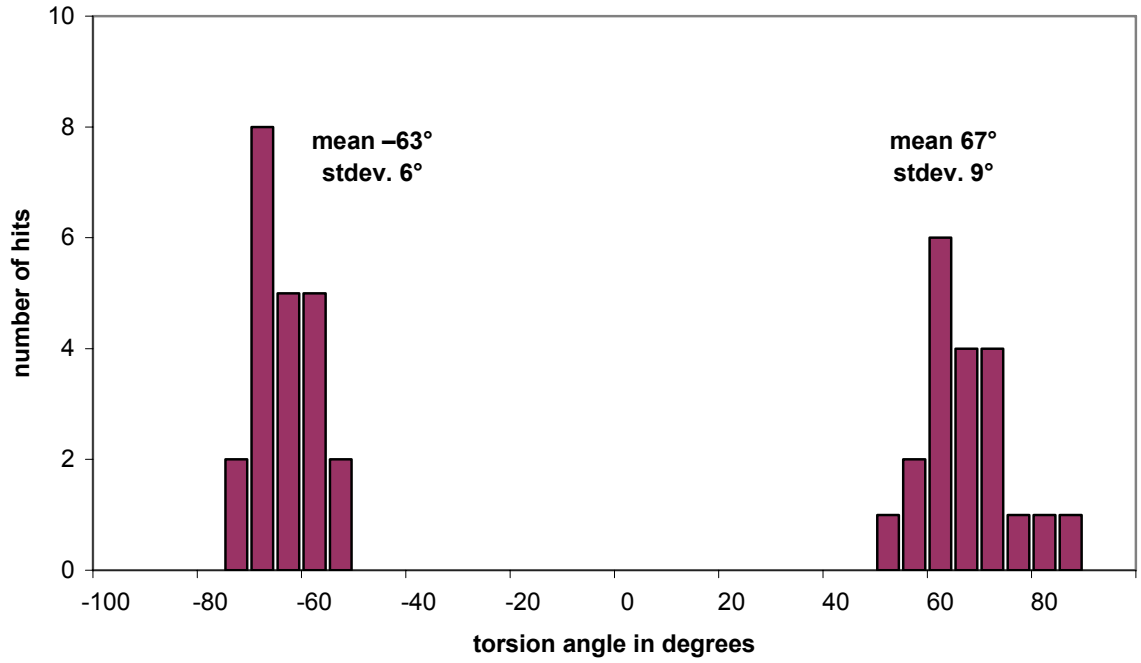


Fig. S3 NOESY spectrum of the heterodimer **1a·1b** in $C_2D_2Cl_4$ (mixing time = 300 ms).

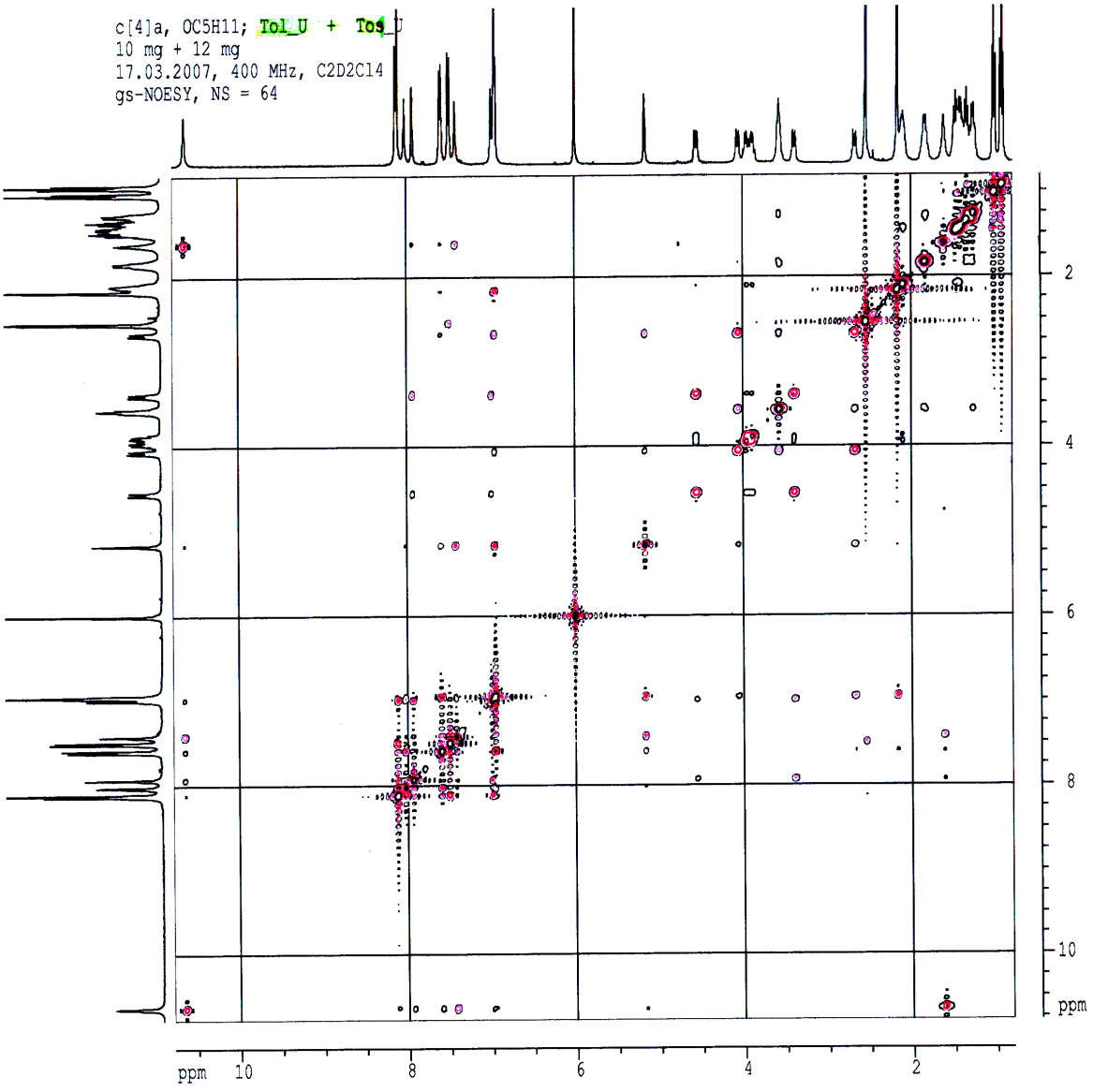
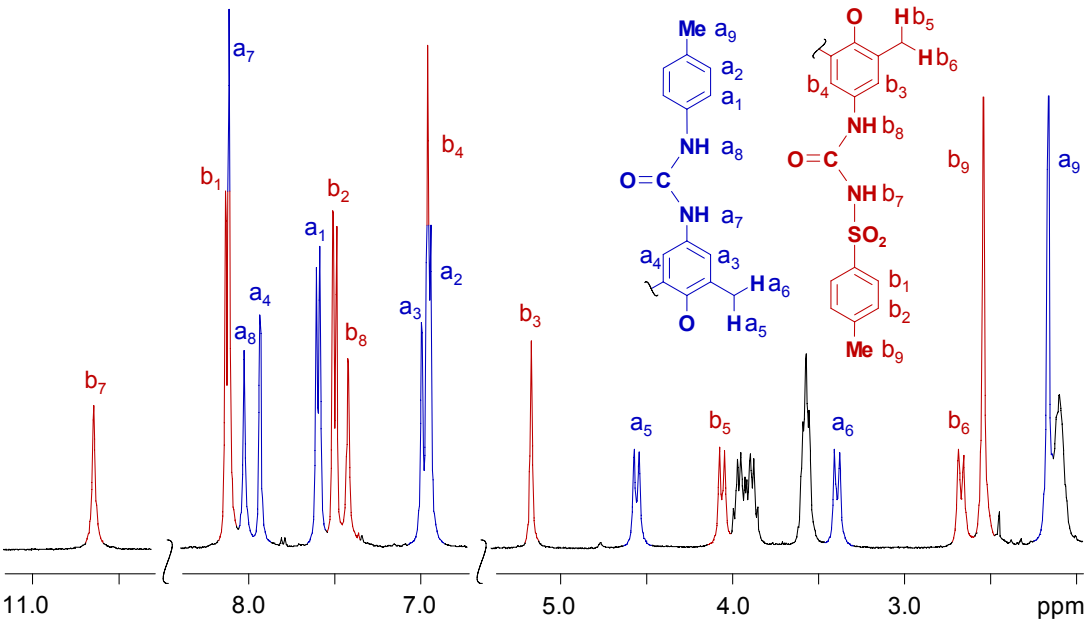


Table S2 Interpretation of NOESY spectrum of the heterodimer **1a·1b** in $C_2D_2Cl_4$.



proton 1	proton 2	intens.
a_1	a_2	++
	a_8	++
	a_9	+
	b_3	+
	b_6	+
	b_7	+
a_2	a_1	++
	a_9	++
a_3	a_4	++
	a_5	+
	a_6	++
	a_7	++
	b_7	+
a_4	a_3	++
	a_5	+
	a_6	++
	a_7	+
	b_7	+
a_5	a_3	+
	a_4	+
	a_6	++
a_6	a_3	++
	a_4	++
	a_5	++
a_7	a_3	++
	a_4	+
	a_8	++
a_8	a_1	++

proton 1	proton 2	intens.
b_1	b_2	++
	b_7	+
	b_9	+
b_2	b_1	++
	b_9	++
b_3	b_4	++
	b_5	+
	b_6	++
	b_7	+
	b_8	++
	a_1	+
	a_8	+
b_4	b_3	++
	b_5	+
	b_6	++
	a_8	+
b_5	b_3	+
	b_4	+
	b_6	++
b_6	b_3	++
	b_4	++
	b_5	++
	a_1	+
b_7	b_1	+
	b_3	+
	b_8	++
	a_1	+
	a_3	+

	a_7	++		a_4	+
	b_3	+	b_8	b_3	++
	b_4	+		b_7	++
a_9	a_1	+	b_9	b_1	+
	a_2	++		b_2	++

Fig. S4 Intermolecular contacts for the heterodimer **1a·1b** (derived from the NOESY spectrum).