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Supporting Information

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Supramolecular architectures of *N,N,N′,N′-tetrakis* (*2-hydroxyethyl*) *ethylenediamine* and tris(2-hydroxyethyl)amine with La(III) picrate and picric acid

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Contents

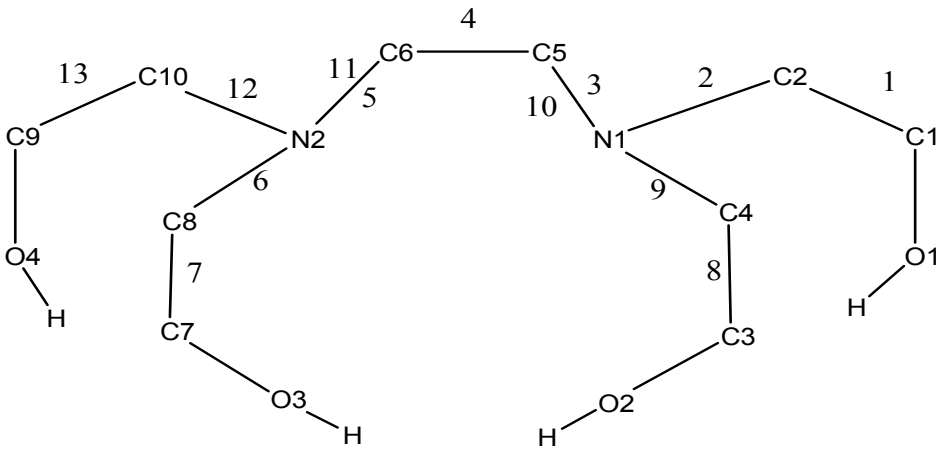

Fig. S1 THEEN

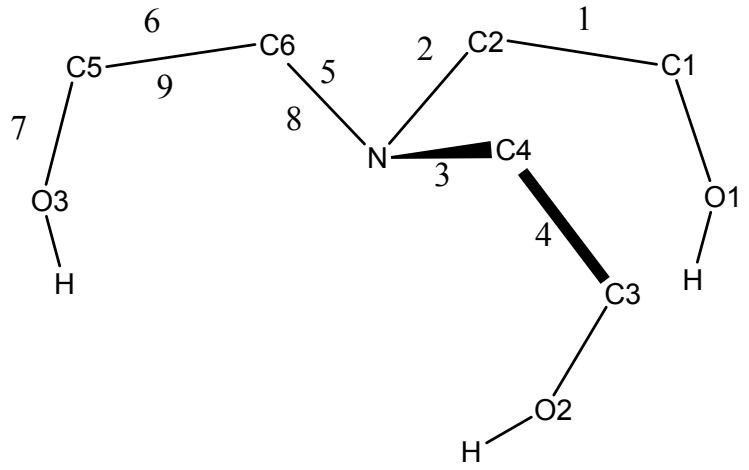

Fig. S2 $TEAH_3$

Table S1

Experimental and optimized bond lengths (Å) and angles (°) for compound (**1**)

Bond distances (Å)	Cal.	Exp.	Dev.	Bond angles ( )	Cal.	Exp.	Dev.
Picrate anion (1)				Compound (1)			
C6-C7	1.459	1.458	0.001	C4- N1 -C2	108.70	110.64	-1.94
C7-C8	1.386	1.385	0.001	C1 -C2 -N1	117.20	111.16	6.04
C8-C9	1.389	1.385	0.004	O1- C1- C2	116.30	112.80	3.50
C9-C10	1.395	1.401	-0.006	C3 -C4 -N1	116.00	114.20	2.09
C10-C11	1.382	1.398	-0.016	O2- C3 -C4	109.10	109.93	-0.83
C6-O3	1.258	1.274	-0.016	N1- C5 -C5	113.80	112.23	1.57
C7-N2	1.451	1.481	-0.030	O4 -N2- O5	122.70	123.30	-0.60
N2-O4	1.241	1.210	0.031	O3 -C6 -C7	124.20	123.04	1.16
N2-O5	1.234	1.227	0.006	O3- C6 -C11	123.30	124.04	-0.74
C9-N3	1.450	1.460	-0.010	C7 -C6-C11	112.40	112.21	0.19
N3-O6	1.235	1.242	-0.007	C8 -C7-C6	123.80	124.28	-0.48
N3-O7	1.234	1.237	-0.003	C8 -C7- N2	116.30	116.11	0.19
C11-N4	1.457	1.467	-0.010	C6 -C7-N2	120.00	119.94	0.06
N4 -O8	1.234	1.245	-0.011	C7- C8 -C9	119.50	119.21	0.29
N4-O9	1.236	1.241	-0.005	C8 -C9-C10	120.80	122.04	-1.24
THEEN				C8- C9- N3	119.50	118.48	1.02
C1-C2	1.545	1.531	0.014	C10- C9 -N3	119.60	119.82	-0.22
C3-C4	1.523	1.526	-0.003	C11-C10- C9	119.90	117.99	1.91
N1-C2	1.528	1.531	-0.003	C10 -C11-C6	123.40	124.84	-1.44
N1-C5	1.513	1.518	-0.005	C10 -C11-N4	116.00	116.55	-0.55
N1-C4	1.514	1.526	-0.012	C6- C11-N4	120.60	118.91	1.69
C1-O1	1.406	1.435	-0.029				
C3-O2	1.424	1.433	-0.009				

Table S2

Comparison of selected experimental and calculated geometric parameters bond lengths (Å) and bond angles (°) for compound (**2**).

Bond length (Å)	Cal.	Exp.	Dev.	Bond angles ( )	Cal.	Exp.	Dev.
Picrate anion				Compound (**2**)			
C7-C8	1.462	1.448	0.014	O1- C1- C2	112.10	111.07	1.03
C8-C9	1.382	1.370	0.012	O2 -C3 -C4	111.40	107.88	3.52
C9-C10	1.393	1.387	0.006	O3- C5 -C6	109.00	110.77	-1.77
C10-C11	1.395	1.377	0.018	O4 -C7 -C12	124.50	125.98	-1.48
C11-C12	1.382	1.372	0.001	O4 -C7- C8	123.10	122.77	0.33
O4-C7	1.253	1.267	-0.014	O5- N2 -O6	122.90	122.98	-0.07
C8-N2	1.450	1.460	-0.010	O5 -N2 -C8	118.60	119. 25	-0.65
N2-O5	1.242	1.232	0.010	O6 -N2 -C8	118.50	118.15	0.34
N2-O6	1.233	1.243	-0.010	O7- N3- O8	124.50	124.01	0.49
C10-N3	1.453	1.466	-0.012	O7 -N3- C10	117.70	117.54	0.16
N3-O7	1.235	1.228	0.007	O8- N3 -C10	117.80	118.94	-1.14
N3-O8	1.234	1.232	0.002	O9 -N4- C12	118.00	118.65	-0.65
C12-N4	1.458	1.459	-0.001	O10 -N4- O9	123.40	121.98	1.42
N4- O9	1.233	1.211	0.022	O10- N4- C12	118.60	119.77	-1.17
N4-O10	1.237	1.208	0.029	C2- N1- C4	113.70	114.34	-0.64
TEA				C2- N1 -C6	113.50	111.76	1.74
N1-C2	1.520	1.519	0.001	C3 -C4 -N1	111.70	112.46	-0.76
N1-C4	1.504	1.518	-0.014	C4- N1 -C6	112.70	110.75	1.95
N1-C6	1.518	1.526	-0.008	C5 -C6 -N1	107.30	111.39	-4.09
C1-O1	1.437	1.417	0.020	C9 -C8 -C7	123.80	125.30	-1.50
C3-O2	1.407	1.413	-0.006	C12 -C7 -C8	112.30	111.66	0.64
C5-O3	1.412	1.413	-0.001	N1- C2 -C1	111.10	109.18	1.92
C1-C2	1. 525	1.516	0.008				
C3 –C4	1.535	1.502	0.033				
C5-C6	1.541	1.525	0.016				

Table S3

Theoretical and experimental hydrogen bond lengths (Å) and bond angles (˚) in the compounds (**1**) and (**2**)

Hydrogen bonding geometry (Theoretical)					Hydrogen bonding geometry (Experimental)			
D-H...A	d(D-H)	d(H-A)	d(D-A)	∠ (DHA)	d(D-H)	d(H-A)	d(D-A)	∠ (DHA)
Compound (**1**)								
N1 -H1C...O1	1.053	2.971	4.030	80.22	0.91	2.557	2.882	101.57
O1 -H1...O3	0.98	2.085	3.065	128.66	0.82	1.875	2.677	165.09
O1 -H1...O9	0.98	1.943	2.923	146.61	0.82	2.580	3.087	121.19
Compound (**2**)								
N1 -H1C...O1	1.046	2.674	3.720	99.04	0.84	2.263	2.770	118.47
N1 -H1C...O2	1.046	2.434	3.480	104.15	0.84	2.423	2.831	110.25
N1 –H1C...O3	1.046	1.915	2.961	123.49	0.84,	2.484	2.918	111.15
O3 -H3...O4	0.98	1.859	2.839	141.76	0.82	1.921	2.737	171.87
O3 -H3...O10	0.98	2.177	3.157	127.09	0.82	2.606	3.077	117.73