Supplementary Materials: Using the Singly Deprotonated Triethanolamine to Prepare Dinuclear Lanthanide(III) Complexes: Synthesis, Structural Characterization and Magnetic Studies

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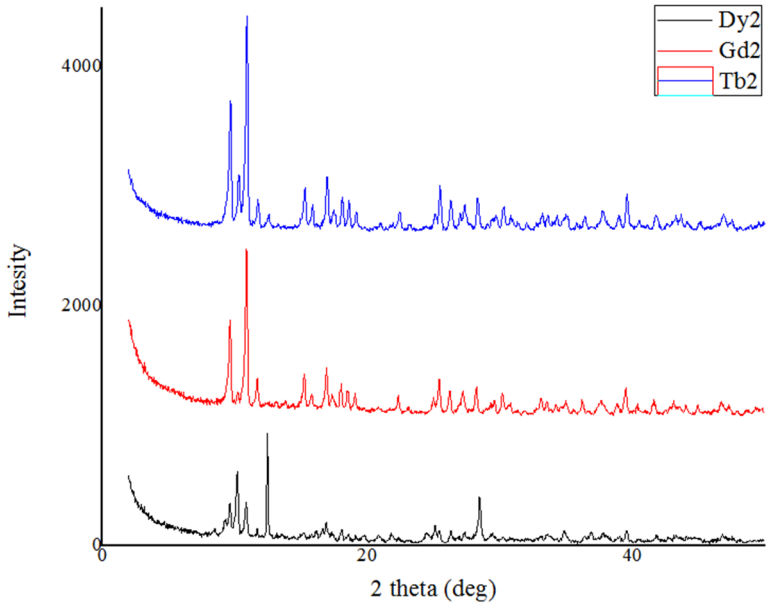

Figure S1. X-ray powder diffraction patterns of complexes **3** (blue), **2** (red) and **4** (black).

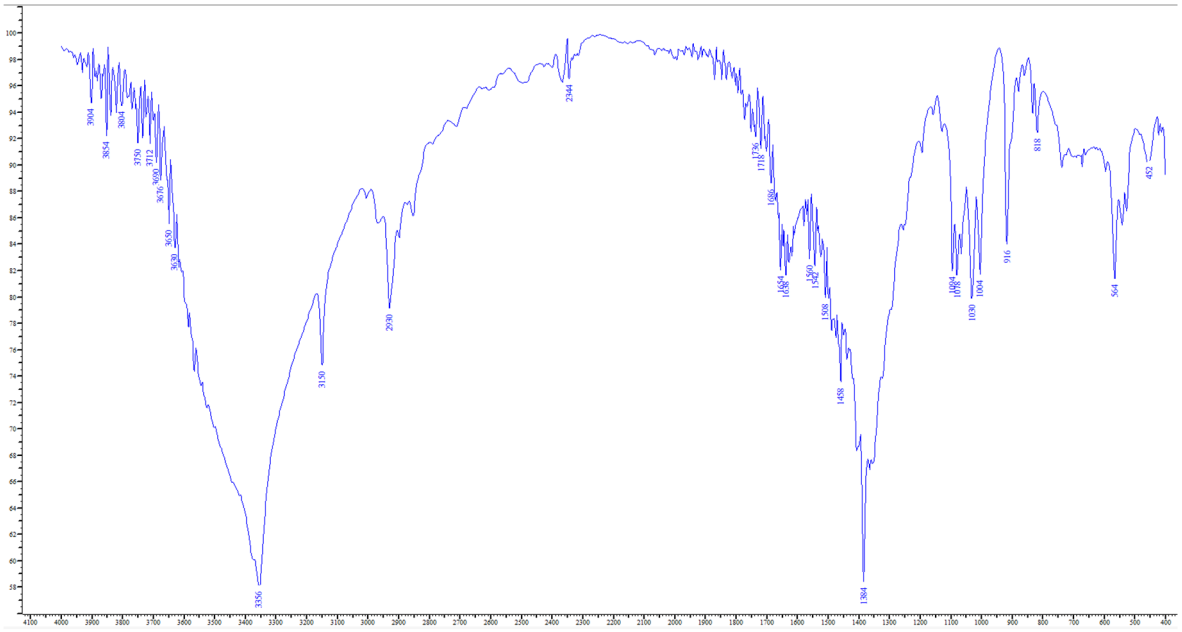

Figure S2. The IR spectrum (KBr, cm^{-1}) of complex 3.

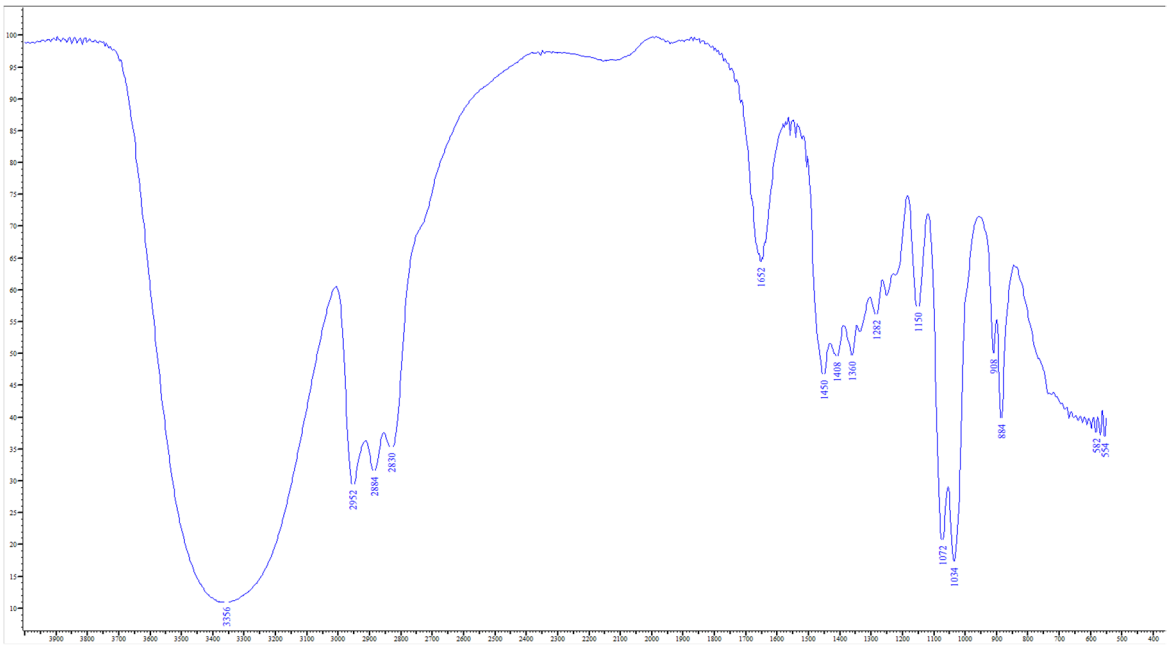

Figure S3. The IR spectrum (liquid between CsI disks, cm^{-1}) of the free $teaH_3$ ligand.

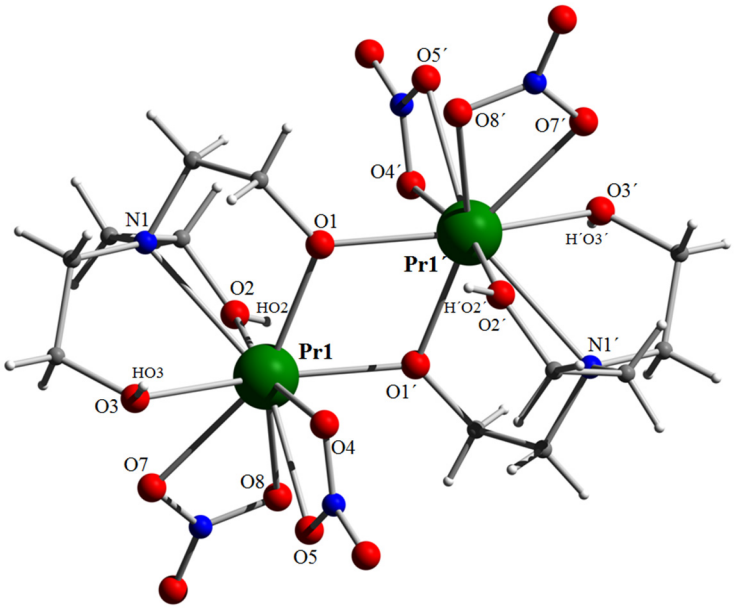

Figure S4. Partially labeled plot of the molecule $[Pr_2(NO_3)_4(teaH_2)_2]$ that is present in the structure of 1·2MeOH. Symmetry operation used to generate equivalent atoms: (′) $-x + 1, -y, -z + 1$. Only the H atoms at O2 and O3 (and their centrosymmetric equivalents) are shown.

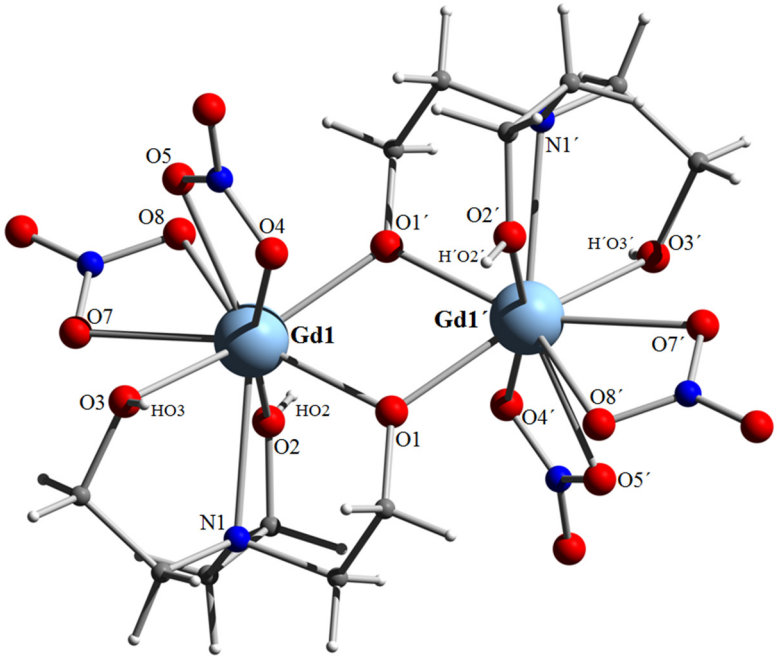

Figure S5. Partially labeled plot of the molecule $[Gd_2(NO_3)_4(teaH_2)_2]$ that is present in the structure of 2·2MeOH. Symmetry operation used to generate equivalent atoms: (′) $-x + 1, -y, -z + 1$. Only the H atoms at O2 and O3 (and their centrosymmetric equivalents) are shown.

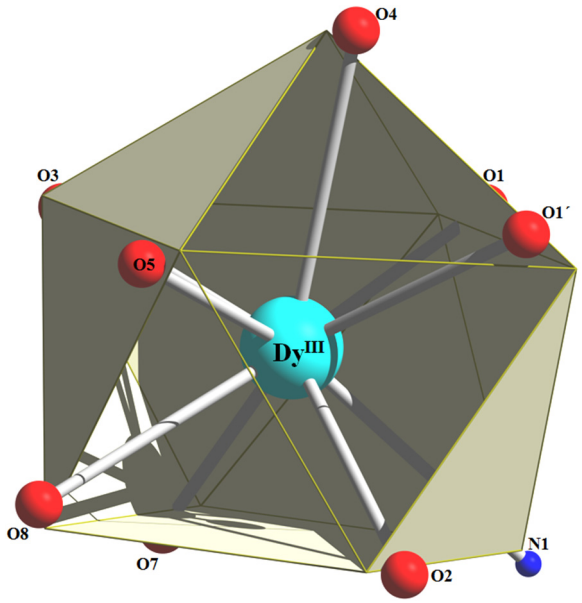

Figure S6. The spherical capped square antiprismatic coordination geometry of Dy1 in the structure of 4·2MeOH. The plotted polyhedron is the ideal, best-fit polyhedron using the program SHAPE. Primed and unprimed atoms are related by the symmetry operation (′) $-x + 1, -y, -z + 1$.

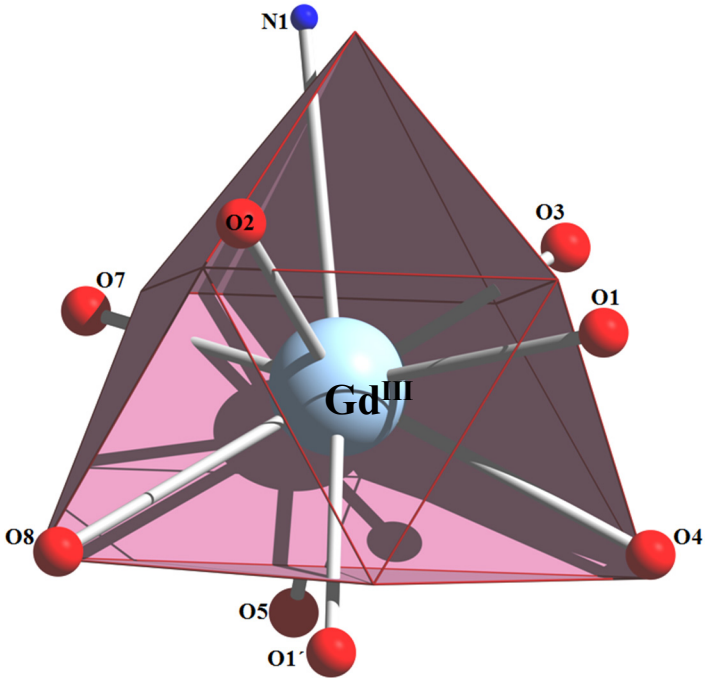

Figure S7. The Johnson tricapped trigonal prismatic coordination geometry of Gd1 in the structure of 2·2MeOH. The plotted polyhedron is the ideal, best-fit polyhedron using the program SHAPE. Primed and unprimed atoms are related by the symmetry operation (′) $-x + 1, -y, -z + 1$.

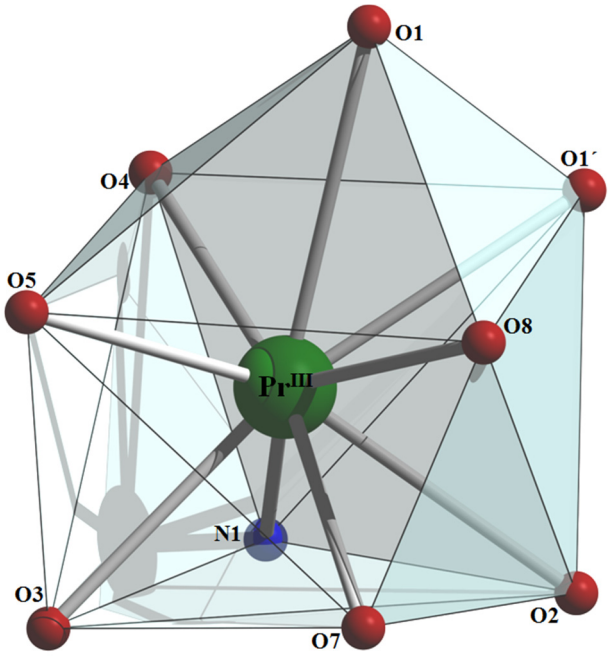

Figure S8. The spherical-relaxed capped cubic coordination geometry of Pr1 in the structure of 1·2MeOH. The plotted polyhedron is the ideal, best-fit polyhedron using the program SHAPE. Primed and unprimed atoms are related by the symmetry operation (′) $-x + 1, -y, -z + 1$.

Table S1. Continuous Shape Measures (CShM) values for the potential coordination polyhedra of Dy1/Dy1′ in the structure of complex $[Dy_2(NO_3)_4(teaH_2)_2]$·2MeOH (4·2MeOH) [a].

Polyhedron	CShM
Enneagon	34.494
Octagonal pyramid	22.687
Heptagonal bipyramid	14.572

Johnson triangular cupola	14.848
Capped cube	5.168
Spherical-relaxed capped cube	4.016
Capped square antiprism	3.864
Spherical capped square antiprism	3.263
Tricapped trigonal prism	4.165
Spherical tricapped trigonal prism	3.830

[a] The coordination polyhedron with the lowest CShM value, i.e., the spherical capped square antiprism, defines the best polyhedron for Dy1 and its centrosymmetric equivalent (Dy1′). Chemically significant distortions give CShM values of 0.1 or higher, while values larger than about 3 (as in the present case) indicate important distortions. This polyhedron is shown in Figure S6.

Table S2. Continuous Shape Measures (CShM) values for the potential coordination polyhedra of Gd1/Gd1′ in the structure of complex $[Gd_2(NO_3)_4(teaH_2)_2]\cdot 2MeOH$ (2·2MeOH) [a].

Polyhedron	**CShM**
Enneagon	41.574
Octagonal pyramid	29.759
Heptagonal bipyramid	30.829
Johnson triangular cupola	22.420
Capped cube	22.032
Spherical-relaxed capped cube	22.233
Capped square antiprism	21.832
Spherical capped square antiprism	22.269
Tricapped trigonal prism	21.255
Spherical tricapped trigonal prism	22.787

[a] The coordination polyhedron with the lowest CShM value, i.e., the tricapped trigonal prism, defines the best polyhedron for Gd1 and its centrosymmetric equivalent (Gd1′). Chemically significant distortions give CShM values of 0.1 or higher, while values larger than about 3 (as in the present case) indicate important distortions. This polyhedron is shown in Figure S7.

Table S3. Continuous Shape Measures (CShM) values for the potential coordination polyhedra of Pr1/Pr1′ in the structure of complex $[Pr_2(NO_3)_4(teaH_2)_2]\cdot 2MeOH$ (1·2MeOH) [a].

Polyhedron	**CShM**
Enneagon	34.283
Octagonal pyramid	22.036
Heptagonal bipyramid	14.161
Johnson triangular cupola	15.074
Capped cube	4.901
Spherical-relaxed capped cube	3.639
Capped square antiprism	4.743
Spherical capped square antiprism	4.100
Tricapped trigonal prism	4.922
Spherical tricapped trigonal prism	4.507

[a] The coordination polyhedron with the lowest CShM value, i.e., the spherical -relaxed capped cube, defines the best polyhedron for Pr1 and its centrosymmetric equivalent (Pr1′). Chemically significant distortions give CShM values of 0.1 or higher, while values larger than about 3 (as in the present case) indicate important distortions. This polyhedron is shown in Figure S8.

Table S4. Continuous Shape Measures (CShM) values for the potential coordination polyhedra of Pr1 in the structure of $[Pr(NO_3)(teaH_3)_2](NO_3)_2$ (6) [a].

Polyhedron	CShM
Decagon	37.851
Enneagonal pyramid	25.260
Octagonal bipyramid	13.586
Pentagonal prism	12.635
Pentagonal antiprism	13.757
Bicapped cube	12.903
Bicapped square antiprism	5.148
Metabidiminished icosahedron	9.469
Augmented tridiminished icosahedron	18.800
Sphenocorona	1.893

[a] The coordination polyhedron with the lowest CShM value, i.e., the sphenocorona, defines the best polyhedron for Pr1. Chemically significant distortions give CShM values of 0.1 or higher, while values larger than about 3 indicate important distortions. The Pr1 polyhedron is shown in Figure 4**b**.

Table S5. H bonds in the crystal structure of complex $[Dy_2(NO_3)_4(teaH_2)_2]\cdot 2MeOH$ (4·2MeOH).

D–H··A	D–H (Å)	H··A (Å)	D··A (Å)	D–H··A(°)	Symmetry Code
O2–H(O2)···O1M	0.74(3)	1.92(3)	2.646(2)	169(3)	x, y, z
O3–H(O3)···O6	0.68(3)	2.11(3)	2.778(2)	167(3)	$-x+2, -y, -z+1$
O3–H(O3)···O4	0.68(3)	2.70(3)	3.248(2)	140(3)	$-x+2, -y, -z+1$
O1M–H(O1M)···O3	0.68(4)	2.34(4)	2.971(2)	154(4)	$x-1, y, z$
C2 [a]–HB(C2)···O8	1.01(3)	2.53(3)	3.411(3)	145(2)	$x, y-1, z$

[a] C2 is the carbon atom of teaH2- that is connected to the nitrogen atom (N1); atom C2 is not labelled in Figure 2. D = donor, A = acceptor.

Table S6. H bonds in the crystal structure of complex $[Pr(NO_3)(teaH_3)_2](NO_3)_2$ (6).

D–H··A	D–H (Å)	H··A (Å)	D··A (Å)	D–H··A(°)	Symmetry Code
O1–H(O1)···O6 [a]	0.74(2)	1.96(2)	2.702(2)	178(2)	$-x+1, y, -z+3/2$
O2–H(O2)···O8 [a]	0.71(2)	1.99(2)	2.693(2)	168(3)	$x, y, z-1$
O3–H(O3)···O8 [a]	0.72(2)	2.00(2)	2.714(2)	173(2)	$x+1/2, -y+1/2, z-1/2$
C2A–H2(C2A)···O7 [a,b]	0.99(2)	2.58(2)	3.537(2)	162(2)	$x+1, -y, z-1/2$
C6–HA(C6)···O8 [a,b]	0.99(2)	2.58(2)	3.533(2)	163(2)	$-x+1/2, -y+1/2, z-1/2$
C3–HB(C3)···O4	0.95(2)	2.65(2)	3.376(2)	133(2)	$-x+1, -y, -z$

[a] Atoms O6, O7 and O8 (not shown in Figure 4) belong to the nitrate counterion; [b] These H bonds are very weak and they might not be taken into account.