Table 6. Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters ($Å^2$ x 10^3) for $[Nd(NO_3)_3(TMSA)_{1.5}]_2$

Atom	x	y	z	U(eq)
H(2A)	-870(2)	8022(1)	3410(1)	29
H(2B)	-2475(2)	8219(1)	2813(1)	29
H(3A)	-997(2)	9023(1)	1899(1)	28
H(3B)	-1113(2)	9444(1)	2803(1)	28
H(5A)	-2841(17)	5949(2)	3248(7)	54
H(5B)	-3653(9)	6843(9)	3002(5)	54
H(5C)	-2094(9)	6801(10)	3677(3)	54
H(6A)	-1270(19)	5415(3)	2284(2)	58
H(6B)	-895(15)	6013(4)	1526(8)	58
H(6C)	-2654(5)	5777(7)	1602(8)	58
H(7A)	1581(8)	9319(8)	4717(2)	37
H(7B)	-48(7)	9202(7)	4113(5)	37
H(7C)	796(14)	10105(2)	4178(5)	37
H(8A)	3766(3)	9674(8)	4147(5)	42
H(8B)	3767(3)	9699(8)	3139(5)	42
H(8C)	3961(3)	8815(2)	3637(10)	42
H(10A)	-1504(2)	10100(1)	245(1)	26
H(10B)	-1197(2)	10038(1)	-723(1)	26
H(11A)	-3376(12)	7484(1)	15(9)	38
H(11B)	-1561(7)	7358(2)	-5(9)	38
H(11C)	-2745(19)	7400(2)	-878(2)	38
H(12A)	-4623(2)	8714(5)	-589(8)	38
H(12B)	-3693(9)	9073(8)	-1309(2)	38
H(12C)	-3664(9)	9579(4)	-433(7)	38

Table 1. Crystal data and structure refinement, Compound 5

Compound	$[Gd(NO_3)_3(TMSA)_{1.5}]_2$
Color / Shape	colorless / parallelepiped
Empirical formula	$C_{12}H_{24}GdN_6O_{12}$
Formula weight	601.62
Temperature	173(2) K
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 8.7282(2) Å α = 90°
(6009 reflections	b = 15.7267(1) Å β = 98.887(1)°
in full θ range)	c = 15.7495(3) Å γ = 90°
Volume	2135.91(7) $Å^3$
Z	4
Density (calculated)	1.871 Mg/m^3
Absorption coefficient	3.176 mm^{-1}
Diffractometer / scan	Siemens SMART / CCD area detector
Radiation / wavelength	MoKα (graphite monochrom.) / 0.71073 Å
F(000)	1192
Crystal size	0.44 x 0.50 x 0.70 mm
θ range for data collection	1.84 to 27.87°
Index ranges	$-9 \le h \le 11$, $-16 \le k \le 20$, $-20 \le \ell \le 20$
Reflections collected	13255
Independent / observed refls.	4919(R_{int} = 0.0364) / 4551([I>2σ(I)])
Absorption correction	SADABS
Range of relat. transm. factors	0.96 and 0.45
Refinement method	Full-matrix least-squares on F^2
Computing	SHELXTL, Ver. 5[1]
Data / restraints / parameters	4917 / 0 / 287
Goodness-of-fit on F^2	1.056
SHELX-93 weight parameters	0.0325, 0.6481
Final R indices [I>2σ(I)]	R1 = 0.0254, wR2 = 0.0657
R indices (all data)	R1 = 0.0281, wR2 = 0.0680
Extinction coefficient	0.0123(4)
Largest diff. peak and hole	1.847 and -1.008 $eÅ^{-3}$

Table 2. Atomic Coordinates [x 10^4] and Equivalent Isotropic Displacement Parameters [$Å^2$ x 10^3] for $[Gd(NO_3)_3(TMSA)_{1.5}]_2$

Atom	x/a	y/b	z/c	U(eq)
Gd	1999(1)	7717(1)	1181(1)	12(1)
O(1)	-348(3)	7420(1)	1655(1)	22(1)
O(2)	1840(2)	8847(1)	2106(1)	20(1)
O(3)	257(2)	8445(1)	178(1)	19(1)
O(4)	3380(3)	6359(1)	1631(1)	37(1)
O(5)	2609(3)	7065(2)	2647(1)	34(1)
O(6)	3797(3)	5852(1)	2935(1)	33(1)
O(7)	4794(2)	8039(2)	1727(2)	31(1)
O(8)	3665(2)	8826(1)	699(1)	23(1)
O(9)	5919(3)	9203(2)	1395(2)	41(1)
O(10)	915(2)	6498(1)	266(1)	22(1)
O(11)	2981(3)	7078(1)	-78(1)	24(1)
O(12)	2078(3)	5907(1)	-712(1)	29(1)
N(1)	-1717(3)	6619(2)	2446(2)	25(1)
N(2)	1745(3)	9261(1)	3460(1)	19(1)
N(3)	-2319(3)	8529(1)	-292(2)	19(1)
N(4)	3278(3)	6404(2)	2419(2)	23(1)
N(5)	4829(3)	8704(2)	1280(2)	23(1)
N(6)	1989(3)	6471(2)	-195(1)	19(1)
C(1)	-1101(3)	7356(2)	2264(2)	17(1)
C(2)	-1364(3)	8121(2)	2808(2)	20(1)
C(3)	-699(3)	8950(2)	2509(2)	19(1)
C(4)	1050(3)	9017(2)	2692(2)	16(1)
C(5)	-2657(4)	6518(3)	3133(2)	40(1)
C(6)	-1580(5)	5873(2)	1909(3)	42(1)
C(7)	932(4)	9500(2)	4176(2)	26(1)
C(8)	3429(4)	9370(2)	3609(2)	30(1)
C(9)	-936(3)	8886(2)	-73(2)	15(1)
C(10)	-826(3)	9845(2)	-123(2)	17(1)
C(11)	-2528(4)	7608(2)	-270(2)	26(1)
C(12)	-3695(3)	9014(2)	-668(2)	27(1)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Torsion Angles [°] for $[Gd(NO_3)_3(TMSA)_{1.5}]_2$

N(1)-C(1)-C(2)-C(3)	-176.2(2)	C(1)-C(2)-C(3)-C(4)	-72.9(3)
C(2)-C(3)-C(4)-N(2)	-82.5(3)	N(3)-C(9)-C(10)-C(10)#1	-178.5(3)
C(9)-C(10)-C(10)#1-C(9)#1	180.0	C(10)-C(10)#1-C(9)#1-N(3)#1	178.5(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z

Table 4. Bond Lengths [Å] and Angles [°] for $[Gd(NO_3)_3(TMSA)_{1.5}]_2$

Gd-O(2)	2.316(2)	Gd-O(3)	2.319(2)
Gd-O(1)	2.334(2)	Gd-O(8)	2.465(2)
Gd-O(11)	2.490(2)	Gd-O(10)	2.495(2)
Gd-O(4)	2.500(2)	Gd-O(5)	2.507(2)
Gd-O(7)	2.509(2)	O(1)-C(1)	1.247(4)
O(2)-C(4)	1.263(3)	O(3)-C(9)	1.262(3)
O(4)-N(4)	1.259(3)	O(5)-N(4)	1.272(3)
O(6)-N(4)	1.227(3)	O(7)-N(5)	1.264(3)
O(8)-N(5)	1.274(3)	O(9)-N(5)	1.225(3)
O(10)-N(6)	1.272(3)	O(11)-N(6)	1.283(3)
O(12)-N(6)	1.215(3)	N(1)-C(1)	1.329(3)
N(1)-C(6)	1.462(4)	N(1)-C(5)	1.464(4)
N(2)-C(4)	1.323(3)	N(2)-C(8)	1.463(4)
N(2)-C(7)	1.471(4)	N(3)-C(9)	1.328(3)
N(3)-C(11)	1.461(3)	N(3)-C(12)	1.468(4)
C(1)-C(2)	1.514(4)	C(2)-C(3)	1.530(4)
C(3)-C(4)	1.512(4)	C(9)-C(10)	1.515(3)
C(10)-C(10)#1	1.514(5)		

O(2)-Gd-O(3)	87.31(7)	O(2)-Gd-O(1)	79.11(7)
O(3)-Gd-O(1)	78.51(7)	O(2)-Gd-O(8)	75.32(7)
O(3)-Gd-O(8)	78.26(7)	O(1)-Gd-O(8)	146.00(7)
O(2)-Gd-O(11)	150.72(7)	O(3)-Gd-O(11)	85.82(7)
O(1)-Gd-O(11)	126.96(7)	O(8)-Gd-O(11)	75.41(7)
O(2)-Gd-O(10)	153.97(7)	O(3)-Gd-O(10)	80.54(7)
O(1)-Gd-O(10)	75.97(7)	O(8)-Gd-O(10)	123.71(7)
O(11)-Gd-O(10)	51.44(7)	O(2)-Gd-O(4)	123.37(7)
O(3)-Gd-O(4)	148.38(7)	O(1)-Gd-O(4)	98.45(8)
O(8)-Gd-O(4)	114.24(8)	O(11)-Gd-O(4)	70.79(7)
O(10)-Gd-O(4)	68.33(7)	O(2)-Gd-O(5)	76.05(7)
O(3)-Gd-O(5)	148.51(8)	O(1)-Gd-O(5)	72.26(8)
O(8)-Gd-O(5)	121.48(8)	O(11)-Gd-O(5)	121.21(7)
O(10)-Gd-O(5)	103.01(8)	O(4)-Gd-O(5)	50.60(7)
O(2)-Gd-O(7)	77.27(8)	O(3)-Gd-O(7)	129.38(7)
O(1)-Gd-O(7)	141.80(8)	O(8)-Gd-O(7)	51.29(7)
O(11)-Gd-O(7)	85.29(8)	O(10)-Gd-O(7)	127.91(7)

O(4)-Gd-O(7)	71.01(8)	O(5)-Gd-O(7)	73.17(8)
C(1)-O(1)-Gd	148.7(2)	C(4)-O(2)-Gd	135.6(2)
C(9)-O(3)-Gd	155.1(2)	N(4)-O(4)-Gd	97.3(2)
N(4)-O(5)-Gd	96.6(2)	N(5)-O(7)-Gd	94.7(2)
N(5)-O(8)-Gd	96.6(2)	N(6)-O(10)-Gd	96.2(2)
N(6)-O(11)-Gd	96.1(2)	C(1)-N(1)-C(6)	120.3(3)
C(1)-N(1)-C(5)	123.0(3)	C(6)-N(1)-C(5)	116.5(3)
C(4)-N(2)-C(8)	119.2(2)	C(4)-N(2)-C(7)	124.6(2)
C(8)-N(2)-C(7)	116.0(2)	C(9)-N(3)-C(11)	121.7(2)
C(9)-N(3)-C(12)	122.6(2)	C(11)-N(3)-C(12)	115.3(2)
O(6)-N(4)-O(4)	122.5(3)	O(6)-N(4)-O(5)	122.0(3)
O(4)-N(4)-O(5)	115.4(2)	O(9)-N(5)-O(7)	122.3(2)
O(9)-N(5)-O(8)	121.6(3)	O(7)-N(5)-O(8)	116.1(2)
O(12)-N(6)-O(10)	122.4(2)	O(12)-N(6)-O(11)	121.9(2)
O(10)-N(6)-O(11)	115.7(2)	O(1)-C(1)-N(1)	121.0(3)
O(1)-C(1)-C(2)	121.0(2)	N(1)-C(1)-C(2)	118.0(2)
C(1)-C(2)-C(3)	113.9(2)	C(4)-C(3)-C(2)	114.8(2)
O(2)-C(4)-N(2)	120.3(2)	O(2)-C(4)-C(3)	119.6(2)
N(2)-C(4)-C(3)	120.1(2)	O(3)-C(9)-N(3)	121.5(2)
O(3)-C(9)-C(10)	120.5(2)	N(3)-C(9)-C(10)	118.0(2)
C(10)#1-C(10)-C(9)	111.9(3)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z

Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)

7.532 (0.008) x + 7.494 (0.024) y + 0.513 (0.028) z = 7.395 (0.015)

*	-0.002 (0.002)	N4
*	0.001 (0.001)	O4
*	0.001 (0.001)	O5
*	0.001 (0.001)	O6
	-0.045 (0.005)	Gd

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Rms deviation of fitted atoms = 0.001

- 4.895 (0.012) x + 8.012 (0.023) y + 11.519 (0.016) z = 6.083 (0.023)

Angle to previous plane (with approximate esd) = 82.44 (0.12)

*	0.002 (0.002)	N5
*	-0.001 (0.001)	O7
*	-0.001 (0.001)	O8
*	-0.001 (0.001)	O9
	0.481 (0.005)	Gd

Rms deviation of fitted atoms = 0.001

- 4.017 (0.011) x - 8.447 (0.019) y + 9.880 (0.017) z = 4.859 (0.013)

Angle to previous plane (with approximate esd) = 85.96 (0.10)

*	0.001 (0.002)	N6
*	0.000 (0.001)	O10
*	0.000 (0.001)	O11
*	0.000 (0.001)	O12
	-0.310 (0.004)	Gd

Rms deviation of fitted atoms = 0.001

- 6.555 (0.009) x - 3.436 (0.024) y + 7.869 (0.020) z = 1.473 (0.019)

Angle to previous plane (with approximate esd) = 25.38 (0.18)

*	-0.006 (0.002)	C1
*	0.002 (0.001)	N1
*	0.002 (0.001)	O1
*	0.002 (0.001)	C2
	0.043 (0.006)	C5
	0.078 (0.006)	C6

Rms deviation of fitted atoms = 0.003

- 0.119 (0.012) x + 15.012 (0.006) y - 4.601 (0.020) z = 12.288 (0.011)

Angle to previous plane (with approximate esd) = 66.15 (0.13)

*	-0.004 (0.002)	C4
*	0.001 (0.001)	N2

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*    0.001 (0.001)   O2
     0.001 (0.001)   C3
     0.041 (0.005)   C7
     0.078 (0.005)   C8

Rms deviation of fitted atoms =    0.002

- 2.787 (0.011) x + 1.174 (0.022) y + 15.477 (0.004) z = 1.195 (0.020)

Angle to previous plane (with approximate esd) = 78.13 ( 0.11 )

*   -0.004 (0.002)   C9
*    0.001 (0.001)   N3
*    0.001 (0.001)   O3
*    0.001 (0.001)   C10
    -0.015 (0.005)   C11
    -0.140 (0.005)   C12

Rms deviation of fitted atoms =    0.002
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Table 5. Anisotropic Displacement Parameters [$Å^2$ x 10^3] for $[Gd(NO_3)_3(TMSA)_{1.5}]_2$

Atom	U11	U22	U33	U23	U13	U12
Gd	18(1)	10(1)	10(1)	0(1)	3(1)	2(1)
O(1)	27(1)	23(1)	18(1)	-7(1)	10(1)	-7(1)
O(2)	24(1)	14(1)	21(1)	-7(1)	7(1)	-1(1)
O(3)	24(1)	13(1)	20(1)	3(1)	-3(1)	2(1)
O(4)	70(2)	21(1)	18(1)	-1(1)	-1(1)	15(1)
O(5)	52(2)	32(1)	21(1)	7(1)	13(1)	17(1)
O(6)	43(1)	24(1)	30(1)	16(1)	-3(1)	2(1)
O(7)	25(1)	30(1)	36(1)	15(1)	-4(1)	2(1)
O(8)	20(1)	24(1)	23(1)	6(1)	-1(1)	-3(1)
O(9)	27(1)	41(1)	50(2)	6(1)	-6(1)	-16(1)
O(10)	24(1)	22(1)	22(1)	-7(1)	8(1)	-1(1)
O(11)	31(1)	23(1)	18(1)	-4(1)	9(1)	-5(1)
O(12)	36(1)	27(1)	26(1)	-14(1)	8(1)	2(1)
N(1)	29(1)	22(1)	25(1)	-1(1)	10(1)	-9(1)
N(2)	23(1)	16(1)	16(1)	0(1)	1(1)	-2(1)
N(3)	21(1)	12(1)	23(1)	-1(1)	0(1)	0(1)
N(4)	27(1)	18(1)	21(1)	7(1)	-2(1)	-2(1)
N(5)	18(1)	26(1)	25(1)	1(1)	3(1)	0(1)
N(6)	24(1)	18(1)	14(1)	-1(1)	1(1)	4(1)
C(1)	14(1)	19(1)	18(1)	-2(1)	2(1)	-2(1)
C(2)	19(1)	23(1)	17(1)	-6(1)	5(1)	-2(1)
C(3)	20(1)	16(1)	20(1)	-3(1)	2(1)	3(1)
C(4)	21(1)	9(1)	18(1)	1(1)	2(1)	0(1)
C(5)	40(2)	51(2)	33(2)	5(2)	15(2)	-19(2)
C(6)	62(2)	19(2)	51(2)	-6(2)	25(2)	-13(2)
C(7)	40(2)	25(2)	16(1)	-5(1)	7(1)	-6(1)
C(8)	24(2)	31(2)	33(2)	-1(1)	-3(1)	-7(1)
C(9)	22(1)	13(1)	11(1)	-1(1)	2(1)	1(1)
C(10)	22(1)	10(1)	16(1)	-1(1)	0(1)	1(1)
C(11)	30(2)	14(1)	30(2)	1(1)	-2(1)	-7(1)
C(12)	19(1)	25(2)	35(2)	-1(1)	-2(1)	1(1)

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^* b^* U_{12}].$$

Table 6. Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters ($Å^2$ x 10^3) for $[Gd(NO_3)_3(TMSA)_{1.5}]_2$

Atom	x	y	z	U(eq)
H(2A)	-886(3)	8009(2)	3409(2)	24
H(2B)	-2493(3)	8193(2)	2800(2)	24
H(3A)	-1035(3)	9009(2)	1882(2)	23
H(3B)	-1147(3)	9431(2)	2793(2)	23
H(5A)	-2776(25)	5912(3)	3251(11)	49
H(5B)	-3681(11)	6773(14)	2954(7)	49
H(5C)	-2143(15)	6803(14)	3654(5)	49
H(6A)	-1197(28)	5390(5)	2275(3)	51
H(6B)	-852(23)	5995(6)	1510(11)	51
H(6C)	-2598(8)	5733(10)	1584(12)	51
H(7A)	1548(12)	9322(12)	4721(2)	32
H(7B)	-83(11)	9219(11)	4107(7)	32
H(7C)	788(22)	10118(2)	4178(8)	32
H(8A)	3757(4)	9594(13)	4189(5)	36
H(8B)	3728(4)	9770(11)	3186(9)	36
H(8C)	3931(4)	8820(3)	3551(14)	36
H(10A)	-1227(3)	10033(2)	-716(2)	20
H(10B)	-1484(3)	10103(2)	266(2)	20
H(11A)	-3329(19)	7471(2)	81(12)	31
H(11B)	-1549(8)	7338(2)	-21(14)	31
H(11C)	-2848(26)	7396(3)	-856(3)	31
H(12A)	-4629(4)	8731(8)	-534(12)	32
H(12B)	-3739(14)	9044(11)	-1293(3)	32
H(12C)	-3635(12)	9590(5)	-428(10)	32

Table 1. Crystal data and structure refinement, compound 6

Compound	$[Yb(NO_3)_3(TMSA)_{1.5}]_2$
Color / Shape	colorless / parallelepiped
Empirical formula	$C_{12}H_{24}N_6O_{12}Yb$
Formula weight	617.41
Temperature	173(2) K
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions (8192 reflections in full θ range)	a = 8.7171(1) Å α = 90° b = 15.6061(1) Å β = 99.152(1)° c = 15.6237(2) Å γ = 90°
Volume	2098.39(4) $Å^3$
Z	4
Density (calculated)	1.954 Mg/m^3
Absorption coefficient	4.529 mm^{-1}
Diffractometer / scan	Siemens SMART / CCD area detector
Radiation / wavelength	MoKα (graphite monochrom.) / 0.71073 Å
F(000)	1216
Crystal size	0.30 x 0.50 x 0.80 mm
θ range for data collection	1.86 to 27.88°
Index ranges	$-11 \le h \le 11$, $-20 \le k \le 19$, $-20 \le \ell \le 10$
Reflections collected	13088
Independent / observed refls.	4868(R_{int} = 0.0280) / 4274([I>2σ(I)])
Absorption correction	SADABS
Range of relat. transm. factors	0.96 and 0.55
Refinement method	Full-matrix least-squares on F^2
Computing	SHELXTL, Ver. 5[1]
Data / restraints / parameters	4864 / 0 / 287
Goodness-of-fit on F^2	1.018
SHELX-93 weight parameters	0.0267, 0.0000
Final R indices [I>2σ(I)]	R1 = 0.0212, wR2 = 0.0509
R indices (all data)	R1 = 0.0257, wR2 = 0.0537
Extinction coefficient	0.0113(2)
Largest diff. peak and hole	1.227 and -1.438 $eÅ^{-3}$

Table 2. Atomic Coordinates [x 10^4] and Equivalent Isotropic Displacement Parameters [$Å^2$ x 10^3] for $[Yb(NO_3)_3(TMSA)_{1.5}]_2$

Atom	x/a	y/b	z/c	U(eq)
Yb	1947(1)	7723(1)	1192(1)	13(1)
O(1)	-315(2)	7391(1)	1646(1)	21(1)
O(2)	1800(2)	8833(1)	2086(1)	19(1)
O(3)	248(2)	8432(1)	209(1)	19(1)
O(4)	3220(3)	6376(1)	1635(1)	36(1)
O(5)	2587(3)	7117(1)	2671(2)	33(1)
O(6)	3733(3)	5881(1)	2948(1)	31(1)
O(7)	4683(2)	8002(1)	1737(2)	29(1)
O(8)	3561(2)	8818(1)	714(1)	21(1)
O(9)	5852(2)	9165(2)	1403(2)	37(1)
O(10)	871(2)	6541(1)	267(1)	22(1)
O(11)	2958(2)	7131(1)	-35(1)	23(1)
O(12)	2068(3)	5960(1)	-709(1)	29(1)
N(1)	-1697(3)	6581(2)	2429(2)	25(1)
N(2)	1720(3)	9258(1)	3445(2)	19(1)
N(3)	-2335(3)	8523(2)	-255(2)	19(1)
N(4)	3190(3)	6443(2)	2436(2)	22(1)
N(5)	4742(3)	8677(2)	1289(2)	22(1)
N(6)	1962(3)	6520(2)	-179(1)	19(1)
C(1)	-1080(3)	7325(2)	2254(2)	18(1)
C(2)	-1378(3)	8097(2)	2796(2)	20(1)
C(3)	-735(3)	8934(2)	2491(2)	19(1)
C(4)	1017(3)	9006(2)	2674(2)	16(1)
C(5)	-2663(4)	6469(3)	3110(2)	39(1)
C(6)	-1533(4)	5828(2)	1889(2)	39(1)
C(7)	917(4)	9514(2)	4164(2)	27(1)
C(8)	3417(3)	9362(2)	3592(2)	31(1)
C(9)	-946(3)	8876(2)	-45(2)	15(1)
C(10)	-829(3)	9844(2)	-105(2)	17(1)
C(11)	-2564(4)	7597(2)	-226(2)	25(1)
C(12)	-3718(3)	9014(2)	-632(2)	26(1)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Torsion Angles [°] for $[Yb(NO_3)_3(TMSA)_{1.5}]_2$

N(1)-C(1)-C(2)-C(3)	-174.9(2)	C(1)-C(2)-C(3)-C(4)	-72.0(3)
C(2)-C(3)-C(4)-N(2)	-82.8(3)	N(3)-C(9)-C(10)-C(10)#1	-176.9(3)
C(9)-C(10)-C(10)#1-C(9)#1	180.0	C(10)-C(10)#1-C(9)#1-N(3)#1	176.9(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z

Table 4. Bond Lengths [Å] and Angles [°] for $[Yb(NO_3)_3(TMSA)_{1.5}]_2$

Yb-O(2)	2.242(2)	Yb-O(3)	2.248(2)
Yb-O(1)	2.259(2)	Yb-O(8)	2.406(2)
Yb-O(11)	2.418(2)	Yb-O(4)	2.426(2)
Yb-O(10)	2.437(2)	Yb-O(7)	2.441(2)
Yb-O(5)	2.476(2)	O(1)-C(1)	1.249(3)
O(2)-C(4)	1.259(3)	O(3)-C(9)	1.261(3)
O(4)-N(4)	1.261(3)	O(5)-N(4)	1.257(3)
O(6)-N(4)	1.230(3)	O(7)-N(5)	1.269(3)
O(8)-N(5)	1.273(3)	O(9)-N(5)	1.222(3)
O(10)-N(6)	1.265(3)	O(11)-N(6)	1.284(3)
O(12)-N(6)	1.217(3)	N(1)-C(1)	1.326(4)
N(1)-C(6)	1.467(4)	N(1)-C(5)	1.468(4)
N(2)-C(4)	1.321(3)	N(2)-C(8)	1.469(4)
N(2)-C(7)	1.470(4)	N(3)-C(9)	1.323(3)
N(3)-C(11)	1.461(3)	N(3)-C(12)	1.470(3)
C(1)-C(2)	1.519(4)	C(2)-C(3)	1.526(4)
C(3)-C(4)	1.513(4)	C(9)-C(10)	1.519(3)
C(10)-C(10)#1	1.511(5)		

O(2)-Yb-O(3)	87.04(7)	O(2)-Yb-O(1)	80.95(7)
O(3)-Yb-O(1)	79.32(7)	O(2)-Yb-O(8)	74.83(7)
O(3)-Yb-O(8)	78.02(6)	O(1)-Yb-O(8)	147.44(7)
O(2)-Yb-O(11)	148.59(7)	O(3)-Yb-O(11)	85.98(7)
O(1)-Yb-O(11)	127.44(7)	O(8)-Yb-O(11)	73.76(7)
O(2)-Yb-O(4)	124.15(7)	O(3)-Yb-O(4)	147.48(7)
O(1)-Yb-O(4)	95.42(8)	O(8)-Yb-O(4)	116.11(8)
O(11)-Yb-O(4)	71.75(7)	O(2)-Yb-O(10)	154.13(7)
O(3)-Yb-O(10)	79.50(7)	O(1)-Yb-O(10)	74.94(7)
O(8)-Yb-O(10)	122.83(7)	O(11)-Yb-O(10)	52.75(7)
O(4)-Yb-O(10)	68.21(7)	O(2)-Yb-O(7)	78.12(7)
O(3)-Yb-O(7)	130.63(7)	O(1)-Yb-O(7)	141.70(8)
O(8)-Yb-O(7)	52.71(6)	O(11)-Yb-O(7)	83.42(7)
O(4)-Yb-O(7)	71.21(8)	O(10)-Yb-O(7)	127.19(7)
O(2)-Yb-O(5)	74.97(7)	O(3)-Yb-O(5)	148.38(8)
O(1)-Yb-O(5)	72.41(8)	O(8)-Yb-O(5)	120.29(8)
O(11)-Yb-O(5)	122.53(7)	O(4)-Yb-O(5)	51.58(7)

O(10)-Yb-O(5)	105.85(7)	O(7)-Yb-O(5)	71.36(8)
C(1)-O(1)-Yb	148.9(2)	C(4)-O(2)-Yb	135.4(2)
C(9)-O(3)-Yb	155.1(2)	N(4)-O(4)-Yb	97.5(2)
N(4)-O(5)-Yb	95.1(2)	N(5)-O(7)-Yb	94.5(2)
N(5)-O(8)-Yb	96.1(2)	N(6)-O(10)-Yb	95.4(2)
N(6)-O(11)-Yb	95.8(2)	C(1)-N(1)-C(6)	120.2(3)
C(1)-N(1)-C(5)	123.5(3)	C(6)-N(1)-C(5)	116.1(3)
C(4)-N(2)-C(8)	119.0(2)	C(4)-N(2)-C(7)	124.7(2)
C(8)-N(2)-C(7)	116.2(2)	C(9)-N(3)-C(11)	121.9(2)
C(9)-N(3)-C(12)	122.8(2)	C(11)-N(3)-C(12)	114.9(2)
O(6)-N(4)-O(5)	122.9(3)	O(6)-N(4)-O(4)	121.3(3)
O(5)-N(4)-O(4)	115.8(2)	O(9)-N(5)-O(7)	122.5(2)
O(9)-N(5)-O(8)	121.9(2)	O(7)-N(5)-O(8)	115.6(2)
O(12)-N(6)-O(10)	122.5(2)	O(12)-N(6)-O(11)	121.9(2)
O(10)-N(6)-O(11)	115.5(2)	O(1)-C(1)-N(1)	120.8(3)
O(1)-C(1)-C(2)	121.2(2)	N(1)-C(1)-C(2)	118.0(3)
C(1)-C(2)-C(3)	113.6(2)	C(4)-C(3)-C(2)	114.4(2)
O(2)-C(4)-N(2)	120.2(2)	O(2)-C(4)-C(3)	119.6(2)
N(2)-C(4)-C(3)	120.2(2)	O(3)-C(9)-N(3)	121.8(2)
O(3)-C(9)-C(10)	120.4(2)	N(3)-C(9)-C(10)	117.8(2)
C(10)#1-C(10)-C(9)	112.2(3)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z

Least squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)

7.703 (0.007) x + 7.062 (0.022) y - 0.344 (0.026) z = 6.926 (0.014)

*	-0.003 (0.002)	N4
*	0.001 (0.001)	O4
*	0.001 (0.001)	O5
*	0.001 (0.001)	O6
	-0.014 (0.005)	Yb

BMPS

Rms deviation of fitted atoms = 0.002

- 4.707 (0.011) x + 8.058 (0.021) y + 11.595 (0.015) z = 6.257 (0.021)

Angle to previous plane (with approximate esd) = 80.58 (0.11)

*	-0.002 (0.002)	N5
*	0.001 (0.001)	O7
*	0.001 (0.001)	O8
*	0.001 (0.001)	O9
	0.432 (0.004)	Yb

Rms deviation of fitted atoms = 0.001

- 3.849 (0.011) x - 8.584 (0.018) y + 9.836 (0.017) z = 5.017 (0.013)

Angle to previous plane (with approximate esd) = 87.06 (0.10)

*	0.001 (0.002)	N6
*	0.000 (0.001)	O10
*	0.000 (0.001)	O11
*	0.000 (0.001)	O12
	-0.310 (0.004)	Yb

Rms deviation of fitted atoms = 0.000

- 6.455 (0.009) x - 3.296 (0.024) y + 8.000 (0.020) z = 1.318 (0.018)

Angle to previous plane (with approximate esd) = 26.44 (0.18)

*	-0.010 (0.002)	C1
*	0.004 (0.001)	N1
*	0.004 (0.001)	O1
*	0.003 (0.001)	C2
	0.045 (0.006)	C5
	0.082 (0.006)	C6

Rms deviation of fitted atoms = 0.006

- 0.153 (0.012) x + 14.863 (0.006) y - 4.652 (0.019) z = 12.129 (0.011)

Angle to previous plane (with approximate esd) = 65.90 (0.12)

*	-0.004 (0.002)	C4
*	0.001 (0.001)	N2

```
*     0.001 (0.001)   O2
*     0.001 (0.001)   C3
      0.060 (0.005)   C7
      0.063 (0.005)   C8

Rms deviation of fitted atoms =    0.002


- 2.710 (0.011) x + 1.348 (0.023) y + 15.372 (0.004) z = 1.389 (0.020)

Angle to previous plane (with approximate esd) = 78.44 ( 0.11 )

*    -0.006 (0.002)   C9
*     0.002 (0.001)   N3
*     0.002 (0.001)   O3
*     0.002 (0.001)   C10
     -0.017 (0.005)   C11
     -0.137 (0.005)   C12

Rms deviation of fitted atoms =    0.003
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Table 5. Anisotropic Displacement Parameters [$Å^2$ x 10^3] for $[Yb(NO_3)_3(TMSA)_{1.5}]_2$

Atom	U11	U22	U33	U23	U13	U12
Yb	16(1)	13(1)	11(1)	0(1)	4(1)	1(1)
O(1)	25(1)	20(1)	20(1)	-5(1)	12(1)	-7(1)
O(2)	21(1)	17(1)	21(1)	-5(1)	9(1)	0(1)
O(3)	18(1)	16(1)	21(1)	4(1)	0(1)	0(1)
O(4)	66(2)	24(1)	17(1)	-2(1)	0(1)	11(1)
O(5)	45(1)	31(1)	25(1)	8(1)	14(1)	14(1)
O(6)	38(1)	27(1)	27(1)	16(1)	0(1)	4(1)
O(7)	23(1)	29(1)	33(1)	13(1)	0(1)	2(1)
O(8)	16(1)	25(1)	21(1)	5(1)	2(1)	0(1)
O(9)	22(1)	44(1)	42(1)	7(1)	-4(1)	-14(1)
O(10)	22(1)	25(1)	23(1)	-6(1)	10(1)	1(1)
O(11)	26(1)	25(1)	18(1)	-4(1)	8(1)	-5(1)
O(12)	36(1)	29(1)	25(1)	-13(1)	12(1)	0(1)
N(1)	25(1)	26(1)	25(1)	-1(1)	11(1)	-9(1)
N(2)	19(1)	20(1)	17(1)	0(1)	3(1)	-1(1)
N(3)	18(1)	17(1)	22(1)	0(1)	1(1)	0(1)
N(4)	24(1)	21(1)	20(1)	6(1)	-1(1)	-4(1)
N(5)	17(1)	26(1)	23(1)	1(1)	3(1)	0(1)
N(6)	22(1)	23(1)	13(1)	0(1)	5(1)	5(1)
C(1)	13(1)	23(1)	17(1)	-1(1)	2(1)	-1(1)
C(2)	18(1)	25(1)	18(1)	-3(1)	6(1)	-2(1)
C(3)	17(1)	20(1)	20(1)	-2(1)	3(1)	4(1)
C(4)	17(1)	11(1)	20(1)	1(1)	4(1)	1(1)
C(5)	37(2)	50(2)	34(2)	2(2)	19(2)	-18(2)
C(6)	53(2)	22(2)	47(2)	-4(2)	24(2)	-10(2)
C(7)	37(2)	28(2)	17(1)	-6(1)	9(1)	-5(1)
C(8)	22(2)	34(2)	34(2)	2(1)	-4(1)	-6(1)
C(9)	19(1)	16(1)	10(1)	0(1)	3(1)	1(1)
C(10)	19(1)	14(1)	16(1)	0(1)	1(1)	1(1)
C(11)	27(2)	20(1)	28(2)	2(1)	0(1)	-6(1)
C(12)	16(1)	27(2)	32(2)	1(1)	-1(1)	-1(1)

The anisotropic displacement factor exponent takes the form:

$$\cdot \quad -2\pi^2 \left[(ha^*)^2 U_{11} + \ldots + 2hka^*b^* U_{12} \right].$$

Table 6. Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters ($Å^2$ x 10^3) for $[Yb(NO_3)_3(TMSA)_{1.5}]_2$

Atom	x	y	z	U(eq)
H(2A)	-902(3)	7993(2)	3406(2)	24
H(2B)	-2512(3)	8160(2)	2781(2)	24
H(3A)	-1080(3)	8990(2)	1858(2)	23
H(3B)	-1187(3)	9418(2)	2776(2)	23
H(5A)	-2729(21)	5858(3)	3245(10)	47
H(5B)	-3708(9)	6692(13)	2907(6)	47
H(5C)	-2197(14)	6780(12)	3631(5)	47
H(6A)	-1156(26)	5342(4)	2261(3)	47
H(6B)	-790(21)	5954(5)	1496(11)	47
H(6C)	-2545(7)	5685(9)	1549(11)	47
H(7A)	1556(11)	9361(11)	4716(2)	32
H(7B)	-85(11)	9217(10)	4111(7)	32
H(7C)	742(20)	10134(3)	4143(8)	32
H(8A)	3732(4)	9709(11)	4113(8)	37
H(8B)	3737(4)	9650(12)	3091(6)	37
H(8C)	3913(3)	8798(2)	3669(13)	37
H(10A)	-1274(3)	10030(2)	-699(2)	20
H(10B)	-1451(3)	10110(2)	302(2)	20
H(11A)	-3283(20)	7464(2)	178(11)	30
H(11B)	-1564(5)	7316(2)	-31(14)	30
H(11C)	-2999(25)	7390(3)	-806(4)	30
H(12A)	-4648(4)	8745(8)	-473(11)	31
H(12B)	-3797(13)	9022(11)	-1265(2)	31
H(12C)	-3630(11)	9602(4)	-410(10)	31

Table 9. Crystal data and structure refinement, compound 7

Compound	$[La(NO_3)_3(TMSA)_2]_n$
Color / Shape	colorless / fragment
Empirical formula	$C_{16}H_{32}LaN_7O_{13}$
Formula weight	669.40
Temperature	173(2) K
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 11.5604(1) Å α = 90°
(7521 reflections	b = 16.7875(2) Å β = 104.712(1)°
in full θ range)	c = 13.8918(2) Å γ = 90°
Volume	2607.60(5) Å^3
Z	4
Density (calculated)	1.705 Mg/m^3
Absorption coefficient	1.712 mm^{-1}
Diffractometer / scan	Siemens SMART / CCD area detector
Radiation / wavelength	MoKα (graphite monochrom.) / 0.71073 Å
F(000)	1352
Crystal size	0.06 x 0.20 x 0.90 mm
θ range for data collection	1.94 to 27.88°
Index ranges	$-14 \le h \le 14$, $-18 \le k \le 21$, $-15 \le \ell \le 18$
Reflections collected	16354
Independent / observed refls.	6066(R_{int} = 0.0383) / 4643([I>2σ(I)])
Absorption correction	SADABS[1]
Range of relat. transm. factors	0.97 and 0.71
Refinement method	Full-matrix least-squares on F^2
Computing	SHELXTL, Ver. 5[2]
Data / restraints / parameters	6066 / 0 / 343
Goodness-of-fit on F^2	0.954
SHELX-93 weight parameters	0.0290, 0.0000
Final R indices [I>2σ(I)]	R1 = 0.0282, wR2 = 0.0559
R indices (all data)	R1 = 0.0469, wR2 = 0.0614
Extinction coefficient	0.00132(14)
Largest diff. peak and hole	0.511 and -0.882 eÅ^{-3}

Table 10. Atomic Coordinates [x 10^4] and Equivalent Isotropic Displacement Parameters [$Å^2$ x 10^3] for $[La(NO_3)_3(TMSA)_2]_n$

Atom	x/a	y/b	z/c	U(eq)
La	6640(1)	1805(1)	3048(1)	14(1)
O(1)	8409(2)	2698(1)	3512(2)	24(1)
O(2)	5947(2)	3106(1)	3595(2)	25(1)
O(3)	6289(2)	2637(1)	1537(1)	19(1)
O(4)	2251(2)	3390(1)	-157(2)	28(1)
O(5)	4634(2)	1674(1)	3818(2)	35(1)
O(6)	4325(2)	1597(1)	2223(2)	31(1)
O(7)	2835(2)	1498(2)	2915(2)	62(1)
O(8)	5947(2)	353(1)	3342(2)	25(1)
O(9)	6061(2)	548(1)	1827(2)	30(1)
O(10)	5253(2)	-540(1)	2215(2)	50(1)
O(11)	8219(2)	1377(1)	1958(2)	26(1)
O(12)	8478(2)	800(1)	3390(2)	27(1)
O(13)	9582(2)	455(1)	2395(2)	40(1)
N(1)	10308(2)	3088(1)	4126(2)	22(1)
N(2)	6067(2)	3808(2)	4989(2)	32(1)
N(3)	7010(2)	3569(1)	671(2)	22(1)
N(4)	2290(2)	4061(1)	1252(2)	22(1)
N(5)	3908(2)	1594(1)	2990(2)	29(1)
N(6)	5745(2)	106(1)	2454(2)	26(1)
N(7)	8780(2)	866(1)	2577(2)	23(1)
C(1)	9140(2)	3181(2)	4024(2)	19(1)
C(2)	8701(2)	3879(2)	4526(2)	24(1)
C(3)	7431(2)	4140(2)	3946(2)	23(1)
C(4)	6432(2)	3652(2)	4173(2)	22(1)
C(5)	10714(3)	2503(2)	3502(3)	32(1)
C(6)	11224(3)	3626(2)	4698(2)	31(1)
C(7)	6572(3)	4441(2)	5712(3)	45(1)
C(8)	5165(3)	3306(2)	5260(3)	49(1)
C(9)	6140(2)	3262(2)	1023(2)	18(1)
C(10)	4949(2)	3691(2)	781(2)	22(1)

C(11)	4009(2)	3225(2)	1153(2)	21(1)
C(12)	2786(2)	3572(2)	720(2)	18(1)
C(13)	6872(3)	4296(2)	59(3)	30(1)
C(14)	8202(2)	3204(2)	898(3)	30(1)
C(15)	1093(2)	4385(2)	839(3)	30(1)
C(16)	2867(3)	4325(2)	2261(3)	43(1)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 11. Torsion Angles [°] for $[La(NO_3)_3(TMSA)_2]_n$

N(1)-C(1)-C(2)-C(3)	151.4(3)	C(1)-C(2)-C(3)-C(4)	82.6(3)
C(2)-C(3)-C(4)-N(2)	80.7(3)	O(1)-C(1)-C(2)-C(3)	-28.0(4)
C(1)-C(2)-C(3)-C(4)	82.6(3)	C(2)-C(3)-C(4)-O(2)	-99.4(3)
N(3)-C(9)-C(10)-C(11)	174.6(3)	C(9)-C(10)-C(11)-C(12)	-168.2(2)
C(10)-C(11)-C(12)-N(4)	-100.0(3)	O(3)-C(9)-C(10)-C(11)	-5.2(4)
C(9)-C(10)-C(11)-C(12)	-168.2(2)	C(10)-C(11)-C(12)-O(4)	79.6(3)

Table 12. Bond Lengths [Å] and Angles [°] for $[La(NO_3)_3(TMSA)_2]_n$

La-O(4)#1	2.436(2)	La-O(3)	2.468(2)
La-O(1)	2.485(2)	La-O(2)	2.509(2)
La-O(8)	2.630(2)	La-O(6)	2.654(2)
La-O(12)	2.660(2)	La-O(9)	2.684(2)
La-O(11)	2.747(2)	La-O(5)	2.798(2)
O(1)-C(1)	1.254(3)	O(2)-C(4)	1.253(3)
O(3)-C(9)	1.255(3)	O(4)-C(12)	1.255(3)
O(4)-La#2	2.436(2)	O(5)-N(5)	1.247(3)
O(6)-N(5)	1.276(3)	O(7)-N(5)	1.228(3)
O(8)-N(6)	1.266(3)	O(9)-N(6)	1.266(3)
O(10)-N(6)	1.231(3)	O(11)-N(7)	1.269(3)
O(12)-N(7)	1.268(3)	O(13)-N(7)	1.233(3)
N(1)-C(1)	1.330(3)	N(1)-C(6)	1.464(3)
N(1)-C(5)	1.464(4)	N(2)-C(4)	1.333(4)
N(2)-C(8)	1.463(4)	N(2)-C(7)	1.477(4)
N(3)-C(9)	1.330(3)	N(3)-C(14)	1.467(3)
N(3)-C(13)	1.472(4)	N(4)-C(12)	1.328(3)
N(4)-C(16)	1.460(4)	N(4)-C(15)	1.462(3)
C(1)-C(2)	1.515(4)	C(2)-C(3)	1.547(4)
C(3)-C(4)	1.513(4)	C(9)-C(10)	1.514(4)
C(10)-C(11)	1.532(4)	C(11)-C(12)	1.506(4)

O(4)#1-La-O(3)	152.84(7)	O(4)#1-La-O(1)	79.06(7)
O(3)-La-O(1)	79.98(6)	O(4)#1-La-O(2)	80.74(7)
O(3)-La-O(2)	76.65(7)	O(1)-La-O(2)	72.63(6)
O(4)#1-La-O(8)	74.73(6)	O(3)-La-O(8)	131.73(6)
O(1)-La-O(8)	141.44(6)	O(2)-La-O(8)	128.78(6)
O(4)#1-La-O(6)	115.02(7)	O(3)-La-O(6)	77.12(6)
O(1)-La-O(6)	149.87(6)	O(2)-La-O(6)	83.17(6)
O(8)-La-O(6)	68.36(6)	O(4)#1-La-O(12)	73.78(7)
O(3)-La-O(12)	117.55(6)	O(1)-La-O(12)	76.65(6)
O(2)-La-O(12)	143.13(6)	O(8)-La-O(12)	69.21(6)
O(6)-La-O(12)	131.74(6)	O(4)#1-La-O(9)	120.13(7)
O(3)-La-O(9)	86.94(6)	O(1)-La-O(9)	134.03(6)
O(2)-La-O(9)	145.92(6)	O(8)-La-O(9)	48.10(6)
O(6)-La-O(9)	63.96(7)	O(12)-La-O(9)	70.95(6)

O(4)#1-La-O(11)	117.93(6)	O(3)-La-O(11)	70.63(6)
O(1)-La-O(11)	71.51(6)	O(2)-La-O(11)	134.67(6)
O(8)-La-O(11)	96.53(6)	O(6)-La-O(11)	117.77(7)
O(12)-La-O(11)	47.14(6)	O(9)-La-O(11)	62.59(6)
O(4)#1-La-O(5)	69.58(7)	O(3)-La-O(5)	113.35(6)
O(1)-La-O(5)	130.98(6)	O(2)-La-O(5)	66.02(6)
O(8)-La-O(5)	63.45(6)	O(6)-La-O(5)	46.50(7)
O(12)-La-O(5)	125.70(6)	O(9)-La-O(5)	94.68(6)
O(11)-La-O(5)	157.09(6)	C(1)-O(1)-La	158.3(2)
C(4)-O(2)-La	134.9(2)	C(9)-O(3)-La	157.7(2)
C(12)-O(4)-La#2	165.8(2)	N(5)-O(5)-La	94.9(2)
N(5)-O(6)-La	101.1(2)	N(6)-O(8)-La	98.1(2)
N(6)-O(9)-La	95.5(2)	N(7)-O(11)-La	95.7(2)
N(7)-O(12)-La	100.0(2)	C(1)-N(1)-C(6)	124.0(2)
C(1)-N(1)-C(5)	119.0(2)	C(6)-N(1)-C(5)	116.1(2)
C(4)-N(2)-C(8)	120.4(3)	C(4)-N(2)-C(7)	124.3(3)
C(8)-N(2)-C(7)	115.1(3)	C(9)-N(3)-C(14)	121.0(2)
C(9)-N(3)-C(13)	123.5(2)	C(14)-N(3)-C(13)	115.4(2)
C(12)-N(4)-C(16)	124.4(2)	C(12)-N(4)-C(15)	120.7(2)
C(16)-N(4)-C(15)	114.9(2)	O(7)-N(5)-O(5)	121.4(3)
O(7)-N(5)-O(6)	121.2(3)	O(5)-N(5)-O(6)	117.5(2)
O(10)-N(6)-O(8)	120.6(3)	O(10)-N(6)-O(9)	121.7(3)
O(8)-N(6)-O(9)	117.6(2)	O(13)-N(7)-O(12)	121.7(3)
O(13)-N(7)-O(11)	121.3(3)	O(12)-N(7)-O(11)	117.0(2)
O(1)-C(1)-N(1)	120.3(3)	O(1)-C(1)-C(2)	120.3(2)
N(1)-C(1)-C(2)	119.4(2)	C(1)-C(2)-C(3)	111.4(2)
C(4)-C(3)-C(2)	114.3(2)	O(2)-C(4)-N(2)	120.1(3)
O(2)-C(4)-C(3)	120.2(3)	N(2)-C(4)-C(3)	119.6(3)
O(3)-C(9)-N(3)	121.7(2)	O(3)-C(9)-C(10)	120.6(2)
N(3)-C(9)-C(10)	117.6(2)	C(9)-C(10)-C(11)	111.4(2)
C(12)-C(11)-C(10)	110.0(2)	O(4)-C(12)-N(4)	120.9(2)
O(4)-C(12)-C(11)	118.3(2)	N(4)-C(12)-C(11)	120.7(3)

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2,-y+1/2,z+1/2 #2 x-1/2,-y+1/2,z-1/2

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)

- 1.352 (0.020) x + 16.630 (0.004) y - 0.541 (0.019) z = 1.953 (0.009)

*	0.008 (0.002)	N5
*	-0.003 (0.001)	O5
*	-0.003 (0.001)	O6
*	-0.003 (0.001)	O7
	-0.013 (0.005)	La

Rms deviation of fitted atoms = 0.005

10.036 (0.009) x - 7.534 (0.025) y - 0.215 (0.019) z = 5.632 (0.006)

Angle to previous plane (with approximate esd) = 55.87 (0.14)

*	0.002 (0.002)	N6
*	-0.001 (0.001)	O8
*	-0.001 (0.001)	O9
*	-0.001 (0.001)	O10
	-0.393 (0.005)	La

Rms deviation of fitted atoms = 0.001

6.788 (0.013) x + 11.686 (0.017) y + 3.478 (0.018) z = 7.869 (0.009)

Angle to previous plane (with approximate esd) = 73.45 (0.10)

*	0.000 (0.002)	N7
*	0.000 (0.001)	O11
*	0.000 (0.001)	O12
*	0.000 (0.001)	O13
	-0.192 (0.004)	La

Rms deviation of fitted atoms = 0.000

Table 13. Anisotropic Displacement Parameters [$Å^2$ x 10^3] for $[La(NO_3)_3(TMSA)_2]_n$

Atom	U11	U22	U33	U23	U13	U12
La	14(1)	17(1)	13(1)	0(1)	4(1)	-2(1)
O(1)	20(1)	23(1)	30(1)	-6(1)	7(1)	-7(1)
O(2)	22(1)	27(1)	27(1)	-10(1)	9(1)	-3(1)
O(3)	18(1)	25(1)	17(1)	5(1)	7(1)	3(1)
O(4)	27(1)	40(1)	16(1)	-4(1)	4(1)	8(1)
O(5)	33(1)	41(1)	33(2)	-10(1)	11(1)	-7(1)
O(6)	23(1)	37(1)	32(1)	10(1)	7(1)	-1(1)
O(7)	19(1)	91(2)	82(2)	-5(2)	22(1)	-2(1)
O(8)	30(1)	24(1)	21(1)	-2(1)	9(1)	-6(1)
O(9)	44(1)	26(1)	26(1)	-4(1)	19(1)	-9(1)
O(10)	78(2)	33(1)	50(2)	-22(1)	39(2)	-30(1)
O(11)	23(1)	30(1)	27(1)	7(1)	8(1)	5(1)
O(12)	27(1)	34(1)	21(1)	6(1)	8(1)	2(1)
O(13)	29(1)	43(1)	55(2)	-1(1)	20(1)	14(1)
N(1)	19(1)	22(1)	24(1)	1(1)	4(1)	-2(1)
N(2)	33(2)	33(2)	35(2)	-16(1)	20(1)	-12(1)
N(3)	18(1)	22(1)	25(2)	2(1)	7(1)	0(1)
N(4)	18(1)	27(1)	20(1)	-6(1)	6(1)	0(1)
N(5)	20(1)	25(1)	46(2)	-1(1)	16(1)	0(1)
N(6)	28(1)	22(1)	31(2)	-6(1)	14(1)	-5(1)
N(7)	17(1)	23(1)	30(2)	-2(1)	7(1)	-1(1)
C(1)	22(1)	21(1)	17(2)	6(1)	8(1)	-4(1)
C(2)	23(2)	26(2)	22(2)	-3(1)	7(1)	-6(1)
C(3)	26(2)	20(1)	25(2)	-1(1)	10(1)	-2(1)
C(4)	20(2)	21(2)	25(2)	-2(1)	6(1)	2(1)
C(5)	25(2)	31(2)	38(2)	-2(2)	7(2)	2(1)
C(6)	24(2)	35(2)	30(2)	-2(2)	1(1)	-6(1)
C(7)	48(2)	50(2)	42(2)	-25(2)	21(2)	-13(2)
C(8)	56(2)	49(2)	58(3)	-18(2)	44(2)	-19(2)
C(9)	19(1)	21(1)	14(2)	-5(1)	3(1)	-3(1)
C(10)	20(1)	21(1)	24(2)	6(1)	4(1)	2(1)
C(11)	19(1)	25(1)	18(2)	4(1)	5(1)	5(1)
C(12)	18(1)	23(1)	15(2)	3(1)	7(1)	-1(1)

C(13)	30(2)	27(2)	36(2)	8(1)	14(2)	-2(1)
C(14)	19(1)	35(2)	39(2)	6(2)	13(1)	5(1)
C(15)	21(2)	37(2)	36(2)	-3(2)	11(1)	5(1)
C(16)	40(2)	60(2)	30(2)	-23(2)	8(2)	-1(2)

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$.

Table 14. Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters ($Å^2$ x 10^3) for $[La(NO_3)_3(TMSA)_2]_n$

Atom	x	y	z	U(eq)
H(2A)	9259(2)	4332(2)	4568(2)	28
H(2B)	8689(2)	3727(2)	5212(2)	28
H(3A)	7316(2)	4705(2)	4103(2)	28
H(3B)	7374(2)	4104(2)	3224(2)	28
H(5A)	10128(9)	2070(6)	3334(12)	47
H(5B)	11489(9)	2286(9)	3865(6)	47
H(5C)	10796(17)	2761(3)	2890(7)	47
H(6A)	10935(8)	3872(10)	5233(10)	46
H(6B)	11393(14)	4042(8)	4258(4)	46
H(6C)	11956(7)	3325(3)	4986(13)	46
H(7A)	6986(18)	4833(7)	5397(6)	68
H(7B)	7140(16)	4206(3)	6288(8)	68
H(7C)	5926(4)	4704(9)	5931(13)	68
H(8A)	4701(15)	3026(11)	4668(5)	73
H(8B)	4629(14)	3638(3)	5534(18)	73
H(8C)	5561(4)	2915(10)	5761(14)	73
H(10A)	4667(2)	3765(2)	52(2)	26
H(10B)	5053(2)	4225(2)	1095(2)	26
H(11A)	4019(2)	2659(2)	955(2)	25
H(11B)	4199(2)	3249(2)	1889(2)	25
H(13A)	6024(3)	4441(7)	-154(13)	45
H(13B)	7177(16)	4200(4)	-527(8)	45
H(13C)	7324(15)	4732(3)	452(5)	45
H(14A)	8177(5)	2687(6)	1221(14)	45
H(14B)	8776(4)	3553(6)	1345(12)	45
H(14C)	8449(8)	3127(11)	280(3)	45
H(15A)	786(8)	4194(10)	154(6)	46
H(15B)	1131(4)	4968(2)	840(14)	46
H(15C)	560(5)	4209(10)	1244(9)	46
H(16A)	3735(3)	4257(13)	2387(6)	65
H(16B)	2571(15)	4007(9)	2740(3)	65
H(16C)	2684(17)	4888(4)	2333(6)	65

Table 1. Crystal data and structure refinement - Compound 8

Compound	$[Ce(NO_3)_3(TMSA)_2]_n$
Color / Shape	colorless / fragment
Empirical formula	$C_{16}H_{32}CeN_7O_{13}$
Formula weight	670.61
Temperature	173(2) K
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 11.5490(3) Å α = 90°
(5793 reflections	b = 16.7235(5) Å β = 104.854(1)°
in full θ range)	c = 13.8387(4) Å γ = 90°
Volume	2583.48(13) Å^3
Z	4
Density (calculated)	1.724 Mg/m^3
Absorption coefficient	1.837 mm^{-1}
Diffractometer / scan	Siemens SMART / CCD area detector
Radiation / wavelength	MoKα (graphite monochrom.) / 0.71073 Å
F(000)	1356
Crystal size	0.14 x 0.34 x 0.50 mm
θ range for data collection	1.95 to 27.92°
Index ranges	$-13 \le h \le 15$, $-21 \le k \le 20$, $-18 \le \ell \le 11$
Reflections collected	16144
Independent / observed refls.	6024(R_{int} = 0.0348) / 5175([I>2σ(I)])
Absorption correction	SADABS[1]
Range of relat. transm. factors	0.97 and 0.75
Refinement method	Full-matrix least-squares on F^2
Computing	SHELXTL, Ver. 5[2]
Data / restraints / parameters	6023 / 0 / 343
Goodness-of-fit on F^2	1.016
SHELX-93 weight parameters	0.0283, 0.0000
Final R indices [I>2σ(I)]	R1 = 0.0220, wR2 = 0.0541
R indices (all data)	R1 = 0.0293, wR2 = 0.0563
Extinction coefficient	0.0019(2)
Largest diff. peak and hole	0.815 and -0.550 eÅ^{-3}

Table 2. Atomic Coordinates [x 10^4] and Equivalent Isotropic Displacement Parameters [$Å^2$ x 10^3] for $[Ce(NO_3)_3(TMSA)_2]_n$

Atom	x/a	y/b	z/c	U(eq)
Ce	6647(1)	1806(1)	3045(1)	14(1)
O(1)	8406(1)	2688(1)	3501(1)	24(1)
O(2)	5952(1)	3090(1)	3592(1)	25(1)
O(3)	6290(1)	2635(1)	1542(1)	19(1)
O(4)	2252(1)	3390(1)	-169(1)	27(1)
O(5)	4624(2)	1677(1)	3817(1)	38(1)
O(6)	4351(1)	1602(1)	2227(1)	31(1)
O(7)	2841(2)	1510(2)	2889(2)	67(1)
O(8)	5952(1)	368(1)	3346(1)	24(1)
O(9)	6064(1)	556(1)	1826(1)	28(1)
O(10)	5264(2)	-534(1)	2223(2)	49(1)
O(11)	8215(1)	1379(1)	1954(1)	25(1)
O(12)	8464(1)	800(1)	3389(1)	28(1)
O(13)	9575(1)	455(1)	2397(2)	40(1)
N(1)	10309(2)	3081(1)	4112(1)	21(1)
N(2)	6071(2)	3808(1)	4986(2)	32(1)
N(3)	7014(2)	3568(1)	674(1)	21(1)
N(4)	2288(2)	4061(1)	1246(1)	22(1)
N(5)	3908(2)	1602(1)	2981(2)	30(1)
N(6)	5752(2)	118(1)	2459(2)	24(1)
N(7)	8768(2)	868(1)	2570(2)	23(1)
C(1)	9136(2)	3174(1)	4016(2)	18(1)
C(2)	8698(2)	3870(1)	4519(2)	23(1)
C(3)	7431(2)	4134(1)	3941(2)	23(1)
C(4)	6433(2)	3645(1)	4170(2)	22(1)
C(5)	10714(2)	2497(1)	3485(2)	30(1)
C(6)	11229(2)	3622(1)	4683(2)	29(1)
C(7)	6570(3)	4441(2)	5699(2)	44(1)
C(8)	5171(3)	3304(2)	5262(2)	49(1)
C(9)	6141(2)	3258(1)	1028(2)	17(1)
C(10)	4950(2)	3688(1)	781(2)	22(1)

C(11)	4007(2)	3220(1)	1147(2)	21(1)
C(12)	2784(2)	3572(1)	709(2)	18(1)
C(13)	6879(2)	4294(1)	57(2)	29(1)
C(14)	8203(2)	3197(1)	902(2)	29(1)
C(15)	1087(2)	4384(2)	829(2)	30(1)
C(16)	2873(2)	4320(2)	2261(2)	45(1)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Torsion Angles [°] for $[Ce(NO_3)_3(TMSA)_2]_n$

N(1)-C(1)-C(2)-C(3)	150.9(2)	C(1)-C(2)-C(3)-C(4)	82.8(2)
C(2)-C(3)-C(4)-N(2)	81.3(3)	O(1)-C(1)-C(2)-C(3)	-28.4(3)
C(1)-C(2)-C(3)-C(4)	82.8(2)	C(2)-C(3)-C(4)-O(2)	-98.7(2)
N(3)-C(9)-C(10)-C(11)	174.4(2)	C(9)-C(10)-C(11)-C(12)	-168.4(2)
C(10)-C(11)-C(12)-N(4)	-100.2(2)	O(3)-C(9)-C(10)-C(11)	-5.3(3)
C(9)-C(10)-C(11)-C(12)	-168.4(2)	C(10)-C(11)-C(12)-O(4)	79.9(2)

Table 4. Bond Lengths [Å] and Angles [°] for $[Ce(NO_3)_3(TMSA)_2]_n$

Ce-O(4)#1	2.412(2)	Ce-O(3)	2.4442(14)
Ce-O(1)	2.4592(14)	Ce-O(2)	2.477(2)
Ce-O(8)	2.602(2)	Ce-O(6)	2.625(2)
Ce-O(12)	2.636(2)	Ce-O(9)	2.663(2)
Ce-O(11)	2.734(2)	Ce-O(5)	2.815(2)
O(1)-C(1)	1.252(2)	O(2)-C(4)	1.259(3)
O(3)-C(9)	1.250(2)	C(4)-C(12)	1.251(3)
O(4)-Ce#2	2.413(2)	O(5)-N(5)	1.245(3)
O(6)-N(5)	1.274(3)	O(7)-N(5)	1.216(2)
O(8)-N(6)	1.261(2)	O(9)-N(6)	1.263(2)
O(10)-N(6)	1.232(2)	O(11)-N(7)	1.260(2)
O(12)-N(7)	1.274(2)	O(13)-N(7)	1.231(2)
N(1)-C(1)	1.335(3)	N(1)-C(5)	1.460(3)
N(1)-C(6)	1.464(3)	N(2)-C(4)	1.330(3)
N(2)-C(7)	1.461(3)	N(2)-C(8)	1.462(3)
N(3)-C(9)	1.333(3)	N(3)-C(14)	1.466(3)
N(3)-C(13)	1.469(3)	N(4)-C(12)	1.329(3)
N(4)-C(16)	1.460(3)	N(4)-C(15)	1.462(3)
C(1)-C(2)	1.510(3)	C(2)-C(3)	1.542(3)
C(3)-C(4)	1.512(3)	C(9)-C(10)	1.511(3)
C(10)-C(11)	1.529(3)	C(11)-C(12)	1.507(3)

O(4)#1-Ce-O(3)	152.89(5)	O(4)#1-Ce-O(1)	79.35(5)
O(3)-Ce-O(1)	79.99(5)	O(4)#1-Ce-O(2)	80.58(6)
O(3)-Ce-O(2)	76.80(5)	O(1)-Ce-O(2)	73.31(5)
O(4)#1-Ce-O(8)	74.38(5)	O(3)-Ce-O(8)	131.93(5)
O(1)-Ce-O(8)	141.44(5)	O(2)-Ce-O(8)	127.91(5)
O(4)#1-Ce-O(6)	114.81(5)	O(3)-Ce-O(6)	77.03(5)
O(1)-Ce-O(6)	149.97(5)	O(2)-Ce-O(6)	82.76(5)
O(8)-Ce-O(6)	68.26(5)	O(4)#1-Ce-O(12)	73.74(5)
O(3)-Ce-O(12)	117.90(5)	O(1)-Ce-O(12)	76.66(5)
O(2)-Ce-O(12)	143.43(5)	O(8)-Ce-O(12)	69.23(5)
O(6)-Ce-O(12)	131.62(5)	O(4)#1-Ce-O(9)	120.15(5)
O(3)-Ce-O(9)	86.90(5)	O(1)-Ce-O(9)	133.77(5)
O(2)-Ce-O(9)	145.60(5)	O(8)-Ce-O(9)	48.50(5)
O(6)-Ce-O(9)	63.97(5)	O(12)-Ce-O(9)	70.93(5)

O(4)#1-Ce-O(11)	118.13(5)	O(3)-Ce-O(11)	70.66(4)
O(1)-Ce-O(11)	71.19(5)	O(2)-Ce-O(11)	135.03(5)
O(8)-Ce-O(11)	97.03(5)	O(6)-Ce-O(11)	117.82(5)
O(12)-Ce-O(11)	47.43(5)	O(9)-Ce-O(11)	62.64(5)
O(4)#1-Ce-O(5)	69.59(5)	O(3)-Ce-O(5)	113.04(5)
O(1)-Ce-O(5)	131.30(5)	O(2)-Ce-O(5)	65.49(5)
O(8)-Ce-O(5)	63.15(5)	O(6)-Ce-O(5)	46.30(5)
O(12)-Ce-O(5)	125.60(5)	O(9)-Ce-O(5)	94.64(5)
O(11)-Ce-O(5)	157.14(5)	C(1)-O(1)-Ce	157.89(14)
C(4)-O(2)-Ce	135.13(14)	C(9)-O(3)-Ce	157.85(14)
C(12)-O(4)-Ce#2	165.9(2)	N(5)-O(5)-Ce	94.20(14)
N(5)-O(6)-Ce	102.70(13)	N(6)-O(8)-Ce	97.97(12)
N(6)-O(9)-Ce	94.96(12)	N(7)-O(11)-Ce	95.46(12)
N(7)-O(12)-Ce	99.87(11)	C(1)-N(1)-C(5)	119.4(2)
C(1)-N(1)-C(6)	124.0(2)	C(5)-N(1)-C(6)	115.8(2)
C(4)-N(2)-C(7)	124.5(2)	C(4)-N(2)-C(8)	120.2(2)
C(7)-N(2)-C(8)	115.2(2)	C(9)-N(3)-C(14)	120.8(2)
C(9)-N(3)-C(13)	123.8(2)	C(14)-N(3)-C(13)	115.3(2)
C(12)-N(4)-C(16)	124.2(2)	C(12)-N(4)-C(15)	120.4(2)
C(16)-N(4)-C(15)	115.4(2)	O(7)-N(5)-O(5)	121.6(2)
O(7)-N(5)-O(6)	121.6(2)	O(5)-N(5)-O(6)	116.8(2)
O(10)-N(6)-O(8)	120.6(2)	O(10)-N(6)-O(9)	121.5(2)
O(8)-N(6)-O(9)	118.0(2)	O(13)-N(7)-O(11)	121.7(2)
O(13)-N(7)-O(12)	121.2(2)	O(11)-N(7)-O(12)	117.1(2)
O(1)-C(1)-N(1)	119.9(2)	O(1)-C(1)-C(2)	120.4(2)
N(1)-C(1)-C(2)	119.7(2)	C(1)-C(2)-C(3)	111.5(2)
C(4)-C(3)-C(2)	114.1(2)	O(2)-C(4)-N(2)	120.4(2)
O(2)-C(4)-C(3)	120.2(2)	N(2)-C(4)-C(3)	119.4(2)
O(3)-C(9)-N(3)	121.7(2)	O(3)-C(9)-C(10)	120.7(2)
N(3)-C(9)-C(10)	117.6(2)	C(9)-C(10)-C(11)	111.5(2)
C(12)-C(11)-C(10)	109.9(2)	O(4)-C(12)-N(4)	121.2(2)
O(4)-C(12)-C(11)	118.2(2)	N(4)-C(12)-C(11)	120.6(2)

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2,-y+1/2,z+1/2 #2 x-1/2,-y+1/2,z-1/2

Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)

- 1.250 (0.018) x + 16.582 (0.003) y - 0.569 (0.016) z = 1.988 (0.008)

*	0.009 (0.002)	N5
*	-0.003 (0.001)	O5
*	-0.003 (0.001)	O6
*	-0.003 (0.001)	O7
	0.002 (0.005)	Ce

Rms deviation of fitted atoms = 0.005

10.036 (0.007) x - 7.431 (0.020) y - 0.171 (0.014) z = 5.642 (0.005)

Angle to previous plane (with approximate esd) = 56.62 (0.12)

*	0.001 (0.002)	N6
*	0.000 (0.001)	O8
*	0.000 (0.001)	O9
*	0.000 (0.001)	O10
	-0.366 (0.004)	Ce

Rms deviation of fitted atoms = 0.000

6.756 (0.011) x + 11.621 (0.013) y + 3.519 (0.014) z = 7.839 (0.007)

Angle to previous plane (with approximate esd) = 73.11 (0.08)

*	-0.004 (0.002)	N7
*	0.001 (0.001)	O11
*	0.001 (0.000)	O12
*	0.001 (0.001)	O13
	-0.179 (0.004)	Ce

Rms deviation of fitted atoms = 0.002