Supplementary Material (ESI) for *CrystEngComm*

Electronic Supplementary Information

Five Supramolecular Compounds of Water-soluble Sulfonylcalix[4]arenetetrasulfonate Showing Two Calixarene Conformations

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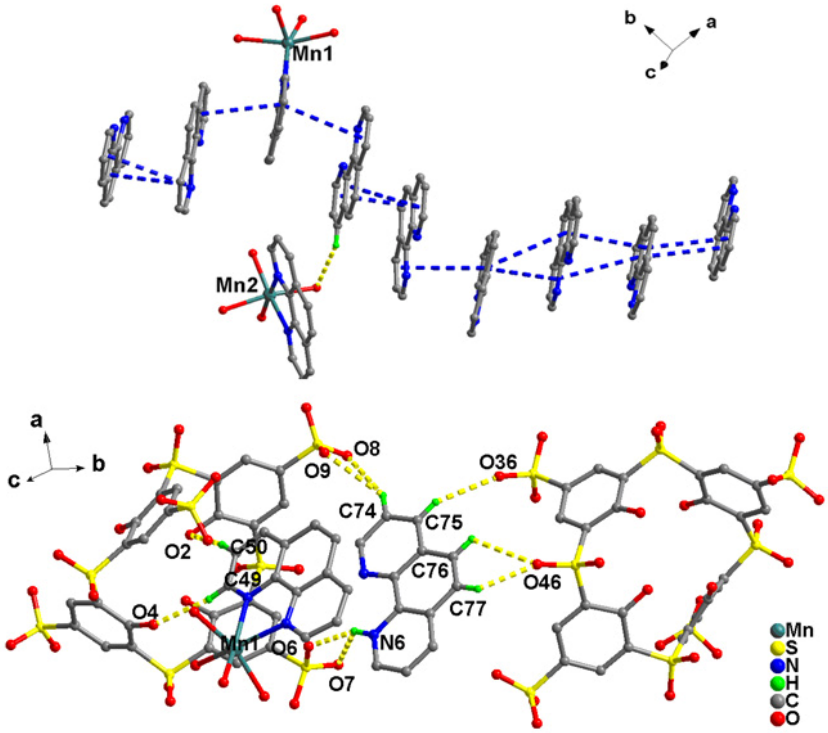
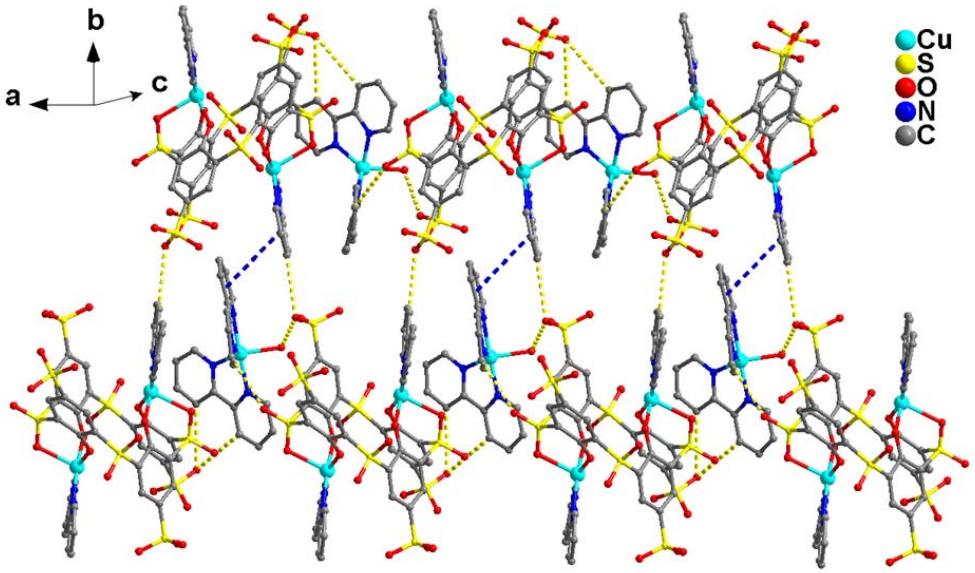
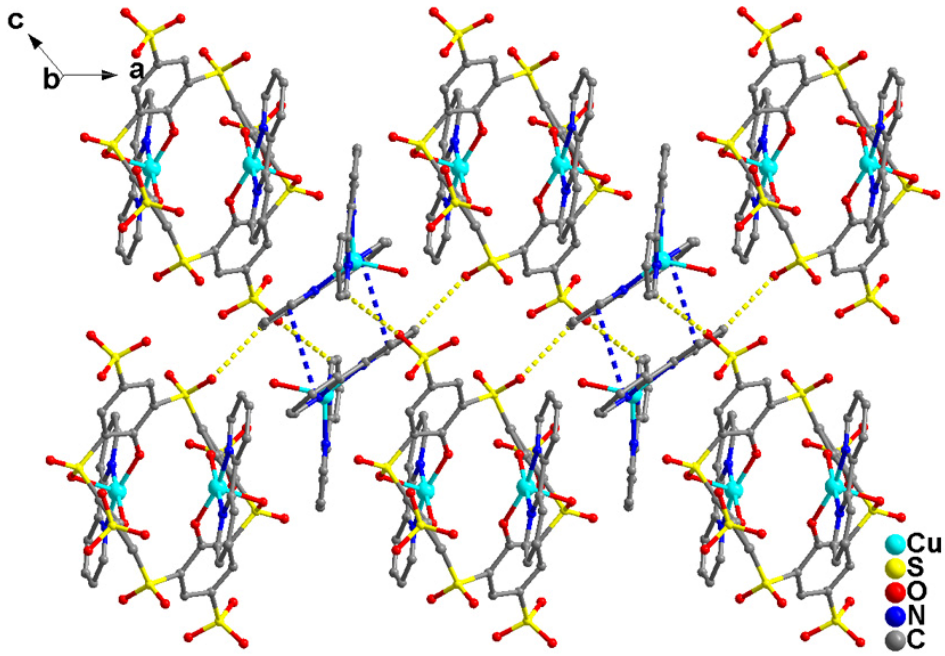


Fig. S1 The supramolecular interactions in 2.

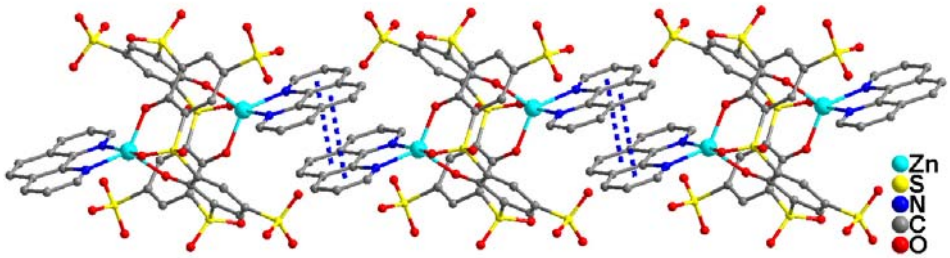


a



b

Fig. S2 Supramolecular network of **4** showing H-bondings and π-π interactions.



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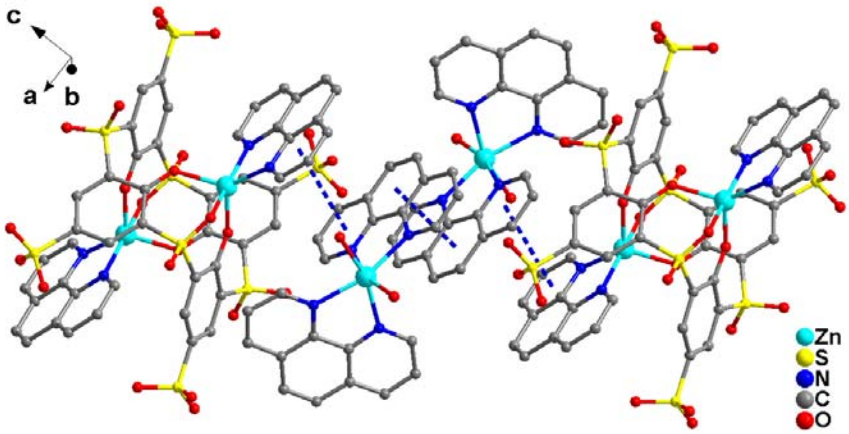

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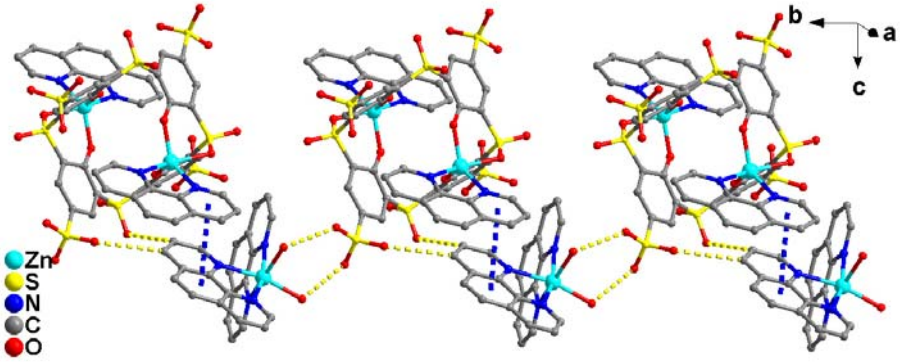

c

Fig. S3 Supramolecular interactions in **5.**

Table S1. Hydrogen–Bonding Geometry (Å, °) for Compounds **1-5**

D–H…A	D–H	H…A	D…A	<D–H…A	Symmetry code
			1		
C(49)–H(49A)…O(15)	0.95	2.38	3.151(9)	138	1-x,1-y,1-z
C(51)–H(51A)…O(2)	0.95	2.49	3.148(12)	127	1-x,1-y,1-z
C(51)–H(51A)…O(20)	0.95	2.39	3.294(12)	159	1-x,1-y,1-z
C(52)–H(52A)…O(19)	0.95	2.38	3.151(12)	138	x, y, z
C(54)–H(54A)…O(7)	0.95	2.58	3.487(10)	160	x, y, z
C(56)–H(56A)…O(8)	0.95	2.39	3.220(12)	146	-x,1-y,1-z
			2		
N(6)–H(6A) …O(6)	0.88	1.89	2.690(7)	150	x, y, z
N(9) –H(9A) …O(42)	0.88	1.89	2.678(7)	148	x,-1+y,z
N(16)–H(16G)…O(35)	0.88	1.92	2.708(7)	148	1-x,1-y,1-z
N(20)–H(20B)…O(23)	0.88	1.99	2.776(7)	148	x,1+y,z
C(101)--H(10C)…O(48)	0.95	2.60	3.122(11)	115	2-x,1-y,1-z
C(115)--H(11F)…O(22)	0.95	2.30	3.248(9)	174	-1+x,y,-1+z
C(121)--H(12A)…O(31)	0.95	2.59	3.411(14)	145	1-x,1-y,1-z
C(127)--H(12H)…O(24)	0.95	2.37	3.290(12)	163	-1+x,y,-1+z
C(134)--H(13B)…O(34)	0.95	2.49	3.274(11)	140	1-x,1-y,1-z
C(135)--H(13C)…O(7)	0.95	2.57	3.471(11)	159	1-x,1-y,1-z
C(137)--H(13E)…O(19)	0.95	2.48	3.185(9)	131	1-x,1-y,1-z
C(138)--H(13F)…O(20)	0.95	2.52	3.411(9)	156	-1+x,y,-1+z
C(49)–H(49A)…O(4)	0.95	2.34	3.274(8)	168	x, y, z
C(54)–H(54A)…O(43)	0.95	2.51	3.425(7)	162	-x,1-y,1-z
C(55)–H(55A)…O(25)	0.95	2.48	3.281(9)	142	-x,1-y,1-z
C(65)–H(65A)…O(33)	0.95	2.50	3.403(9)	159	-x,1-y,1-z
C(67)–H(67A)…O(43)	0.95	2.59	3.403(10)	143	-x,1-y,1-z
C(75)–H(75A)…O(56)	0.95	2.57	3.289(9)	133	x,1+y,z
C(77)–H(77A)…O(46)	0.95	2.39	3.125(9)	134	x, y, z
C(78)–H(78A)…O(26)	0.95	2.43	3.225(9)	141	1-x,1-y,1-z
C(80)–H(80A)…O(38)	0.95	2.41	3.158(9)	136	1-x,1-y,1-z
C(85)–H(85A)…O(48)	0.95	2.32	3.028(11)	131	2-x,1-y,1-z
C(92)–H(92A)…O(11)	0.95	2.60	3.329(10)	134	x, y, z
C(99)–H(99A)…O(39)	0.95	2.27	3.193(10)	165	2-x,1-y,1-z
			3		

C(39)–H(39)…O(4)	0.93	2.51	3.426(8)	169	1/2-x,1/2-y,1-z
C(40)–H(40)..O(3)	0.93	2.47	3.393(8)	171	1/2-x,1/2-y,1-z
C(44)–H(44)…O(5)	0.93	2.58	3.160(9)	121	x,1+y,z
			4		
O(13)–H(13A)…O(3)	0.80	1.87	2.658(4)	172	2-x,-y,2-z
O(13)–H(13B)… O(8)	0.88	1.82	2.681(4)	167	1-x,-y,1-z
C(29)–H(29)…O(8)	0.95	2.41	3.361(5)	176	x, y, z
C(34)–H(34)…O(10)	0.95	2.54	3.147(5)	122	2-x,-y,2-z
C(20)–H(20)…O(3)	0.95	2.28	3.155(5)	152	2-x,-1/2+y,5/2-z
C(16)–H(16)…O(6)	0.95	2.52	3.155(5)	124	1-x,-1/2+y,3/2-z
			5		
O(13)–H(13B)…O(9)	0.84	1.89	2.718(4)	169	x, y, z
O(13)–H(13A)…O(10)	0.89	1.84	2.712(6)	169	-1+x,y,z
O(14)–H(14B)…O(8)	0.84	1.91	2.731(4)	167	x, y, z
C(26)–H(26A)…O(6)	0.95	2.59	3.377(7)	141	x,-1+y,z
C(27)–H(27A)…O(7)	0.95	2.55	3.490(6)	171	x,-1+y,z
C(40)–H(40A)…O(8)	0.95	2.27	3.216(7)	175	1-x,1-y,-z
C(41)–H(41A)…O(12)	0.95	2.57	3.383(7)	144	1-x,1-y,1-z
C(42)–H(42A)…O(12)	0.95	2.53	3.353(7)	145	1-x,1-y,1-z
C(43)–H(43A)…O(4)	0.95	2.43	3.294(6)	152	x, y, z

Table S2. Selected Bond Distances (Å) for Compounds **1-5**

		1	
Na(1)–O(5)	2.244(5)	Na(1)–O(25)	2.355(5)
Na(1)–O(23)	2.316(5)	Na(1)–O(26)	2.421(7)
Na(1)–O(15)	2.319(5)	Na(1)–N(1)	2.857(7)
		2	
Mn(1)–O(50)	2.145(5)	Mn(2)–O(53)	2.143(5)
Mn(1)–O(49)	2.188(5)	Mn(2)–O(54)	2.178(5)
Mn(1)–O(52)	2.211(5)	Mn(2)–O(56)	2.194(5)
Mn(1)–O(51)	2.247(5)	Mn(2)–O(55)	2.215(5)
Mn(1)–N(1)	2.263(5)	Mn(2)–N(4)	2.243(5)
Mn(1)–N(2)	2.297(5)	Mn(2)–N(3)	2.276(5)
		3	
Cu(1)–O(2)	1.920(3)	Cu(2)–N(5)	1.978(4)
Cu(1)–O(1)	1.923(3)	Cu(2)–N(4)	1.980(4)
Cu(1)–N(2)	2.008(4)	Cu(2)–N(3)	2.016(5)
Cu(1)–N(1)	2.017(4)	Cu(2)–N(6)	2.036(4)
Cu(1)–O(9)	2.359(4)	Cu(2)–O(6)	2.182(4)
		4	
Cu(1)–O(1)	1.924(2)	Cu(2)–N(3)	1.981(3)
Cu(1)–O(2)	1.940(2)	Cu(2)–N(6)	1.994(3)
Cu(1)–N(1)	1.991(3)	Cu(2)–N(4)	2.042(3)
Cu(1)–N(2)	1.996(3)	Cu(2)–N(5)	2.075(3)
Cu(1)–O(9)	2.279(2)	Cu(2)–O(13)	2.089(2)
		5	
Zn(1)–O(2)	1.980(3)	Zn(2)–O(14)	2.082(3)
Zn(1)–O(1)	1.986(3)	Zn(2)–O(13)	2.128(3)
Zn(1)–N(2)	2.074(4)	Zn(2)–N(6)	2.158(4)
Zn(1)–N(1)	2.099(4)	Zn(2)–N(4)	2.161(4)
Zn(1)–O(3)	2.152(3)	Zn(2)–N(5)	2.183(4)
Zn(2)–N(3)	2.217(4)		