Electronic Supplementary Information

Inclusion of unique four-clawed crown-like nitrate-water cluster $[(NO_3)_6(H_2O)_6]^{6-}$ anions into the inter-spaces of a 3D H-bonded cationic net formed by a cationic calix[4]arene

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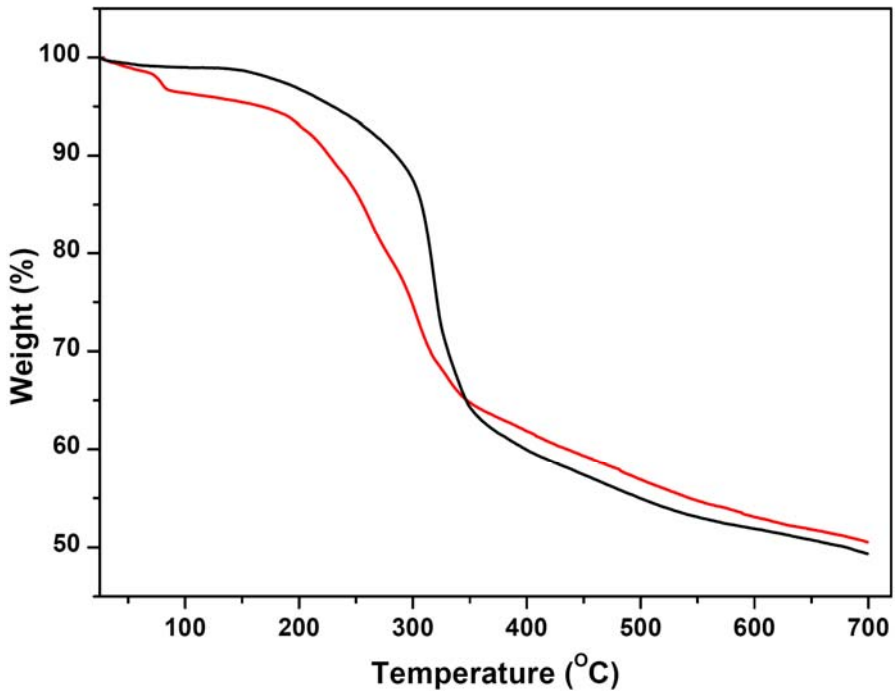
Table S1. Hydrogen-bonding interactions in **4** and **5.**·····**S5-S6**



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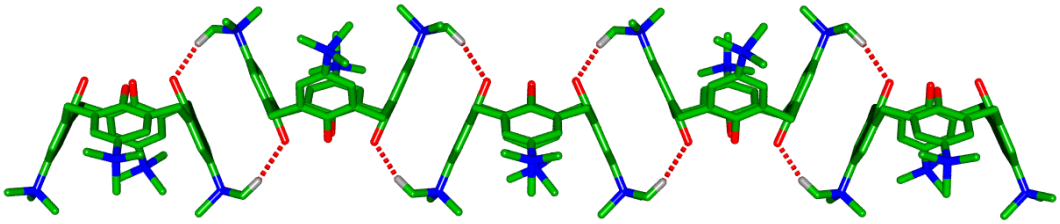

Figure S2. View of the one-dimensional chain structure formed via H-bonding interactions in **4** extending along the *c* axis.

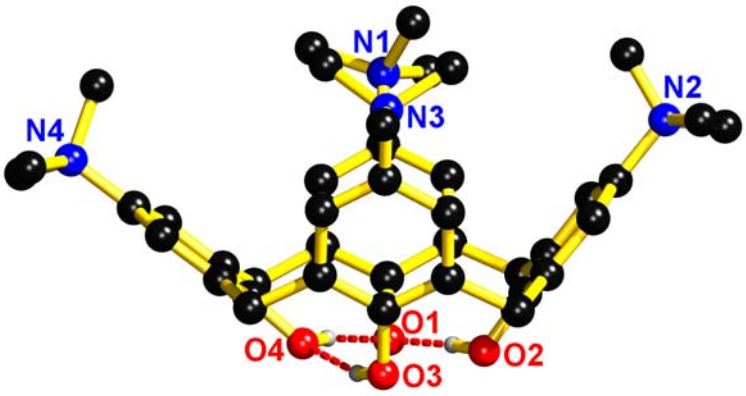

Figure S3. View of the structure of the $[H_3L]^{3+}$ trication of **5**.

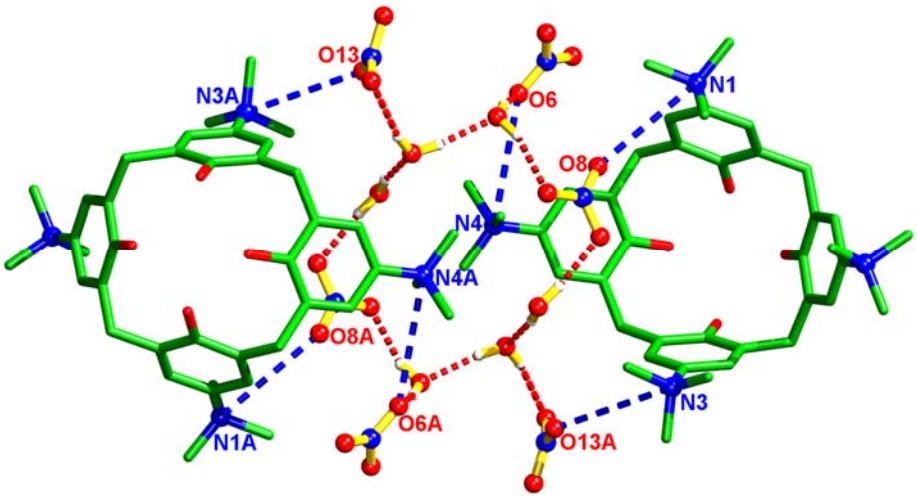

Figure S4. View of electrostatic interactions (O8···N1 = 3.789(1) Å, O13···N3 = 3.867(5) Å and O6···N4 = 3.948(1) Å, dashed blue lines) among the oxygen atoms (O3, O8 and O13) of NO_3^- and N atoms (N1, N3 and N4) of NMe_3^+ groups in **5**. Symmetry codes: A, $-x, -y, -z + 1$.

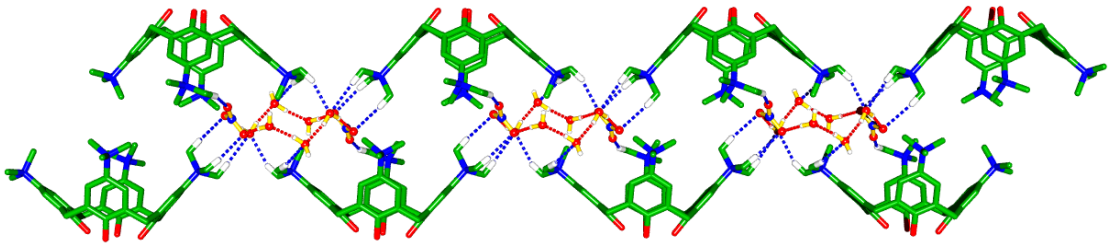

Figure S5. View of the one-dimensional chain structure formed via H-bonding interactions in **5** extending along the *a* axis.

Table S1. Geometry parameters for hydrogen-bonding interactions in **4** and **5.**

Interactions	D−H [Å]	H···A [Å]	D···A [Å]	Angle (D−H···A) [°]
Compound **2**				
O1−H1A···O4	0.83(2)	1.91(6)	2.596(9)	139(8)
O2−H2A···O1	0.86(2)	1.89(3)	2.712(8)	161(6)
O4−H4A···O3	0.86(2)	1.75(3)	2.586(8)	163(6)
C7−H7B···O3[a]	0.98	2.34	3.290(16)	162.5
C8−H8B···F6[b]	0.98	2.45	3.342(17)	151.7
C13−H13···F3[c]	0.95	2.51	3.40(2)	156.6
C15−H15···F14[d]	0.95	2.38	3.302(14)	163.5
C18−H18C···F3[c]	0.98	2.33	3.30(2)	173.1
C29−H29A···F4	0.98	2.49	3.39(2)	152.6
C29−H29B···O1[e]	0.98	2.13	3.10(2)	167.7
C37−H37A···F1	0.98	2.46	3.36(2)	153.4
C38−H38A···F8[f]	0.98	2.52	3.40(2)	148.9
C38−H38B···F1	0.98	2.52	3.411(17)	150.8
C39−H39B···F7[f]	0.98	2.41	3.333(16)	156.2
Compound **3**				
O2−H2A···O1	0.94(4)	1.62(4)	2.553(3	171(4)
O3−H3A···O4	0.86(4)	1.83(4)	2.661(3)	163(4)
O4−H4A···O1	0.867(18)	1.62(2)	2.462(3)	164(4)
O1W−HW1A···O2W	0.85	1.93	2.768(4)	168.2
O1W−HW1B···O10[a]	0.85	1.98	2.819(5)	170.5
O2W−HW2A···O3W	0.85	1.90	2.738(5)	169.7
O3W−HW3A···O6	0.85	1.98	2.810(4)	165.5
O3W−HW3B···O9	0.85	2.01	2.825(5)	161.4
C8−H8A···O8	0.97	2.42	3.330(6)	156.8
C9−H9A···O1[b]	0.97	2.33	3.260(4)	160.9
C9−H9B···O12[c]	0.97	2.48	3.434(9)	168.6
C17−H17A···O1W	0.97	2.55	3.505(6)	167.1
C18−H18B···O11[c]	0.97	2.52	3.450(10)	159.8
C18−H18C···O10[d]	0.97	2.58	3.506(7)	160.2
C19−H19A···O7[e]	0.97	2.51	3.390(6)	150.4
C19−H19B···O9[f]	0.97	2.42	3.360(6)	163.4
C19−H19C···O2[g]	0.97	2.59	3.487(6)	154.4
C28−H28B···O7[h]	0.97	2.44	3.339(5)	154.5

C29−H29A···O13^{i}	0.97	2.46	3.371(7)	156.6
C38−H38A···O2W^{i}	0.97	2.46	3.405(5)	165.9
C39−H39A···O3^{j}	0.97	2.43	3.381(4)	166.1
C39−H39B···O6	0.97	2.39	3.306(4)	158.0
C39−H39C···O1W	0.97	2.44	3.356(4)	157.8

Symmetry codes for **4**: a, 1 − *x*, 1 − *y*, − 1/2 + *z*; b, 2 − *x*, 1 − *y*, − 1/2 + *z*; c, 3/2 − *x*, 1/2 + *y*, − 1/2 + *z*; d, 3/2 − *x*, 1/2 + *y*, 1/2 + *z*; e, 1 − *x*, 1 − *y*, 1/2 + *z*; f, 1/2 + *x*, 1/2 − *y*, − 1 + *z*.

Symmetry codes for **5**: a, − *x*, − *y*, 1 − *z*; b, − *x*, 1 − *y*, − *z*; c, − *x*, 1 − *y*, 1 − *z*; d, 1 − *x*,1 − *y*,1 − *z*; e, 1 + *x*, *y*, *z*; f, 1 − *x*, 1 − *y*, 1 − *z*; g, 1 − *x*, 1 − *y*, − *z*; h, 1 + *x*, *y*, *z*; i, − *x*, − *y*, 1 − *z*; j, − *x*, − *y*, − *z*.
