Electronic Supplementary Information

Unusual bridging of three nitrates with two bridgehead protons in an octaprotonated azacryptand

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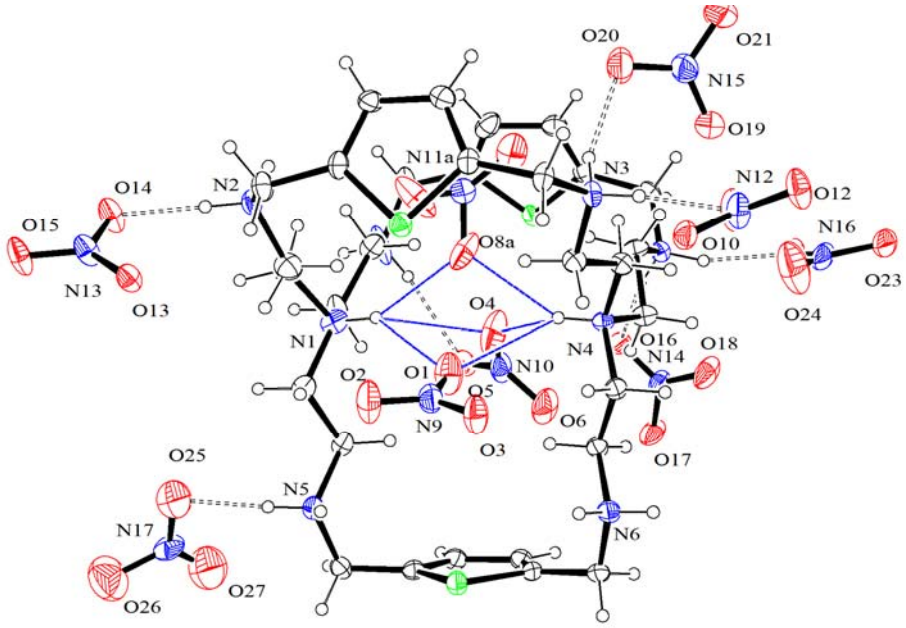

Figure S1. ORTEP views of the nitrate complex of **L** with 30% probability factor for the thermal ellipsoid.

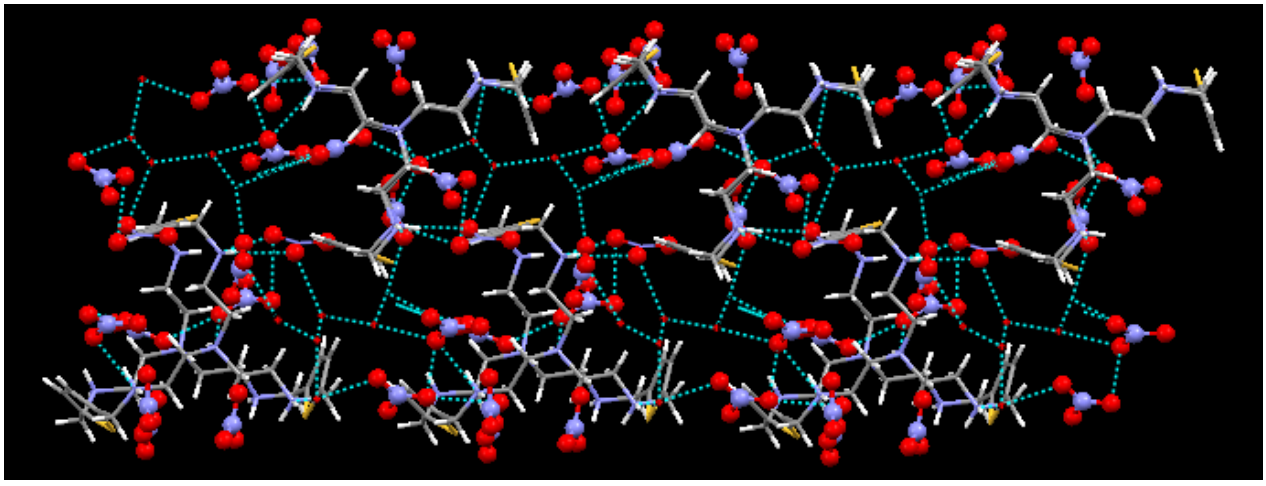

Figure S2. Packing view of the nitrate complex showing hydrogen bonding interactions.

Table S1. interatomic distances for hydrogen bonding interactions (Å) in $[H_8\mathbf{L}(NO_3)_3](NO_3)_5]\cdot HNO_3\cdot 6H_2O$.

atoms	distances (Å)	atoms	distances (Å)
N1─H1···O1	3.156 (7)	N4─H4···O1	3.290 (6)
N1─H1···O8A	3.122 (12)	N4─H4···O4	3.370 (8)
N1─H1···O4	3.370 (8)	N4─H4···O8A	3.099 (10)
N2─H2···O14	2.734 (6)	N6─H6···O3ii	2.893 (7)
N3─H3···O20	2.763 (7)	N7─H7···O5iii	2.798 (10)
N3─H3···O11	2.731 (6)	N7─H7···O5	3.113 (9)
N5─H5···O25	2.814 (8)	N8─H8···O16	2.797 (6)
N5─H5···O15i	2.868 (6)	N8─H8···O22	2.783 (6)

Symmetry codes: (i) $-x+2, y-1/2, -z+3/2$; (ii) $-x+2, -y, -z+1$; (iii) $-x+1, -y, -z+1$.

Table S2. Interatomic distances for NO bonds in nitrates and nitric acid (Å) in $[H_8\mathbf{L}(NO_3)_3](NO_3)_5]\cdot HNO_3\cdot 6H_2O$.

atoms	distances (Å)	atoms	distances (Å)
N9─O2	1.211 (7)	N13─O13	1.235 (6)
N9─O3	1.244 (7)	N13─O15	1.255 (6)
N9─O1	1.249 (7)	N13─O14	1.274 (6)
N10─O4	1.232 (9)	N14─O16	1.222 (6)
N10─O6	1.236 (8)	N14─O18	1.237 (7)
N10─O5	1.265 (8)	N14─O17	1.253 (7)
N11A─O7	1.256 (11)	N15─O19	1.238 (7)
N11A─O8A	1.211 (12)	N15─O21	1.242 (7)
N11A─O9A	1.302 (13)	N15─O20	1.286 (7)
N11B─O7	1.220 (12)	N16─O24	1.212 (11)
N11B─O9B	1.204 (13)	N16─O22	1.282 (10)
N11B─O8B	1.234 (14)	N16─O23	1.294 (8)
N12─O10	1.224 (6)	N17─O27	1.167 (10)
N12─O12	1.244 (6)	N17─O25	1.180 (9)
N12─O11	1.271 (7)	N17─O26	1.366 (10)

Disorder Models:

Hydrogen atoms on the water molecules could not be reliably located, and were not included in the model. The nitrate ion containing N11 is disordered into two orientations, each of which was assigned half occupancy. The six N-O distances in the disordered nitrate were restrained to 1.25(2) Å. The water molecule nearest to the disordered nitrate, O6W, is also disordered into two sites separated by 1.81 Å. Their populations were constrained to sum to unity, and they refined to 0.638(13) and 0.362(13).

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