X-ray crystallographic, luminescence and NMR studies of phenacyldiphenylphosphine oxide with the Ln(III) ions Sm, Eu, Gd, Tb and Dy

Supplementary Information

Erin Leach,[a] Justin R. Shady,[a] Adam C. Boyden,[a] Anne-lise Emig,[a] Alyssa T. Henry,[b] Emily K. Connor,[b] Richard J. Staples,[c] Stephanie Schaertel,[a] and Eric J. Werner,[b] Shannon M. Biros[a]*

[a]Department of Chemistry, Grand Valley State University, Allendale, MI 49401, USA;

[b]Department of Chemistry, Biochemistry and Physics, The University of Tampa, 401 W. Kennedy Blvd., Tampa, FL 33606, USA;

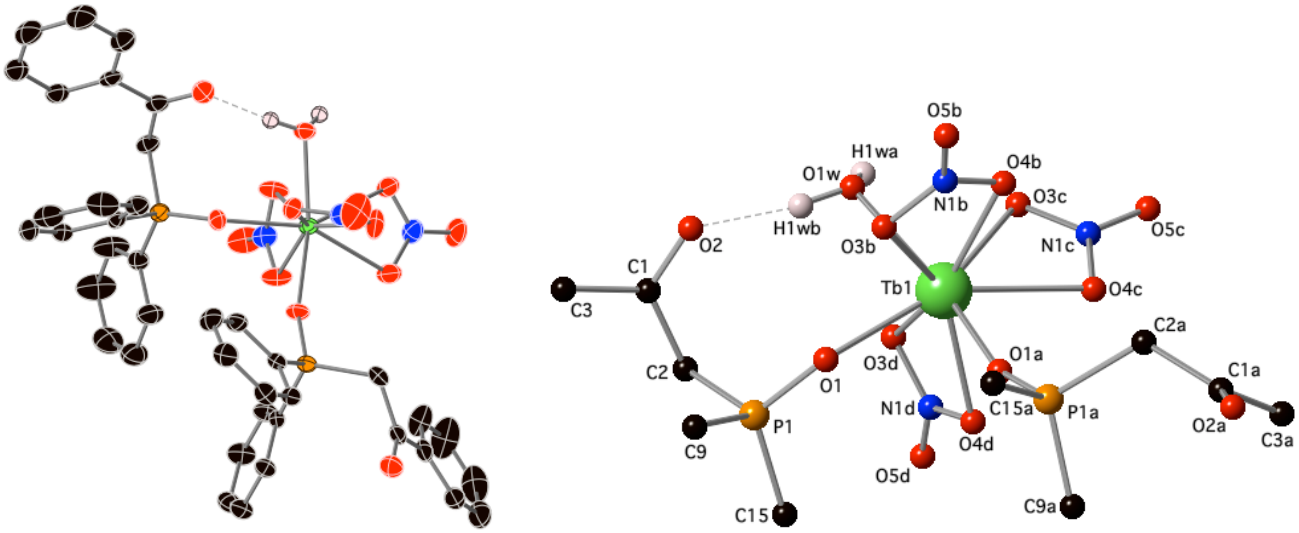
[c]Center for Crystallographic Research, Department of Chemistry, Michigan State University, 578 S. Shaw Lane, East Lansing, MI 48824, USA.

* Corresponding author: Shannon M. Biros, biross@gvsu.edu, +1.616.331.8955

I. X-Ray crystallography details

For all figures in this section thermal ellipsoids are shown at the 50% probability level, and the numbering scheme for all atoms but the pendant phenyl rings are shown with a ball and stick model. Standard CPK colors are used throughout, and all non-polar hydrogen atoms have been omitted for clarity.

A. $Tb(NO_3)_3(4)_2(H_2O)$



Experimental

Single crystals of $C_{40}H_{36}N_3O_{14}P_2Tb$ were grown at 4 °C by slow diffusion of hexane into a solution of the 1:3 $Tb(NO_3)_3$-4 complex in chloroform and used as received. A suitable crystal was selected and mounted using paratone oil on a nylon loop on a Bruker APEX-II CCD diffractometer. The crystal was kept at 173(2) K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimization.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of $Tb(NO_3)_3(4)_2(H_2O)$

Crystal Data for $C_{40}H_{36}N_3O_{14}P_2Tb$ (M =1003.58 g/mol): triclinic, space group P-1 (no. 2), a = 11.2287(12) Å, b = 11.6265(12) Å, c = 18.433(2) Å, α = 72.0460(10)°, β = 75.8340(10)°, γ = 66.6960(10)°, V = 2081.6(4) Å^3, Z = 2, T = 173.15 K, μ(MoKα) = 1.846 mm^{-1}, *Dcalc* = 1.601 g/cm^3, 34436 reflections measured (3.926° ≤ 2Θ ≤ 50.75°), 7587 unique (R_{int} = 0.0518, R_{sigma} = 0.0428) which were used in all calculations. The final R_1 was 0.0293 (I > 2σ(I)) and wR_2 was 0.0654 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.
Details:
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups
 At 1.5 times of:
  All O(H,H) groups
2.a Rotating group:
 O1W(H1WA,H1WB)
2.b Secondary CH2 refined with riding coordinates:
 C2(H2A,H2B), C2A(H2AA,H2AB)

2.c Aromatic/amide H refined with riding coordinates:
C4(H4), C5(H5), C6(H6), C7(H7), C8(H8), C10(H10), C11(H11), C12(H12), C13(H13), C14(H14), C16(H16), C17(H17), C18(H18), C19(H19), C20(H20), C4A(H4A), C5A(H5A), C6A(H6A), C7A(H7A), C8A(H8A), C10A(H10A), C11A(H11A), C12A(H12A), C13A(H13A), C14A(H14A), C16A(H16A), C17A(H17A), C18A(H18A), C19A(H19A), C20A(H20A)

Table 1 Crystal data and structure refinement for $Tb(NO_3)_3(4)_2(H_2O)$

Structure Number	**7**
CCDC Number	1484662
Empirical formula	$C_{40}H_{36}N_3O_{14}P_2Tb$
Formula weight	1003.58
Temperature/K	173.15
Crystal system	triclinic
Space group	P-1
a/Å	11.2287(12)
b/Å	11.6265(12)
c/Å	18.433(2)
α/°	72.0460(10)
β/°	75.8340(10)
γ/°	66.6960(10)
Volume/Å^3	2081.6(4)
Z	2
ϱ_{calc}g/cm^3	1.601
μ/mm^{-1}	1.846
F(000)	1008.0
Crystal size/mm^3	0.286 × 0.102 × 0.095
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.926 to 50.75
Index ranges	$-13 \le h \le 13$, $-13 \le k \le 14$, $-22 \le l \le 22$
Reflections collected	34436
Independent reflections	7587 [R_{int} = 0.0518, R_{sigma} = 0.0428]
Data/restraints/parameters	7587/0/542
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0293, wR_2 = 0.0618
Final R indexes [all data]	R_1 = 0.0371, wR_2 = 0.0654
Largest diff. peak/hole / e Å^{-3}	1.05/-0.41

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **$Tb(NO_3)_3(4)_2(H_2O)$**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Tb1	5173.3(2)	8888.3(2)	6775.7(2)	21.38(6)
P1	5441.8(8)	12003.5(8)	6670.1(5)	21.92(19)
O1	5093(2)	10818(2)	6887.7(12)	26.9(5)
O2	2872(2)	12783(2)	5846.5(15)	39.5(6)
C1	3414(3)	13510(3)	5839.9(19)	28.8(8)
C2	4890(3)	13032(3)	5760.1(19)	28.4(8)
C3	2612(3)	14838(3)	5931.4(18)	28.6(8)

C4	1256(4)	15216(3)	5980(2)	40.2(9)
C5	454(4)	16425(4)	6100(2)	50.7(11)
C6	1003(4)	17247(4)	6170(2)	50.3(11)
C7	2323(4)	16894(4)	6124(2)	42.6(10)
C8	3142(4)	15689(3)	6006.0(19)	33.9(9)
C9	4601(3)	12947(3)	7365.0(17)	22.4(7)
C10	3392(3)	12883(3)	7749.8(19)	32.0(8)
C11	2646(4)	13724(4)	8213(2)	46.0(11)
C12	3093(5)	14620(4)	8285(2)	52.0(12)
C13	4278(5)	14684(3)	7905(2)	47.8(11)
C14	5050(4)	13846(3)	7446(2)	33.6(9)
C15	7158(3)	11661(3)	6605.1(19)	27.5(8)
C16	7894(4)	12224(4)	5999(2)	50.3(11)
C17	9221(4)	11897(5)	6008(3)	61.5(13)
C18	9806(4)	11015(4)	6618(3)	52.0(11)
C19	9076(4)	10468(4)	7232(3)	52.6(12)
C20	7763(4)	10771(4)	7222(2)	44.4(10)
P1A	6134.6(8)	7362.9(8)	8741.3(5)	21.01(19)
O1A	5924(2)	8108(2)	7932.8(12)	27.8(5)
O2A	6792(2)	4484(2)	10067.2(14)	34.8(6)
C1A	6974(3)	4652(3)	9369(2)	25.4(8)
C2A	6011(3)	5796(3)	8896.2(19)	26.3(8)
C3A	8106(3)	3755(3)	8971(2)	29.0(8)
C4A	8524(4)	4072(4)	8193(2)	48.8(11)
C5A	9595(5)	3208(5)	7854(3)	70.1(15)
C6A	10226(4)	2021(5)	8288(3)	65.7(15)
C7A	9816(4)	1688(4)	9055(3)	53.8(12)
C8A	8756(4)	2544(3)	9409(2)	39.8(10)
C9A	7734(3)	7134(3)	8899.2(18)	20.3(7)
C10A	8674(3)	7280(3)	8261(2)	30.7(8)
C11A	9903(3)	7134(4)	8370(2)	36.8(9)
C12A	10202(3)	6845(3)	9101(2)	33.3(9)
C13A	9274(3)	6680(3)	9732(2)	30.9(8)
C14A	8047(3)	6824(3)	9630.8(19)	25.4(8)
C15A	4950(3)	8197(3)	9425.8(18)	22.1(7)
C16A	4308(3)	9516(3)	9162(2)	30.0(8)
C17A	3410(4)	10214(3)	9667(2)	36.6(9)
C18A	3145(4)	9611(4)	10428(2)	37.3(9)
C19A	3786(3)	8301(3)	10693(2)	31.4(8)
C20A	4678(3)	7595(3)	10188.6(18)	25.8(8)
O3B	3146(2)	9727(2)	7640.9(13)	28.5(5)
O4B	3605(3)	7821(2)	7500.5(16)	43.1(7)
O5B	1893(3)	8631(3)	8281.9(19)	65.5(9)
N1B	2848(3)	8725(3)	7822.8(18)	33.9(7)
O3C	5215(3)	7661(2)	5886.7(14)	42.2(7)
O4C	6370(3)	6563(2)	6804.4(14)	41.0(7)
O5C	6313(3)	5628(2)	5958.3(15)	44.7(7)
N1C	5980(3)	6579(3)	6209.1(17)	32.8(7)
O3D	6341(2)	9761(2)	5527.5(13)	35.6(6)
O4D	7522(2)	8619(2)	6429.3(13)	36.6(6)
O5D	8419(3)	9477(3)	5315.1(15)	50.9(8)
N1D	7478(3)	9280(3)	5739.7(17)	32.7(7)

O1W	3528(2)	10208(2)	5990.6(12)	27.7(5)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **$Tb(NO_3)_3(4)_2(H_2O)$**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Tb1	23.97(10)	20.11(9)	18.31(9)	-6.45(6)	-6.43(6)	-2.41(7)
P1	25.1(5)	22.0(4)	17.2(4)	-5.1(3)	-3.0(4)	-6.3(4)
O1	33.0(14)	23.4(12)	27.1(13)	-10.2(10)	-5.3(11)	-8.8(10)
O2	38.1(15)	30.2(14)	51.2(17)	-12.3(12)	-14.9(13)	-5.7(12)
C1	31(2)	30.3(19)	19.6(18)	-3.8(15)	-6.9(15)	-4.3(16)
C2	30(2)	27.4(18)	21.4(18)	-5.8(15)	-4.2(15)	-2.5(15)
C3	31(2)	27.7(18)	18.5(18)	-1.3(14)	-8.4(15)	-1.1(15)
C4	38(2)	33(2)	44(2)	-8.0(18)	-8.5(19)	-5.3(18)
C5	35(2)	44(2)	59(3)	-17(2)	-11(2)	7(2)
C6	56(3)	33(2)	51(3)	-18(2)	-17(2)	7(2)
C7	55(3)	34(2)	39(2)	-7.8(18)	-18(2)	-9(2)
C8	40(2)	31(2)	27(2)	-1.8(16)	-11.0(17)	-9.6(17)
C9	31.1(19)	18.2(16)	16.0(17)	-2.8(13)	-5.7(14)	-6.1(14)
C10	35(2)	34(2)	21.9(19)	-6.1(16)	-4.2(16)	-7.7(17)
C11	41(2)	57(3)	27(2)	-16(2)	1.2(18)	-3(2)
C12	62(3)	46(3)	37(2)	-27(2)	-21(2)	14(2)
C13	73(3)	24(2)	52(3)	-15.2(19)	-36(2)	-3(2)
C14	46(2)	27.4(19)	31(2)	-2.1(16)	-18.9(18)	-11.4(17)
C15	27.7(19)	29.1(19)	25.1(19)	-7.4(15)	-3.8(15)	-8.3(15)
C16	30(2)	73(3)	32(2)	3(2)	-1.3(18)	-15(2)
C17	34(2)	90(4)	43(3)	3(3)	5(2)	-24(2)
C18	27(2)	61(3)	65(3)	-20(2)	-7(2)	-9(2)
C19	42(3)	50(3)	62(3)	8(2)	-27(2)	-17(2)
C20	35(2)	47(2)	47(3)	12(2)	-17.8(19)	-20.7(19)
P1A	21.3(4)	23.2(4)	17.9(4)	-5.3(3)	-5.1(3)	-5.4(4)
O1A	30.0(13)	32.9(13)	17.8(12)	-5.3(10)	-8.5(10)	-5.6(11)
O2A	40.1(15)	38.1(14)	28.3(15)	-7.9(11)	-7.1(12)	-14.4(12)
C1A	28.6(19)	27.2(18)	27(2)	-7.3(15)	-6.0(15)	-15.1(15)
C2A	24.0(18)	31.7(19)	27.3(19)	-13.0(15)	-5.3(15)	-8.5(15)
C3A	28.8(19)	26.1(18)	39(2)	-12.2(16)	-5.5(16)	-13.1(16)
C4A	52(3)	34(2)	51(3)	-15(2)	7(2)	-11(2)
C5A	73(4)	57(3)	68(3)	-32(3)	28(3)	-20(3)
C6A	39(3)	53(3)	109(5)	-48(3)	7(3)	-9(2)
C7A	39(3)	34(2)	93(4)	-24(2)	-24(3)	-2(2)
C8A	34(2)	32(2)	58(3)	-14.9(19)	-20(2)	-5.6(18)
C9A	22.9(17)	18.2(16)	21.8(18)	-4.3(13)	-5.0(14)	-8.3(14)
C10A	30(2)	40(2)	22.3(19)	-4.5(16)	-5.4(15)	-12.5(17)
C11A	26(2)	51(2)	29(2)	-6.4(18)	1.3(16)	-14.4(18)
C12A	25.1(19)	39(2)	39(2)	-11.3(17)	-8.1(17)	-11.0(17)
C13A	32(2)	37(2)	26(2)	-4.8(16)	-7.6(16)	-14.7(17)
C14A	24.8(18)	31.3(19)	21.2(18)	-6.8(15)	-3.1(14)	-10.6(15)
C15A	19.6(17)	27.0(17)	22.0(18)	-7.5(14)	-4.5(14)	-8.2(14)
C16A	36(2)	29.4(19)	23.9(19)	-7.3(15)	-9.7(16)	-6.7(16)
C17A	38(2)	28.0(19)	37(2)	-13.2(17)	-6.2(18)	0.2(17)
C18A	32(2)	45(2)	36(2)	-23.4(19)	-1.0(17)	-6.9(18)
C19A	34(2)	39(2)	24.2(19)	-9.2(16)	0.7(16)	-17.4(17)

C20A	25.3(19)	26.7(18)	25.6(19)	-6.0(15)	-6.6(15)	-7.6(15)
O3B	26.5(13)	25.3(13)	31.1(14)	-8.8(11)	-1.3(11)	-6.5(10)
O4B	44.9(16)	26.0(13)	61.5(19)	-15.9(13)	-2.5(14)	-14.3(12)
O5B	41.6(18)	63(2)	83(2)	-10.5(18)	18.8(17)	-31.0(16)
N1B	31.3(18)	34.5(18)	34.7(18)	-2.2(15)	-4.9(15)	-14.5(15)
O3C	66.9(19)	23.9(13)	34.5(15)	-10.5(11)	-26.5(14)	-0.5(13)
O4C	50.4(17)	30.9(14)	38.0(16)	-13.0(12)	-22.1(13)	2.6(12)
O5C	65.0(19)	28.0(14)	41.3(16)	-18.8(12)	-4.1(14)	-10.2(13)
N1C	41.7(19)	27.4(17)	28.1(17)	-10.4(14)	-0.9(14)	-10.2(14)
O3D	25.7(14)	54.3(16)	21.1(13)	-8.3(12)	-4.8(11)	-7.8(12)
O4D	27.0(14)	42.6(15)	24.8(14)	0.1(12)	-6.7(11)	-0.5(11)
O5D	30.0(15)	71(2)	35.0(16)	-5.6(14)	9.7(13)	-14.1(14)
N1D	29.3(18)	35.3(17)	28.1(18)	-14.0(14)	-0.2(15)	-3.0(14)
O1W	30.7(13)	26.4(12)	23.5(13)	-7.4(10)	-10(1)	-2.5(10)

Table 4 Bond Lengths for **$Tb(NO_3)_3(4)_2(H_2O)$**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Tb1	O1	2.281(2)	C19	C20	1.377(5)
Tb1	O1A	2.273(2)	P1A	O1A	1.497(2)
Tb1	O3B	2.470(2)	P1A	C2A	1.811(3)
Tb1	O4B	2.445(3)	P1A	C9A	1.792(3)
Tb1	N1B	2.877(3)	P1A	C15A	1.793(3)
Tb1	O3C	2.464(2)	O2A	C1A	1.218(4)
Tb1	O4C	2.488(2)	C1A	C2A	1.519(4)
Tb1	N1C	2.909(3)	C1A	C3A	1.486(5)
Tb1	O3D	2.485(2)	C3A	C4A	1.377(5)
Tb1	O4D	2.472(2)	C3A	C8A	1.393(5)
Tb1	N1D	2.921(3)	C4A	C5A	1.382(6)
Tb1	O1W	2.358(2)	C5A	C6A	1.367(7)
P1	O1	1.491(2)	C6A	C7A	1.359(7)
P1	C2	1.820(3)	C7A	C8A	1.384(5)
P1	C9	1.786(3)	C9A	C10A	1.392(4)
P1	C15	1.788(3)	C9A	C14A	1.380(4)
O2	C1	1.217(4)	C10A	C11A	1.379(5)
C1	C2	1.511(5)	C11A	C12A	1.376(5)
C1	C3	1.486(5)	C12A	C13A	1.380(5)
C3	C4	1.396(5)	C13A	C14A	1.373(5)
C3	C8	1.393(5)	C15A	C16A	1.395(4)
C4	C5	1.388(5)	C15A	C20A	1.383(4)
C5	C6	1.375(6)	C16A	C17A	1.378(5)
C6	C7	1.360(6)	C17A	C18A	1.379(5)
C7	C8	1.389(5)	C18A	C19A	1.386(5)
C9	C10	1.389(5)	C19A	C20A	1.380(4)
C9	C14	1.386(4)	O3B	N1B	1.262(3)
C10	C11	1.380(5)	O4B	N1B	1.269(4)
C11	C12	1.373(6)	O5B	N1B	1.213(4)
C12	C13	1.363(6)	O3C	N1C	1.268(4)
C13	C14	1.377(5)	O4C	N1C	1.270(4)
C15	C16	1.373(5)	O5C	N1C	1.216(3)
C15	C20	1.386(5)	O3D	N1D	1.281(4)

C16	C17	1.388(5)	O4D	N1D	1.268(4)	
C17	C18	1.365(6)	O5D	N1D	1.207(4)	
C18	C19	1.368(6)				

Table 5 Bond Angles for **$Tb(NO_3)_3(4)_2(H_2O)$**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Tb1	O3B	72.63(8)	C5	C4	C3	120.1(4)
O1	Tb1	O4B	124.28(8)	C6	C5	C4	119.7(4)
O1	Tb1	N1B	98.36(8)	C7	C6	C5	121.0(4)
O1	Tb1	O3C	145.58(8)	C6	C7	C8	120.3(4)
O1	Tb1	O4C	150.88(8)	C7	C8	C3	119.9(4)
O1	Tb1	N1C	160.31(8)	C10	C9	P1	118.1(3)
O1	Tb1	O3D	75.70(8)	C14	C9	P1	121.1(3)
O1	Tb1	O4D	80.14(8)	C14	C9	C10	120.2(3)
O1	Tb1	N1D	76.49(8)	C11	C10	C9	119.2(4)
O1	Tb1	O1W	83.04(8)	C12	C11	C10	120.2(4)
O1A	Tb1	O1	84.21(8)	C13	C12	C11	120.5(4)
O1A	Tb1	O3B	78.95(8)	C12	C13	C14	120.5(4)
O1A	Tb1	O4B	80.94(9)	C13	C14	C9	119.3(4)
O1A	Tb1	N1B	78.26(8)	C16	C15	P1	124.7(3)
O1A	Tb1	O3C	128.00(8)	C16	C15	C20	118.8(3)
O1A	Tb1	O4C	77.41(8)	C20	C15	P1	116.5(3)
O1A	Tb1	N1C	102.81(8)	C15	C16	C17	120.1(4)
O1A	Tb1	O3D	126.17(8)	C18	C17	C16	120.4(4)
O1A	Tb1	O4D	76.47(8)	C17	C18	C19	120.0(4)
O1A	Tb1	N1D	101.20(8)	C18	C19	C20	120.0(4)
O1A	Tb1	O1W	151.55(8)	C19	C20	C15	120.7(4)
O3B	Tb1	N1B	25.90(7)	O1A	P1A	C2A	109.42(14)
O3B	Tb1	O4C	124.44(8)	O1A	P1A	C9A	110.03(14)
O3B	Tb1	N1C	126.52(8)	O1A	P1A	C15A	111.15(14)
O3B	Tb1	O3D	136.75(8)	C9A	P1A	C2A	108.58(14)
O3B	Tb1	O4D	144.81(8)	C9A	P1A	C15A	108.25(15)
O3B	Tb1	N1D	148.95(8)	C15A	P1A	C2A	109.35(15)
O4B	Tb1	O3B	51.90(8)	P1A	O1A	Tb1	161.87(15)
O4B	Tb1	N1B	26.00(8)	O2A	C1A	C2A	119.1(3)
O4B	Tb1	O3C	78.23(9)	O2A	C1A	C3A	121.5(3)
O4B	Tb1	O4C	75.08(9)	C3A	C1A	C2A	119.3(3)
O4B	Tb1	N1C	75.28(8)	C1A	C2A	P1A	117.1(2)
O4B	Tb1	O3D	150.17(9)	C4A	C3A	C1A	122.6(3)
O4B	Tb1	O4D	144.69(8)	C4A	C3A	C8A	119.3(3)
O4B	Tb1	N1D	159.15(8)	C8A	C3A	C1A	118.1(3)
N1B	Tb1	N1C	101.07(9)	C3A	C4A	C5A	120.2(4)
N1B	Tb1	N1D	174.85(8)	C6A	C5A	C4A	120.0(5)
O3C	Tb1	O3B	120.30(9)	C7A	C6A	C5A	120.4(4)
O3C	Tb1	N1B	99.98(9)	C6A	C7A	C8A	120.6(4)
O3C	Tb1	O4C	51.35(8)	C7A	C8A	C3A	119.4(4)
O3C	Tb1	N1C	25.62(8)	C10A	C9A	P1A	118.4(2)
O3C	Tb1	O3D	74.75(9)	C14A	C9A	P1A	121.8(2)
O3C	Tb1	O4D	94.74(9)	C14A	C9A	C10A	119.8(3)
O3C	Tb1	N1D	84.43(9)	C11A	C10A	C9A	119.3(3)

O4C	Tb1	N1B	99.74(9)	C12A	C11A	C10A	120.6(3)
O4C	Tb1	N1C	25.72(8)	C11A	C12A	C13A	119.9(3)
O4C	Tb1	N1D	85.08(9)	C14A	C13A	C12A	120.0(3)
N1C	Tb1	N1D	84.06(8)	C13A	C14A	C9A	120.4(3)
O3D	Tb1	N1B	153.04(8)	C16A	C15A	P1A	117.1(2)
O3D	Tb1	O4C	97.17(8)	C20A	C15A	P1A	122.9(2)
O3D	Tb1	N1C	85.47(8)	C20A	C15A	C16A	120.0(3)
O3D	Tb1	N1D	25.85(7)	C17A	C16A	C15A	119.7(3)
O4D	Tb1	N1B	154.71(8)	C16A	C17A	C18A	120.2(3)
O4D	Tb1	O4C	73.76(9)	C17A	C18A	C19A	120.3(3)
O4D	Tb1	N1C	83.64(8)	C20A	C19A	C18A	119.8(3)
O4D	Tb1	O3D	51.35(7)	C19A	C20A	C15A	120.1(3)
O4D	Tb1	N1D	25.50(7)	N1B	O3B	Tb1	95.36(18)
O1W	Tb1	O3B	72.99(8)	N1B	O4B	Tb1	96.36(19)
O1W	Tb1	O4B	85.43(8)	O3B	N1B	Tb1	58.74(16)
O1W	Tb1	N1B	78.58(8)	O3B	N1B	O4B	116.3(3)
O1W	Tb1	O3C	72.44(8)	O4B	N1B	Tb1	57.64(16)
O1W	Tb1	O4C	122.86(8)	O5B	N1B	Tb1	177.9(3)
O1W	Tb1	N1C	97.65(8)	O5B	N1B	O3B	121.8(3)
O1W	Tb1	O3D	74.63(8)	O5B	N1B	O4B	121.9(3)
O1W	Tb1	O4D	125.79(8)	N1C	O3C	Tb1	97.18(18)
O1W	Tb1	N1D	100.38(8)	N1C	O4C	Tb1	95.99(18)
O1	P1	C2	110.85(15)	O3C	N1C	Tb1	57.19(15)
O1	P1	C9	109.91(14)	O3C	N1C	O4C	115.5(3)
O1	P1	C15	112.98(14)	O4C	N1C	Tb1	58.29(15)
C9	P1	C2	105.51(15)	O5C	N1C	Tb1	178.8(2)
C9	P1	C15	108.07(15)	O5C	N1C	O3C	121.7(3)
C15	P1	C2	109.21(16)	O5C	N1C	O4C	122.8(3)
P1	O1	Tb1	156.21(14)	N1D	O3D	Tb1	96.40(19)
O2	C1	C2	119.3(3)	N1D	O4D	Tb1	97.45(19)
O2	C1	C3	119.5(3)	O3D	N1D	Tb1	57.75(16)
C3	C1	C2	121.2(3)	O4D	N1D	Tb1	57.05(16)
C1	C2	P1	110.2(2)	O4D	N1D	O3D	114.8(3)
C4	C3	C1	117.6(3)	O5D	N1D	Tb1	178.1(2)
C8	C3	C1	123.3(3)	O5D	N1D	O3D	121.9(3)
C8	C3	C4	119.0(3)	O5D	N1D	O4D	123.3(3)

Table 6 Hydrogen Bonds for **$Tb(NO_3)_3(4)_2(H_2O)$**

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1W	H1WA	O3D[1]	0.89	1.91	2.755(3)	158.1
O1W	H1WB	O2	0.89	1.84	2.727(3)	172.0

[1]1-X,2-Y,1-Z

Table 7 Torsion Angles for **$Tb(NO_3)_3(4)_2(H_2O)$**

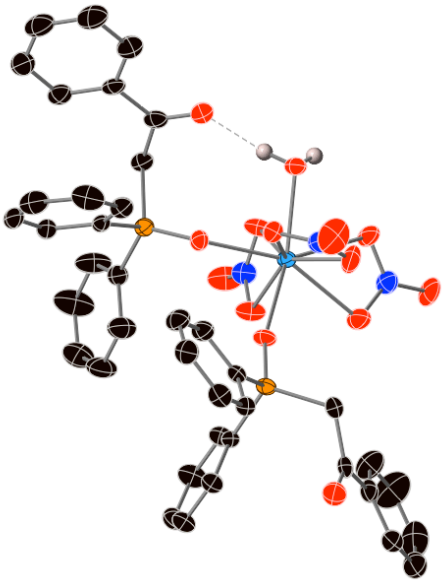
A	B	C	D	Angle/°	A	B	C	D	Angle/°
Tb1	O3B	N1B	O4B	-2.1(3)	C15	C16	C17	C18	0.0(7)
Tb1	O3B	N1B	O5B	177.7(3)	C16	C15	C20	C19	0.8(6)
Tb1	O4B	N1B	O3B	2.2(3)	C16	C17	C18	C19	-1.4(7)
Tb1	O4B	N1B	O5B	-177.6(3)	C17	C18	C19	C20	2.5(7)
Tb1	O3C	N1C	O4C	0.4(3)	C18	C19	C20	C15	-2.2(7)

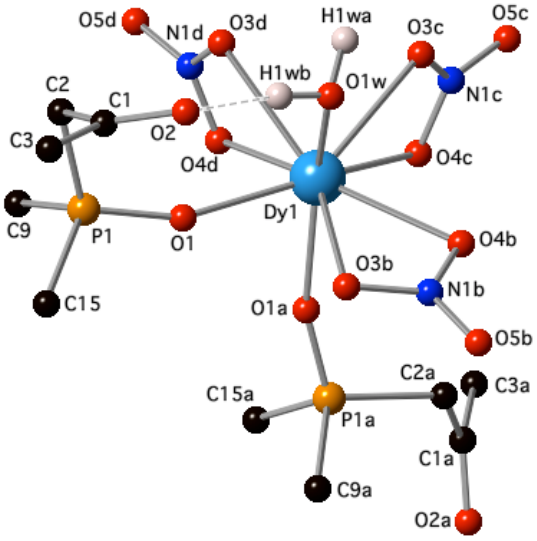
Tb1	O3C	N1C	O5C	-179.3(3)	C20	C15	C16	C17	0.3(6)
Tb1	O4C	N1C	O3C	-0.4(3)	P1A	C9A	C10A	C11A	178.7(3)
Tb1	O4C	N1C	O5C	179.3(3)	P1A	C9A	C14A	C13A	-178.7(3)
Tb1	O3D	N1D	O4D	0.4(3)	P1A	C15A	C16A	C17A	-178.5(3)
Tb1	O3D	N1D	O5D	-177.8(3)	P1A	C15A	C20A	C19A	177.9(3)
Tb1	O4D	N1D	O3D	-0.4(3)	O1A	P1A	C2A	C1A	140.3(2)
Tb1	O4D	N1D	O5D	177.8(3)	O1A	P1A	C9A	C10A	-19.0(3)
P1	C9	C10	C11	-171.5(3)	O1A	P1A	C9A	C14A	160.8(2)
P1	C9	C14	C13	170.5(3)	O1A	P1A	C15A	C16A	-19.8(3)
P1	C15	C16	C17	179.5(3)	O1A	P1A	C15A	C20A	161.4(3)
P1	C15	C20	C19	-178.4(3)	O2A	C1A	C2A	P1A	77.3(4)
O1	P1	C2	C1	64.0(3)	O2A	C1A	C3A	C4A	-163.6(4)
O1	P1	C9	C10	-29.7(3)	O2A	C1A	C3A	C8A	16.8(5)
O1	P1	C9	C14	158.8(3)	C1A	C3A	C4A	C5A	179.1(4)
O1	P1	C15	C16	131.6(3)	C1A	C3A	C8A	C7A	-179.9(3)
O1	P1	C15	C20	-49.2(3)	C2A	P1A	O1A	Tb1	33.6(5)
O2	C1	C2	P1	-76.6(4)	C2A	P1A	C9A	C10A	100.7(3)
O2	C1	C3	C4	-3.4(5)	C2A	P1A	C9A	C14A	-79.5(3)
O2	C1	C3	C8	173.5(3)	C2A	P1A	C15A	C16A	-140.7(3)
C1	C3	C4	C5	177.2(3)	C2A	P1A	C15A	C20A	40.4(3)
C1	C3	C8	C7	-177.1(3)	C2A	C1A	C3A	C4A	17.2(5)
C2	P1	O1	Tb1	66.3(4)	C2A	C1A	C3A	C8A	-162.4(3)
C2	P1	C9	C10	89.8(3)	C3A	C1A	C2A	P1A	-103.5(3)
C2	P1	C9	C14	-81.6(3)	C3A	C4A	C5A	C6A	1.5(7)
C2	P1	C15	C16	7.7(4)	C4A	C3A	C8A	C7A	0.5(5)
C2	P1	C15	C20	-173.1(3)	C4A	C5A	C6A	C7A	-0.7(8)
C2	C1	C3	C4	178.3(3)	C5A	C6A	C7A	C8A	-0.2(7)
C2	C1	C3	C8	-4.8(5)	C6A	C7A	C8A	C3A	0.3(6)
C3	C1	C2	P1	101.7(3)	C8A	C3A	C4A	C5A	-1.4(6)
C3	C4	C5	C6	0.0(6)	C9A	P1A	O1A	Tb1	152.8(4)
C4	C3	C8	C7	-0.3(5)	C9A	P1A	C2A	C1A	20.1(3)
C4	C5	C6	C7	-0.1(7)	C9A	P1A	C15A	C16A	101.2(3)
C5	C6	C7	C8	-0.1(6)	C9A	P1A	C15A	C20A	-77.7(3)
C6	C7	C8	C3	0.2(6)	C9A	C10A	C11A	C12A	0.1(5)
C8	C3	C4	C5	0.1(5)	C10A	C9A	C14A	C13A	1.1(5)
C9	P1	O1	Tb1	-177.4(3)	C10A	C11A	C12A	C13A	1.1(6)
C9	P1	C2	C1	-55.0(3)	C11A	C12A	C13A	C14A	-1.1(5)
C9	P1	C15	C16	-106.6(3)	C12A	C13A	C14A	C9A	0.0(5)
C9	P1	C15	C20	72.6(3)	C14A	C9A	C10A	C11A	-1.1(5)
C9	C10	C11	C12	0.5(5)	C15A	P1A	O1A	Tb1	-87.3(5)
C10	C9	C14	C13	-0.7(5)	C15A	P1A	C2A	C1A	-97.8(3)
C10	C11	C12	C13	-0.3(6)	C15A	P1A	C9A	C10A	-140.7(3)
C11	C12	C13	C14	-0.5(6)	C15A	P1A	C9A	C14A	39.1(3)
C12	C13	C14	C9	1.0(5)	C15A	C16A	C17A	C18A	-0.2(5)
C14	C9	C10	C11	0.0(5)	C16A	C15A	C20A	C19A	-1.0(5)
C15	P1	O1	Tb1	-56.6(4)	C16A	C17A	C18A	C19A	0.5(6)
C15	P1	C2	C1	-170.9(2)	C17A	C18A	C19A	C20A	-1.0(5)
C15	P1	C9	C10	-153.4(3)	C18A	C19A	C20A	C15A	1.3(5)
C15	P1	C9	C14	35.1(3)	C20A	C15A	C16A	C17A	0.4(5)

Table 8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **Tb(NO$_3$)$_3$(4)$_2$(H$_2$O)**

Atom	*x*	*y*	*z*	U(eq)
H2A	5195	13776	5604	34
H2B	5271	12541	5355	34
H4	881	14645	5932	48
H5	-469	16683	6134	61
H6	452	18074	6251	60
H7	2685	17475	6173	51
H8	4063	15444	5976	41
H10	3082	12267	7695	38
H11	1821	13685	8482	55
H12	2572	15199	8603	62
H13	4574	15312	7957	57
H14	5882	13885	7188	40
H16	7494	12839	5573	60
H17	9726	12290	5587	74
H18	10719	10780	6615	62
H19	9474	9880	7666	63
H20	7267	10366	7642	53
H2AA	5114	5842	9152	32
H2AB	6116	5625	8386	32
H4A	8075	4888	7888	59
H5A	9893	3438	7319	84
H6A	10956	1426	8052	79
H7A	10260	859	9351	65
H8A	8475	2309	9946	48
H10A	8471	7479	7756	37
H11A	10548	7233	7937	44
H12A	11046	6761	9171	40
H13A	9484	6466	10237	37
H14A	7411	6710	10067	30
H16A	4488	9931	8638	36
H17A	2972	11113	9490	44
H18A	2519	10096	10772	45
H19A	3612	7892	11219	38
H20A	5106	6694	10366	31
H1WA	3758	10040	5525	42
H1WB	3394	11040	5932	42

B. $Dy(NO_3)_3(4)_2(H_2O)$





Experimental

Single crystals of $C_{40}H_{36}DyN_3O_{14}P_2$ were grown at 4 °C by slow diffusion of hexane into a solution of the 1:3 $Dy(NO_3)_3$-4 complex in chloroform and used as received. A suitable crystal was selected and mounted using paratone oil on a nylon loop on a Bruker APEX-II CCD diffractometer. The crystal was kept at 173(2) K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimization.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of $Dy(NO_3)_3(4)_2(H_2O)$

Crystal Data for $C_{40}H_{36}DyN_3O_{14}P_2$ (M =1007.16 g/mol): triclinic, space group P-1 (no. 2), a = 11.2313(7) Å, b = 11.6143(7) Å, c = 18.4094(11) Å, α = 72.0480(10)°, β = 75.8590(10)°, γ = 66.6400(10)°, V = 2076.6(2) Å^3, Z = 2, T = 173.15 K, μ(MoKα) = 1.947 mm^{-1}, *Dcalc* = 1.611 g/cm^3, 29641 reflections measured (3.932° ≤ 2Θ ≤ 51.42°), 7902 unique (R_{int} = 0.0512, R_{sigma} = 0.0508) which were used in all calculations. The final R_1 was 0.0321 (I > 2σ(I)) and wR_2 was 0.0702 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups
 At 1.5 times of:
  All O(H,H) groups
2.a Rotating group:
 O1W(H1WA,H1WB)
2.b Secondary CH2 refined with riding coordinates:
 C2(H2A,H2B), C2A(H2AA,H2AB)
2.c Aromatic/amide H refined with riding coordinates:
 C4(H4), C5(H5), C6(H6), C7(H7), C8(H8), C10(H10), C11(H11), C12(H12),
 C13(H13), C14(H14), C16(H16), C17(H17), C18(H18), C19(H19), C20(H20), C4A(H4A),
  C5A(H5A), C6A(H6A), C7A(H7A), C8A(H8A), C10A(H10A), C11A(H11A), C12A(H12A),
 C13A(H13A), C14A(H14A), C16A(H16A), C17A(H17A), C18A(H18A), C19A(H19A),
 C20A(H20A)

Table 1 Crystal data and structure refinement for $Dy(NO_3)_3(4)_2(H_2O)$

Structure number	**8**
CCDC Number	1484660
Empirical formula	$C_{40}H_{36}DyN_3O_{14}P_2$
Formula weight	1007.16
Temperature/K	173(2)
Crystal system	triclinic
Space group	P-1
a/Å	11.2313(7)
b/Å	11.6143(7)
c/Å	18.4094(11)
α/°	72.0480(10)
β/°	75.8590(10)
γ/°	66.6400(10)
Volume/Å^3	2076.6(2)
Z	2
ϱ_{calc}g/cm^3	1.611
μ/mm^{-1}	1.947
F(000)	1010.0
Crystal size/mm^3	0.245 × 0.151 × 0.086
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.932 to 51.42
Index ranges	-13 ≤ h ≤ 13, -14 ≤ k ≤ 14, -22 ≤ l ≤ 22
Reflections collected	29641
Independent reflections	7902 [R_{int} = 0.0512, R_{sigma} = 0.0508]
Data/restraints/parameters	7902/0/542
Goodness-of-fit on F^2	1.017
Final R indexes [I>=2σ (I)]	R_1 = 0.0321, wR_2 = 0.0656
Final R indexes [all data]	R_1 = 0.0435, wR_2 = 0.0702
Largest diff. peak/hole / e Å^{-3}	0.69/-0.39

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $Dy(NO_3)_3(4)_2(H_2O)$. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Dy1	5177.2(2)	8885.7(2)	6775.1(2)	21.72(6)
P1	5440.7(9)	11991.6(9)	6671.7(5)	22.8(2)
O1	5093(2)	10802(2)	6891.5(13)	27.1(6)
O2	2870(3)	12772(3)	5851.5(16)	39.4(7)
C1	3411(4)	13502(4)	5844.3(19)	31.2(9)
C2	4886(4)	13018(3)	5766.8(19)	28.7(9)
C3	2619(4)	14836(4)	5931.7(19)	30.0(9)
C4	1262(4)	15216(4)	5979(2)	41.6(10)
C5	470(5)	16418(4)	6096(3)	51.7(12)
C6	999(5)	17246(4)	6167(3)	53.3(13)
C7	2337(5)	16891(4)	6120(2)	46.7(11)
C8	3147(4)	15683(4)	6003(2)	35.3(10)
C9	7161(4)	11645(3)	6606(2)	28.7(9)
C10	7900(4)	12214(5)	6000(2)	50.3(12)
C11	9218(4)	11886(5)	6006(3)	64.4(15)
C12	9812(4)	10999(5)	6615(3)	52.8(12)

C13	9082(4)	10457(4)	7225(3)	56.5(13)
C14	7766(4)	10762(4)	7222(2)	46.9(11)
C15	4600(3)	12932(3)	7364.7(18)	23.4(8)
C16	3392(4)	12876(4)	7757.2(19)	31.2(9)
C17	2651(4)	13723(4)	8214(2)	47.4(12)
C18	3095(5)	14622(4)	8281(3)	54.2(14)
C19	4279(5)	14674(4)	7906(2)	47.6(12)
C20	5055(4)	13833(3)	7444(2)	34.6(9)
P1A	6136.3(9)	7361.4(9)	8737.0(5)	22.4(2)
O1A	5926(2)	8102(2)	7929.1(12)	28.6(6)
O2A	6795(3)	4484(3)	10065.9(14)	38.6(7)
C1A	6979(4)	4648(3)	9367(2)	25.8(8)
C2A	6009(4)	5792(3)	8898(2)	29.0(9)
C3A	8109(4)	3754(4)	8972(2)	31.5(9)
C4A	8517(5)	4072(4)	8190(3)	51.6(12)
C5A	9602(6)	3199(5)	7853(3)	74.2(17)
C6A	10235(5)	2004(5)	8296(4)	69.6(16)
C7A	9826(5)	1675(4)	9067(3)	58.8(14)
C8A	8757(4)	2545(4)	9410(3)	43.4(11)
C9A	4951(3)	8197(3)	9419.5(19)	23.8(8)
C10A	4675(3)	7600(3)	10188.8(19)	27.2(8)
C11A	3787(4)	8311(4)	10691(2)	33.8(9)
C12A	3140(4)	9617(4)	10429(2)	38.8(10)
C13A	3414(4)	10212(4)	9666(2)	38.7(10)
C14A	4313(4)	9511(4)	9161(2)	32.3(9)
C15A	7730(3)	7132(3)	8891.7(19)	22.8(8)
C16A	8047(4)	6820(3)	9628(2)	28.1(9)
C17A	9275(4)	6682(4)	9724(2)	34.1(9)
C18A	10194(4)	6841(4)	9097(2)	34.3(9)
C19A	9907(4)	7123(4)	8363(2)	39.8(10)
C20A	8677(4)	7264(4)	8256(2)	33.1(9)
O3B	3164(2)	9713(2)	7636.9(13)	28.8(6)
O4B	3623(3)	7816(3)	7485.8(17)	43.6(7)
O5B	1900(3)	8625(3)	8265(2)	67.2(10)
N1B	2861(3)	8717(3)	7811.8(19)	35.8(8)
O3C	5221(3)	7675(2)	5888.3(15)	42.3(7)
O4C	6368(3)	6565(2)	6805.2(15)	42.7(7)
O5C	6319(3)	5634(2)	5957.4(15)	45.3(8)
N1C	5983(3)	6594(3)	6204.2(18)	33.9(8)
O3D	6332(2)	9759(3)	5527.9(13)	36.2(7)
O4D	7515(2)	8607(3)	6426.3(14)	37.9(7)
O5D	8411(3)	9469(3)	5313.4(16)	51.1(8)
N1D	7472(3)	9277(3)	5735.8(18)	33.5(8)
O1W	3538(2)	10195(2)	5994.2(13)	28.5(6)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $Dy(NO_3)_3(4)_2(H_2O)$. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Dy1	24.94(11)	20.41(10)	18.38(9)	-6.59(6)	-6.59(7)	-2.87(7)
P1	25.6(5)	22.3(5)	19.3(4)	-5.2(4)	-3.7(4)	-6.5(4)
O1	31.6(15)	24.5(13)	26.6(13)	-9.3(11)	-4.1(11)	-8.9(11)

O2	35.0(17)	30.6(16)	51.6(18)	-10.2(13)	-15.3(13)	-4.8(13)
C1	34(2)	34(2)	19.7(18)	-3.8(16)	-8.6(16)	-5.8(19)
C2	33(2)	27(2)	20.6(18)	-6.6(15)	-3.8(16)	-4.0(17)
C3	31(2)	30(2)	20.1(18)	-0.2(15)	-8.1(16)	-3.5(18)
C4	36(3)	37(2)	46(2)	-9(2)	-7(2)	-6(2)
C5	38(3)	43(3)	60(3)	-16(2)	-8(2)	5(2)
C6	62(3)	36(3)	49(3)	-16(2)	-19(2)	8(2)
C7	60(3)	37(3)	45(3)	-12(2)	-20(2)	-9(2)
C8	46(3)	32(2)	23.8(19)	-3.6(17)	-9.4(18)	-8(2)
C9	30(2)	29(2)	27.1(19)	-8.5(16)	-4.4(16)	-7.9(17)
C10	34(3)	70(3)	30(2)	6(2)	-0.9(19)	-15(2)
C11	30(3)	106(4)	43(3)	-2(3)	6(2)	-28(3)
C12	24(2)	69(3)	61(3)	-19(3)	-6(2)	-9(2)
C13	42(3)	52(3)	67(3)	11(2)	-31(3)	-13(2)
C14	40(3)	49(3)	48(3)	9(2)	-14(2)	-21(2)
C15	30(2)	19.9(19)	19.2(17)	-2.7(14)	-6.4(15)	-7.5(16)
C16	38(2)	32(2)	20.7(18)	-6.0(16)	-2.6(17)	-9.4(18)
C17	38(3)	61(3)	29(2)	-18(2)	2.3(19)	-1(2)
C18	68(4)	45(3)	40(3)	-30(2)	-22(2)	13(3)
C19	75(4)	24(2)	49(3)	-13(2)	-37(3)	-3(2)
C20	47(3)	27(2)	34(2)	-3.3(17)	-17.4(19)	-12.5(19)
P1A	23.1(5)	25.1(5)	18.3(4)	-4.9(4)	-6.1(4)	-5.8(4)
O1A	30.5(15)	33.2(15)	19.0(12)	-5.0(11)	-8.9(11)	-5.5(12)
O2A	46.2(18)	40.3(17)	30.2(15)	-6.9(12)	-6.3(13)	-16.5(14)
C1A	29(2)	22.1(19)	33(2)	-8.1(16)	-6.1(17)	-13.4(17)
C2A	31(2)	30(2)	31(2)	-12.0(16)	-6.7(17)	-10.3(18)
C3A	26(2)	27(2)	47(2)	-15.9(18)	-4.2(18)	-10.7(18)
C4A	55(3)	38(3)	54(3)	-18(2)	7(2)	-12(2)
C5A	80(4)	59(4)	70(4)	-32(3)	24(3)	-17(3)
C6A	41(3)	55(4)	116(5)	-50(4)	6(3)	-8(3)
C7A	52(3)	35(3)	98(4)	-28(3)	-28(3)	-5(2)
C8A	44(3)	34(2)	60(3)	-15(2)	-20(2)	-12(2)
C9A	25(2)	28(2)	21.3(18)	-6.8(15)	-5.7(15)	-9.3(16)
C10A	27(2)	26(2)	28.5(19)	-6.3(16)	-6.0(16)	-8.2(17)
C11A	37(2)	43(2)	23.6(19)	-9.6(18)	2.2(17)	-18(2)
C12A	36(3)	44(3)	38(2)	-23(2)	-1.3(19)	-8(2)
C13A	41(3)	30(2)	40(2)	-12.0(18)	-10.3(19)	-0.7(19)
C14A	37(2)	32(2)	25.5(19)	-6.9(17)	-7.0(17)	-8.1(19)
C15A	25(2)	20.8(19)	22.8(18)	-3.5(14)	-7.4(15)	-6.8(16)
C16A	27(2)	34(2)	23.4(18)	-7.3(16)	-2.3(16)	-10.8(18)
C17A	36(2)	41(2)	29(2)	-7.3(18)	-10.6(18)	-14(2)
C18A	27(2)	38(2)	42(2)	-11.7(19)	-6.4(18)	-12.5(19)
C19A	28(2)	59(3)	30(2)	-8(2)	1.9(17)	-18(2)
C20A	32(2)	40(2)	27(2)	-7.3(17)	-7.4(17)	-10.9(19)
O3B	27.8(15)	28.0(14)	29.4(13)	-7.6(11)	-0.9(11)	-9.9(12)
O4B	45.0(19)	26.2(15)	62.4(19)	-13.5(14)	-4.5(15)	-14.9(14)
O5B	41(2)	67(2)	85(3)	-11.6(19)	19.8(18)	-32.4(18)
N1B	29(2)	36(2)	41(2)	-0.9(16)	-7.1(16)	-15.1(17)
O3C	65(2)	22.4(15)	38.2(15)	-11.8(12)	-24.3(14)	0.1(14)
O4C	54.2(19)	31.1(16)	41.0(16)	-13.2(13)	-20.5(14)	-1.3(14)
O5C	69(2)	26.7(16)	41.3(16)	-20.5(13)	-4.1(15)	-10.2(15)
N1C	40(2)	30.0(19)	31.0(18)	-11.6(15)	-2.3(15)	-9.5(16)

O3D	25.2(15)	54.6(18)	22.8(13)	-8.1(12)	-6.4(11)	-6.7(13)
O4D	28.8(16)	44.5(17)	25.8(14)	-0.2(12)	-5.1(11)	-3.1(13)
O5D	29.9(17)	70(2)	35.6(16)	-4.4(15)	7.8(14)	-12.9(16)
N1D	32(2)	35.7(19)	27.6(18)	-14.2(15)	0.3(16)	-3.6(16)
O1W	31.2(15)	26.1(14)	25.5(13)	-8.0(11)	-10.0(11)	-2.2(12)

Table 4 Bond Lengths for GVS414a.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Dy1	O1	2.264(2)	C19	C20	1.384(6)
Dy1	O1A	2.263(2)	P1A	O1A	1.493(2)
Dy1	O3B	2.453(2)	P1A	C2A	1.812(4)
Dy1	O4B	2.429(3)	P1A	C9A	1.789(3)
Dy1	N1B	2.863(3)	P1A	C15A	1.784(4)
Dy1	O3C	2.443(2)	O2A	C1A	1.219(4)
Dy1	O4C	2.478(3)	C1A	C2A	1.518(5)
Dy1	N1C	2.891(3)	C1A	C3A	1.478(5)
Dy1	O3D	2.477(2)	C3A	C4A	1.380(6)
Dy1	O4D	2.458(3)	C3A	C8A	1.390(5)
Dy1	N1D	2.915(3)	C4A	C5A	1.391(6)
Dy1	O1W	2.344(2)	C5A	C6A	1.379(7)
P1	O1	1.494(2)	C6A	C7A	1.363(7)
P1	C2	1.810(3)	C7A	C8A	1.385(6)
P1	C9	1.791(4)	C9A	C10A	1.390(5)
P1	C15	1.779(3)	C9A	C14A	1.386(5)
O2	C1	1.219(4)	C10A	C11A	1.378(5)
C1	C2	1.509(5)	C11A	C12A	1.382(5)
C1	C3	1.486(5)	C12A	C13A	1.379(5)
C3	C4	1.396(5)	C13A	C14A	1.380(5)
C3	C8	1.385(5)	C15A	C16A	1.388(5)
C4	C5	1.376(6)	C15A	C20A	1.390(5)
C5	C6	1.366(6)	C16A	C17A	1.373(5)
C6	C7	1.379(6)	C17A	C18A	1.368(5)
C7	C8	1.386(5)	C18A	C19A	1.375(5)
C9	C10	1.378(5)	C19A	C20A	1.382(5)
C9	C14	1.380(5)	O3B	N1B	1.260(4)
C10	C11	1.377(6)	O4B	N1B	1.270(4)
C11	C12	1.368(6)	O5B	N1B	1.212(4)
C12	C13	1.362(6)	O3C	N1C	1.260(4)
C13	C14	1.378(6)	O4C	N1C	1.270(4)
C15	C16	1.389(5)	O5C	N1C	1.219(4)
C15	C20	1.390(5)	O3D	N1D	1.280(4)
C16	C17	1.373(5)	O4D	N1D	1.271(4)
C17	C18	1.370(6)	O5D	N1D	1.202(4)
C18	C19	1.355(7)			

Table 5 Bond Angles for $Dy(NO_3)_3(4)_2(H_2O)$.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O1	Dy1	O3B	72.62(8)	C5	C4	C3	119.9(4)

O1	Dy1	O4B	124.54(9)	C6	C5	C4	120.6(4)
O1	Dy1	N1B	98.46(9)	C5	C6	C7	120.4(4)
O1	Dy1	O3C	145.57(8)	C6	C7	C8	119.7(4)
O1	Dy1	O4C	150.92(9)	C3	C8	C7	120.3(4)
O1	Dy1	N1C	160.30(9)	C10	C9	P1	124.8(3)
O1	Dy1	O3D	75.95(9)	C10	C9	C14	118.6(4)
O1	Dy1	O4D	80.57(9)	C14	C9	P1	116.6(3)
O1	Dy1	N1D	76.75(9)	C11	C10	C9	120.4(4)
O1	Dy1	O1W	83.30(8)	C12	C11	C10	120.6(4)
O1A	Dy1	O1	84.20(8)	C13	C12	C11	119.4(4)
O1A	Dy1	O3B	78.92(8)	C12	C13	C14	120.6(4)
O1A	Dy1	O4B	81.20(9)	C13	C14	C9	120.4(4)
O1A	Dy1	N1B	78.45(9)	C16	C15	P1	119.0(3)
O1A	Dy1	O3C	128.02(8)	C16	C15	C20	119.8(3)
O1A	Dy1	O4C	77.22(8)	C20	C15	P1	120.7(3)
O1A	Dy1	N1C	102.86(9)	C17	C16	C15	119.6(4)
O1A	Dy1	O3D	126.44(9)	C18	C17	C16	120.4(4)
O1A	Dy1	O4D	76.68(8)	C19	C18	C17	120.4(4)
O1A	Dy1	N1D	101.46(9)	C18	C19	C20	120.8(4)
O1A	Dy1	O1W	151.60(9)	C19	C20	C15	119.0(4)
O3B	Dy1	N1B	25.98(8)	O1A	P1A	C2A	109.48(16)
O3B	Dy1	O4C	124.16(9)	O1A	P1A	C9A	111.19(15)
O3B	Dy1	N1C	126.53(9)	O1A	P1A	C15A	109.97(15)
O3B	Dy1	O3D	136.80(8)	C9A	P1A	C2A	109.03(17)
O3B	Dy1	O4D	145.22(9)	C15A	P1A	C2A	108.60(16)
O3B	Dy1	N1D	149.19(9)	C15A	P1A	C9A	108.53(16)
O4B	Dy1	O3B	52.14(9)	P1A	O1A	Dy1	162.16(16)
O4B	Dy1	N1B	26.16(8)	O2A	C1A	C2A	118.6(3)
O4B	Dy1	O3C	77.90(10)	O2A	C1A	C3A	121.6(3)
O4B	Dy1	O4C	74.70(10)	C3A	C1A	C2A	119.8(3)
O4B	Dy1	N1C	75.03(9)	C1A	C2A	P1A	117.1(3)
O4B	Dy1	O3D	149.53(9)	C4A	C3A	C1A	122.3(4)
O4B	Dy1	O4D	144.49(9)	C4A	C3A	C8A	119.5(4)
O4B	Dy1	N1D	158.66(9)	C8A	C3A	C1A	118.1(4)
N1B	Dy1	N1C	100.97(10)	C3A	C4A	C5A	119.7(4)
N1B	Dy1	N1D	175.17(9)	C6A	C5A	C4A	119.9(5)
O3C	Dy1	O3B	120.30(9)	C7A	C6A	C5A	120.6(5)
O3C	Dy1	N1B	99.78(10)	C6A	C7A	C8A	119.9(5)
O3C	Dy1	O4C	51.52(8)	C7A	C8A	C3A	120.2(4)
O3C	Dy1	N1C	25.60(8)	C10A	C9A	P1A	123.3(3)
O3C	Dy1	O3D	74.45(9)	C14A	C9A	P1A	117.3(3)
O3C	Dy1	O4D	94.31(9)	C14A	C9A	C10A	119.4(3)
O3C	Dy1	N1D	84.11(9)	C11A	C10A	C9A	120.3(3)
O4C	Dy1	N1B	99.48(10)	C10A	C11A	C12A	120.1(4)
O4C	Dy1	N1C	25.92(8)	C13A	C12A	C11A	119.6(4)
O4C	Dy1	N1D	85.17(9)	C12A	C13A	C14A	120.6(4)
N1C	Dy1	N1D	83.79(9)	C13A	C14A	C9A	119.9(4)
O3D	Dy1	N1B	152.73(9)	C16A	C15A	P1A	121.6(3)
O3D	Dy1	O4C	97.32(9)	C16A	C15A	C20A	119.5(3)
O3D	Dy1	N1C	85.22(9)	C20A	C15A	P1A	118.9(3)
O3D	Dy1	N1D	25.87(8)	C17A	C16A	C15A	119.9(3)
O4D	Dy1	N1B	155.08(9)	C18A	C17A	C16A	120.4(4)

O4D	Dy1	O4C	73.55(9)	C17A	C18A	C19A	120.5(4)
O4D	Dy1	N1C	83.20(9)	C18A	C19A	C20A	120.0(4)
O4D	Dy1	O3D	51.46(8)	C19A	C20A	C15A	119.7(3)
O4D	Dy1	N1D	25.60(8)	N1B	O3B	Dy1	95.5(2)
O1W	Dy1	O3B	73.04(8)	N1B	O4B	Dy1	96.3(2)
O1W	Dy1	O4B	85.10(9)	O3B	N1B	Dy1	58.52(17)
O1W	Dy1	N1B	78.31(9)	O3B	N1B	O4B	116.0(3)
O1W	Dy1	O3C	72.21(9)	O4B	N1B	Dy1	57.50(18)
O1W	Dy1	O4C	122.73(9)	O5B	N1B	Dy1	178.3(3)
O1W	Dy1	N1C	97.39(9)	O5B	N1B	O3B	121.9(4)
O1W	Dy1	O3D	74.55(8)	O5B	N1B	O4B	122.1(3)
O1W	Dy1	O4D	125.87(8)	N1C	O3C	Dy1	97.5(2)
O1W	Dy1	N1D	100.33(9)	N1C	O4C	Dy1	95.5(2)
O1	P1	C2	110.91(16)	O3C	N1C	Dy1	56.90(17)
O1	P1	C9	112.87(16)	O3C	N1C	O4C	115.5(3)
O1	P1	C15	109.74(15)	O4C	N1C	Dy1	58.57(17)
C9	P1	C2	109.37(17)	O5C	N1C	Dy1	179.5(3)
C15	P1	C2	105.38(16)	O5C	N1C	O3C	122.6(3)
C15	P1	C9	108.26(17)	O5C	N1C	O4C	122.0(3)
P1	O1	Dy1	155.91(15)	N1D	O3D	Dy1	96.5(2)
O2	C1	C2	119.0(3)	N1D	O4D	Dy1	97.7(2)
O2	C1	C3	120.1(4)	O3D	N1D	Dy1	57.59(17)
C3	C1	C2	120.9(4)	O4D	N1D	Dy1	56.69(18)
C1	C2	P1	110.6(2)	O4D	N1D	O3D	114.3(3)
C4	C3	C1	117.1(4)	O5D	N1D	Dy1	178.2(3)
C8	C3	C1	123.7(4)	O5D	N1D	O3D	122.3(3)
C8	C3	C4	119.2(4)	O5D	N1D	O4D	123.4(3)

Table 6 Hydrogen Bonds for $Dy(NO_3)_3(4)_2(H_2O)$.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1W	H1WA	O3D[1]	0.87	1.94	2.755(3)	154.8
O1W	H1WB	O2	0.87	1.87	2.725(4)	165.5

[1]1-X,2-Y,1-Z

Table 7 Torsion Angles for $Dy(NO_3)_3(4)_2(H_2O)$.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Dy1	O3B	N1B	O4B	-1.8(3)	C15	C16	C17	C18	0.3(6)
Dy1	O3B	N1B	O5B	178.1(3)	C16	C15	C20	C19	-1.0(5)
Dy1	O4B	N1B	O3B	1.8(3)	C16	C17	C18	C19	-1.0(6)
Dy1	O4B	N1B	O5B	-178.0(3)	C17	C18	C19	C20	0.7(6)
Dy1	O3C	N1C	O4C	1.0(3)	C18	C19	C20	C15	0.3(6)
Dy1	O3C	N1C	O5C	-179.8(3)	C20	C15	C16	C17	0.7(5)
Dy1	O4C	N1C	O3C	-1.0(3)	P1A	C9A	C10A	C11A	177.5(3)
Dy1	O4C	N1C	O5C	179.8(3)	P1A	C9A	C14A	C13A	-178.3(3)
Dy1	O3D	N1D	O4D	0.8(3)	P1A	C15A	C16A	C17A	-178.4(3)
Dy1	O3D	N1D	O5D	-177.9(3)	P1A	C15A	C20A	C19A	178.4(3)
Dy1	O4D	N1D	O3D	-0.8(3)	O1A	P1A	C2A	C1A	139.8(3)
Dy1	O4D	N1D	O5D	177.9(3)	O1A	P1A	C9A	C10A	161.5(3)

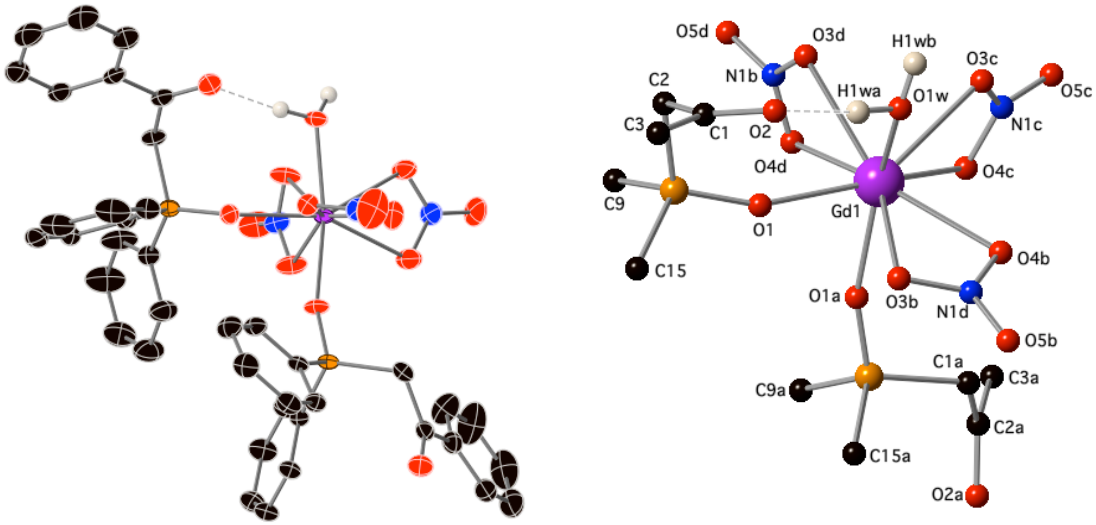
P1	C9	C10	C11	179.6(4)	O1A	P1A	C9A	C14A	-20.3(3)
P1	C9	C14	C13	-178.8(4)	O1A	P1A	C15A	C16A	161.0(3)
P1	C15	C16	C17	-171.1(3)	O1A	P1A	C15A	C20A	-19.4(3)
P1	C15	C20	C19	170.7(3)	O2A	C1A	C2A	P1A	77.8(4)
O1	P1	C2	C1	64.1(3)	O2A	C1A	C3A	C4A	-164.1(4)
O1	P1	C9	C10	132.0(4)	O2A	C1A	C3A	C8A	17.2(5)
O1	P1	C9	C14	-49.4(4)	C1A	C3A	C4A	C5A	178.8(4)
O1	P1	C15	C16	-29.6(3)	C1A	C3A	C8A	C7A	-179.7(4)
O1	P1	C15	C20	158.7(3)	C2A	P1A	O1A	Dy1	34.1(5)
O2	C1	C2	P1	-76.5(4)	C2A	P1A	C9A	C10A	40.7(3)
O2	C1	C3	C4	-3.3(5)	C2A	P1A	C9A	C14A	-141.1(3)
O2	C1	C3	C8	173.7(3)	C2A	P1A	C15A	C16A	-79.2(3)
C1	C3	C4	C5	177.1(4)	C2A	P1A	C15A	C20A	100.4(3)
C1	C3	C8	C7	-176.8(3)	C2A	C1A	C3A	C4A	16.6(5)
C2	P1	O1	Dy1	66.1(4)	C2A	C1A	C3A	C8A	-162.2(3)
C2	P1	C9	C10	8.0(4)	C3A	C1A	C2A	P1A	-102.9(3)
C2	P1	C9	C14	-173.4(3)	C3A	C4A	C5A	C6A	2.4(8)
C2	P1	C15	C16	89.9(3)	C4A	C3A	C8A	C7A	1.5(6)
C2	P1	C15	C20	-81.9(3)	C4A	C5A	C6A	C7A	-1.5(9)
C2	C1	C3	C4	178.4(3)	C5A	C6A	C7A	C8A	0.6(8)
C2	C1	C3	C8	-4.7(5)	C6A	C7A	C8A	C3A	-0.6(7)
C3	C1	C2	P1	101.9(3)	C8A	C3A	C4A	C5A	-2.4(7)
C3	C4	C5	C6	-0.2(6)	C9A	P1A	O1A	Dy1	-86.4(5)
C4	C3	C8	C7	0.0(5)	C9A	P1A	C2A	C1A	-98.4(3)
C4	C5	C6	C7	0.3(7)	C9A	P1A	C15A	C16A	39.2(3)
C5	C6	C7	C8	-0.3(7)	C9A	P1A	C15A	C20A	-141.2(3)
C6	C7	C8	C3	0.1(6)	C9A	C10A	C11A	C12A	1.6(6)
C8	C3	C4	C5	0.0(6)	C10A	C9A	C14A	C13A	0.0(6)
C9	P1	O1	Dy1	-57.1(4)	C10A	C11A	C12A	C13A	-1.7(6)
C9	P1	C2	C1	-170.8(3)	C11A	C12A	C13A	C14A	1.0(6)
C9	P1	C15	C16	-153.1(3)	C12A	C13A	C14A	C9A	-0.1(6)
C9	P1	C15	C20	35.1(3)	C14A	C9A	C10A	C11A	-0.8(5)
C9	C10	C11	C12	-0.4(8)	C15A	P1A	O1A	Dy1	153.4(5)
C10	C9	C14	C13	-0.2(7)	C15A	P1A	C2A	C1A	19.7(3)
C10	C11	C12	C13	-1.3(8)	C15A	P1A	C9A	C10A	-77.4(3)
C11	C12	C13	C14	2.2(8)	C15A	P1A	C9A	C14A	100.8(3)
C12	C13	C14	C9	-1.5(8)	C15A	C16A	C17A	C18A	-0.5(6)
C14	C9	C10	C11	1.1(7)	C16A	C15A	C20A	C19A	-2.0(6)
C15	P1	O1	Dy1	-177.9(3)	C16A	C17A	C18A	C19A	-0.9(6)
C15	P1	C2	C1	-54.6(3)	C17A	C18A	C19A	C20A	0.9(6)
C15	P1	C9	C10	-106.3(4)	C18A	C19A	C20A	C15A	0.6(6)
C15	P1	C9	C14	72.3(3)	C20A	C15A	C16A	C17A	2.0(5)

Table 8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for $Dy(NO_3)_3(4)_2(H_2O)$.

Atom	*x*	*y*	*z*	U(eq)
H2A	5193	13760	5610	34
H2B	5265	12525	5361	34
H4	886	14644	5931	50
H5	-452	16674	6126	62
H6	442	18072	6250	64

H7	2701	17471	6168	56
H8	4069	15436	5971	42
H10	7497	12835	5575	60
H11	9720	12280	5584	77
H12	10726	10763	6612	63
H13	9484	9862	7657	68
H14	7271	10362	7646	56
H16	3080	12256	7710	37
H17	1826	13685	8485	57
H18	2570	15213	8591	65
H19	4580	15296	7962	57
H20	5886	13870	7185	42
H2AA	5114	5839	9159	35
H2AB	6105	5620	8388	35
H4A	8058	4883	7883	62
H5A	9907	3427	7319	89
H6A	10963	1403	8062	83
H7A	10272	852	9369	71
H8A	8467	2313	9947	52
H10A	5101	6698	10369	33
H11A	3620	7902	11219	41
H12A	2511	10103	10772	47
H13A	2980	11113	9487	46
H14A	4494	9928	8636	39
H16A	7414	6701	10066	34
H17A	9488	6475	10228	41
H18A	11037	6757	9168	41
H19A	10554	7220	7931	48
H20A	8478	7451	7750	40
H1WA	3747	9974	5557	43
H1WB	3464	10998	5911	43

C. $Gd(NO_3)_3(4)_2(H_2O)$



Experimental

Single crystals of $C_{40}H_{36}GdN_3O_{14}P_2$ were grown by slow solvent evaporation of a 1:3 $Gd(NO_3)_3$-4 complex in 2:5:5 diethyl ether/pentane/ethanol and used as received. A suitable crystal was selected and mounted using a small amount of paratone oil on a nylon loop on a Bruker APEX-II CCD diffractometer. The crystal was kept at 173(2) K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of $Gd(NO_3)_3(4)_2(H_2O)$

Crystal Data for $C_{40}H_{36}GdN_3O_{14}P_2$ (M =1001.91 g/mol): triclinic, space group P-1 (no. 2), a = 11.23800(10) Å, b = 11.6353(2) Å, c = 18.4819(2) Å, α = 72.0301(6)°, β = 75.7452(6)°, γ = 66.7376(6)°, V = 2090.38(5) Å^3, Z = 2, T = 173.01 K, μ(CuKα) = 11.592 mm^{-1}, *Dcalc* = 1.592 g/cm^3, 30211 reflections measured (5.078° ≤ 2Θ ≤ 144.48°), 7956 unique (R_{int} = 0.0389, R_{sigma} = 0.0359) which were used in all calculations. The final R_1 was 0.0242 (I > 2σ(I)) and wR_2 was 0.0613 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups
 At 1.5 times of:
  All O(H) groups
2.a Rotating group:
 O1W(H1WA)
2.b Secondary CH2 refined with riding coordinates:
 C2(H2A,H2B), C1A(H1AA,H1AB)
2.c Aromatic/amide H refined with riding coordinates:
 C4(H4), C5(H5), C6(H6), C7(H7), C8(H8), C10(H10), C11(H11), C12(H12),
 C13(H13), C14(H14), C16(H16), C17(H17), C18(H18), C19(H19), C20(H20), C4A(H4A),
  C5A(H5A), C6A(H6A), C7A(H7A), C8A(H8A), C10A(H10A), C11A(H11A), C12A(H12A),
 C13A(H13A), C14A(H14A), C16A(H16A), C17A(H17A), C18A(H18A), C19A(H19A),
 C20A(H20A)

Table 1 Crystal data and structure refinement for $Gd(NO_3)_3(4)_2(H_2O)$

Structure number	**6**
CCDC number	1484664
Empirical formula	$C_{40}H_{36}GdN_3O_{14}P_2$
Formula weight	1001.91
Temperature/K	173(2)
Crystal system	triclinic
Space group	P-1
a/Å	11.23800(10)
b/Å	11.6353(2)
c/Å	18.4819(2)
α/°	72.0301(6)
β/°	75.7452(6)
γ/°	66.7376(6)
Volume/Å^3	2090.38(5)
Z	2
ϱ_{calc}g/cm^3	1.592
μ/mm^{-1}	11.592
F(000)	1006.0
Crystal size/mm^3	0.36 × 0.091 × 0.042
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	5.078 to 144.48
Index ranges	-12 ≤ h ≤ 13, -14 ≤ k ≤ 14, -22 ≤ l ≤ 22
Reflections collected	30211
Independent reflections	7956 [R_{int} = 0.0389, R_{sigma} = 0.0359]
Data/restraints/parameters	7956/0/546
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0242, wR_2 = 0.0603
Final R indexes [all data]	R_1 = 0.0257, wR_2 = 0.0612
Largest diff. peak/hole / e Å^{-3}	0.67/-0.43

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $Gd(NO_3)_3(4)_2(H_2O)$. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Gd1	9825.1(2)	6111.8(2)	3224.6(2)	17.92(5)
P1	9552.9(5)	2984.1(5)	3330.7(3)	19.20(11)
O1	9903.5(15)	4174.8(15)	3113.1(9)	24.9(3)
O2	12115.9(17)	2211.1(17)	4154.8(11)	36.4(4)
C1	11578(2)	1481(2)	4159.2(13)	26.6(5)
C2	10099(2)	1952(2)	4236.8(12)	25.2(5)
C3	12385(2)	153(2)	4065.2(13)	27.2(5)
C4	13739(3)	-221(3)	4015.7(16)	37.1(6)
C5	14541(3)	-1417(3)	3898.5(19)	47.6(7)
C6	14015(3)	-2259(3)	3826.8(18)	48.0(8)
C7	12677(3)	-1902(3)	3873.8(17)	42.2(7)
C8	11861(3)	-698(2)	3993.4(14)	31.3(5)
C9	7835(2)	3328(2)	3395.7(14)	26.1(5)

C10	7094(3)	2757(3)	4003.0(16)	46.2(8)
C11	5772(3)	3087(4)	4000(2)	57.1(9)
C12	5183(3)	3967(3)	3390(2)	47.6(7)
C13	5917(3)	4531(3)	2772(2)	51.8(8)
C14	7233(3)	4216(3)	2778.7(17)	42.5(7)
C15	10401(2)	2044(2)	2635.9(12)	22.1(4)
C16	9942(3)	1139(2)	2555.4(15)	31.1(5)
C17	10714(3)	306(3)	2090.9(18)	45.7(8)
C18	11911(3)	372(3)	1715.6(18)	52.3(9)
C19	12356(3)	1272(3)	1785.5(16)	46.5(7)
C20	11608(2)	2115(2)	2247.4(14)	30.2(5)
P1A	8861.1(5)	7641.2(5)	1253.5(3)	18.89(11)
O1A	9066.9(15)	6895.5(16)	2064.3(9)	26.5(3)
O2A	8198.7(18)	10525.6(18)	-70.7(10)	33.6(4)
C1A	8987(2)	9212(2)	1098.8(14)	25.7(5)
C2A	8020(2)	10352(2)	625.2(13)	24.2(5)
C3A	6897(2)	11244(2)	1028.1(15)	28.6(5)
C4A	6472(3)	10911(3)	1810.6(19)	47.9(7)
C5A	5398(4)	11785(4)	2146(3)	68.6(11)
C6A	4758(3)	12977(3)	1721(3)	63.7(11)
C7A	5184(3)	13317(3)	944(2)	52.3(8)
C8A	6240(3)	12462(3)	590.9(18)	38.7(6)
C9A	7262(2)	7868(2)	1097.8(13)	21.1(4)
C10A	6322(2)	7715(2)	1735.8(14)	29.5(5)
C11A	5086(2)	7862(3)	1630.5(15)	34.7(6)
C12A	4790(2)	8152(3)	896.8(15)	31.3(5)
C13A	5715(2)	8328(2)	262.8(14)	28.7(5)
C14A	6952(2)	8182(2)	360.7(13)	24.3(5)
C15A	10051(2)	6802(2)	573.2(12)	20.7(4)
C16A	10696(2)	5483(2)	832.9(14)	28.6(5)
C17A	11591(3)	4787(3)	327.9(16)	35.8(6)
C18A	11857(3)	5386(3)	-436.2(16)	36.2(6)
C19A	11224(2)	6696(3)	-701.3(14)	31.7(5)
C20A	10322(2)	7415(2)	-201.1(13)	25.3(5)
O3B	11855.3(15)	5267.8(15)	2355.5(10)	27.3(3)
O4B	11414.2(18)	7170.3(18)	2492.6(12)	40.1(4)
O5B	13123(2)	6342(3)	1703.5(17)	66.2(7)
N1B	12166(2)	6261(2)	2168.1(13)	33.3(5)
O3C	9792(2)	7352.8(17)	4111.8(11)	40.0(5)
O4C	8622(2)	8449.3(18)	3204.2(11)	39.4(4)
O5C	8680(2)	9378.6(18)	4049.9(11)	41.5(5)
N1C	9013(2)	8429(2)	3797.8(12)	30.6(4)
O3D	8641.3(16)	5241.8(19)	4477.0(9)	34.1(4)
O4D	7461.9(16)	6371.0(18)	3573.9(10)	35.1(4)
O5D	6569.2(18)	5507(2)	4682.2(12)	48.1(5)
N1D	7507(2)	5708(2)	4258.0(12)	29.4(4)
O1W	11476.7(16)	4783.2(16)	4013.4(10)	25.6(3)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $Gd(NO_3)_3(4)_2(H_2O)$. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**

Gd1	17.99(7)	19.74(7)	13.67(7)	-5.42(4)	-4.54(4)	-1.66(4)
P1	18.9(3)	22.1(3)	14.1(2)	-4.59(19)	-1.96(19)	-4.51(19)
O1	27.6(8)	23.4(8)	24.3(8)	-7.8(6)	-3.9(6)	-7.6(6)
O2	29.6(9)	30.2(9)	47.7(11)	-10.7(8)	-14.5(8)	-2.3(7)
C1	26.4(12)	28.4(12)	18.9(11)	-3.0(9)	-5.7(9)	-3.6(9)
C2	23.0(11)	29.4(12)	15(1)	-3.6(9)	-2.1(8)	-2.3(9)
C3	27.1(12)	27.1(12)	18.8(11)	-1.5(9)	-5.9(9)	-2.1(9)
C4	27.3(13)	35.0(14)	41.6(15)	-9.0(11)	-6.0(11)	-2.5(10)
C5	28.3(14)	44.2(17)	55.3(19)	-14.9(14)	-6.9(13)	5.7(11)
C6	51.8(19)	32.7(15)	45.7(17)	-16.7(12)	-15.6(14)	10.3(12)
C7	55.1(18)	33.5(14)	38.2(15)	-9.3(11)	-19.0(13)	-7.8(12)
C8	34.1(13)	30.4(12)	24.2(12)	-3.7(10)	-8.8(10)	-5(1)
C9	23.3(11)	28.7(12)	23.6(11)	-8.1(9)	-2.0(9)	-5.6(9)
C10	25.2(13)	71(2)	26.4(14)	2.0(13)	-1.5(10)	-12.0(12)
C11	26.6(15)	91(3)	41.2(17)	-2.8(16)	3.6(12)	-21.6(15)
C12	20.8(13)	61.9(19)	55.8(19)	-15.0(15)	-7.5(12)	-7.7(12)
C13	35.8(16)	54.2(19)	59(2)	7.1(15)	-24.1(15)	-13.7(13)
C14	32.9(14)	48.7(17)	40.2(16)	10.2(13)	-14.9(12)	-18.0(12)
C15	27.2(11)	21.4(11)	14.3(10)	-2.8(8)	-4.7(8)	-4.9(8)
C16	41.7(14)	24.5(12)	29.3(13)	-4.3(9)	-15.6(10)	-9(1)
C17	67(2)	28.6(13)	46.7(17)	-15.5(12)	-35.1(15)	-0.6(12)
C18	56(2)	47.3(17)	43.5(17)	-32.5(14)	-22.8(15)	18.5(14)
C19	37.6(15)	62.3(19)	24.4(13)	-19.2(13)	2.3(11)	1.1(13)
C20	28.1(12)	35.9(13)	22.6(12)	-10.2(10)	0.0(9)	-6.8(10)
P1A	16.9(2)	24.3(3)	13.7(2)	-4.28(19)	-4.42(18)	-4.11(19)
O1A	24.5(8)	34.1(9)	15.4(8)	-3.7(6)	-7.0(6)	-3.6(6)
O2A	35.5(9)	38.5(10)	26.4(9)	-6.8(7)	-5.9(7)	-12.1(7)
C1A	22.9(11)	30.4(12)	27.0(12)	-11.1(9)	-5.6(9)	-8.2(9)
C2A	24.7(11)	25.6(11)	25.7(12)	-6.3(9)	-4.2(9)	-11.9(9)
C3A	23.6(11)	27.6(12)	37.5(14)	-11.4(10)	-4.4(10)	-9.0(9)
C4A	51.9(18)	37.7(16)	43.1(17)	-13.0(13)	9.4(13)	-11.1(13)
C5A	65(2)	61(2)	68(3)	-32.3(19)	29.6(19)	-20.2(18)
C6A	37.8(17)	49(2)	105(3)	-48(2)	8.7(18)	-4.9(14)
C7A	35.1(15)	33.0(15)	91(3)	-23.1(16)	-22.6(16)	0.9(11)
C8A	35.5(14)	32.8(14)	51.7(17)	-12.7(12)	-17.4(12)	-7.1(11)
C9A	20(1)	21.7(10)	19.9(11)	-4.9(8)	-3.9(8)	-5.1(8)
C10A	24.8(12)	40.4(14)	20.2(11)	-4.7(10)	-2.5(9)	-10.4(10)
C11A	22.3(12)	51.1(16)	28.6(13)	-9.3(11)	2(1)	-14.0(11)
C12A	18.8(11)	40.4(14)	35.6(14)	-11.5(11)	-4.8(9)	-8.8(9)
C13A	25.9(12)	36.8(13)	24.3(12)	-8(1)	-7.5(9)	-9(1)
C14A	21.9(11)	32.6(12)	19.2(11)	-6.5(9)	-3.2(8)	-9.9(9)
C15A	18.2(10)	27.2(11)	16.8(10)	-7.2(8)	-3.2(8)	-5.9(8)
C16A	29.6(12)	30.3(12)	22.5(11)	-5.4(9)	-7.2(9)	-5.5(9)
C17A	35.5(14)	30.7(13)	34.0(14)	-11.2(11)	-7.2(11)	0.1(10)
C18A	30.9(13)	43.6(15)	33.9(14)	-23.0(12)	0.9(10)	-5.5(11)
C19A	31.0(13)	42.7(14)	23.6(12)	-11.2(10)	-0.2(9)	-14.6(10)
C20A	24.8(11)	29.9(12)	21.2(11)	-5.1(9)	-3.2(9)	-10.0(9)
O3B	24.1(8)	27.6(8)	28.2(9)	-7.1(7)	-0.8(6)	-8.2(6)
O4B	37.1(10)	30.3(9)	53.5(12)	-12.2(9)	-1.6(9)	-13.5(8)
O5B	39.0(12)	66.4(16)	83.5(19)	-15.2(14)	24.2(12)	-29.8(11)
N1B	23.4(10)	34.9(12)	38.0(12)	-4.3(9)	-1.1(9)	-11.7(8)
O3C	56.9(12)	28.2(9)	31.5(10)	-10.8(7)	-21.8(9)	0.6(8)

O4C	46.4(11)	31.7(9)	35.9(10)	-14.4(8)	-18.2(8)	2.8(8)
O5C	57.9(12)	28.3(9)	37.6(11)	-18.5(8)	-0.4(9)	-9.7(8)
N1C	36.6(11)	27.5(10)	26.1(11)	-11.9(8)	-2.0(8)	-6.9(8)
O3D	24.6(9)	54.8(11)	17.9(8)	-7.1(7)	-4.8(6)	-8.7(8)
O4D	21.9(8)	43.5(10)	25.1(9)	-2.6(7)	-3.8(7)	0.1(7)
O5D	26.3(10)	67.2(14)	36.1(11)	-6.7(10)	8.0(8)	-12.5(9)
N1D	23.9(10)	33.5(11)	22.2(10)	-10.8(8)	1.6(8)	-0.9(8)
O1W	25.8(8)	27.9(8)	20.4(8)	-7.5(6)	-9.7(6)	-1.6(6)

Table 4 Bond Lengths for $Gd(NO_3)_3(4)_2(H_2O)$.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Gd1	O1	2.2914(16)	C19	C20	1.382(4)
Gd1	O1A	2.2882(15)	P1A	O1A	1.5041(15)
Gd1	O3B	2.4797(16)	P1A	C1A	1.818(2)
Gd1	O4B	2.4608(19)	P1A	C9A	1.794(2)
Gd1	N1B	2.896(2)	P1A	C15A	1.794(2)
Gd1	O3C	2.4827(18)	O2A	C2A	1.217(3)
Gd1	O4C	2.5068(18)	C1A	C2A	1.523(3)
Gd1	N1C	2.927(2)	C2A	C3A	1.485(3)
Gd1	O3D	2.5007(17)	C3A	C4A	1.389(4)
Gd1	O4D	2.4908(17)	C3A	C8A	1.402(4)
Gd1	N1D	2.935(2)	C4A	C5A	1.388(4)
Gd1	O1W	2.3739(15)	C5A	C6A	1.369(6)
P1	O1	1.4985(16)	C6A	C7A	1.382(6)
P1	C2	1.818(2)	C7A	C8A	1.382(4)
P1	C9	1.791(2)	C9A	C10A	1.394(3)
P1	C15	1.787(2)	C9A	C14A	1.392(3)
O2	C1	1.219(3)	C10A	C11A	1.386(4)
C1	C2	1.515(3)	C11A	C12A	1.384(4)
C1	C3	1.490(3)	C12A	C13A	1.384(4)
C3	C4	1.395(4)	C13A	C14A	1.383(3)
C3	C8	1.387(4)	C15A	C16A	1.397(3)
C4	C5	1.376(4)	C15A	C20A	1.406(3)
C5	C6	1.378(5)	C16A	C17A	1.378(4)
C6	C7	1.381(5)	C17A	C18A	1.385(4)
C7	C8	1.389(4)	C18A	C19A	1.387(4)
C9	C10	1.382(4)	C19A	C20A	1.388(3)
C9	C14	1.388(3)	O3B	N1B	1.261(3)
C10	C11	1.380(4)	O4B	N1B	1.277(3)
C11	C12	1.371(5)	O5B	N1B	1.215(3)
C12	C13	1.384(5)	O3C	N1C	1.268(3)
C13	C14	1.379(4)	O4C	N1C	1.269(3)
C15	C16	1.400(3)	O5C	N1C	1.217(3)
C15	C20	1.391(3)	O3D	N1D	1.286(3)
C16	C17	1.383(4)	O4D	N1D	1.263(3)
C17	C18	1.373(5)	O5D	N1D	1.206(3)
C18	C19	1.375(5)			

Table 5 Bond Angles for $Gd(NO_3)_3(4)_2(H_2O)$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Gd1	O3B	72.49(6)	C5	C4	C3	120.4(3)
O1	Gd1	O4B	123.89(6)	C4	C5	C6	120.4(3)
O1	Gd1	N1B	97.98(6)	C5	C6	C7	119.9(3)
O1	Gd1	O3C	145.83(6)	C6	C7	C8	120.1(3)
O1	Gd1	O4C	150.96(6)	C3	C8	C7	120.3(3)
O1	Gd1	N1C	160.15(6)	C10	C9	P1	124.66(19)
O1	Gd1	O3D	75.77(6)	C10	C9	C14	118.9(2)
O1	Gd1	O4D	79.82(6)	C14	C9	P1	116.42(19)
O1	Gd1	N1D	76.13(6)	C11	C10	C9	120.3(3)
O1	Gd1	O1W	83.00(6)	C12	C11	C10	120.5(3)
O1A	Gd1	O1	84.18(6)	C11	C12	C13	119.8(3)
O1A	Gd1	O3B	78.95(6)	C14	C13	C12	119.8(3)
O1A	Gd1	O4B	81.04(7)	C13	C14	C9	120.7(3)
O1A	Gd1	N1B	78.25(6)	C16	C15	P1	120.58(19)
O1A	Gd1	O3C	127.85(6)	C20	C15	P1	118.37(18)
O1A	Gd1	O4C	77.69(6)	C20	C15	C16	120.6(2)
O1A	Gd1	N1C	102.92(6)	C17	C16	C15	119.0(3)
O1A	Gd1	O3D	125.88(6)	C18	C17	C16	120.2(3)
O1A	Gd1	O4D	76.35(6)	C17	C18	C19	121.0(3)
O1A	Gd1	N1D	100.82(6)	C18	C19	C20	120.2(3)
O1A	Gd1	O1W	151.68(6)	C19	C20	C15	119.1(3)
O3B	Gd1	N1B	25.66(6)	O1A	P1A	C1A	109.35(10)
O3B	Gd1	O3C	120.21(6)	O1A	P1A	C9A	109.86(10)
O3B	Gd1	O4C	124.74(6)	O1A	P1A	C15A	111.03(10)
O3B	Gd1	N1C	126.81(6)	C9A	P1A	C1A	108.62(10)
O3B	Gd1	O3D	136.91(6)	C9A	P1A	C15A	108.49(10)
O3B	Gd1	O4D	144.41(6)	C15A	P1A	C1A	109.45(11)
O3B	Gd1	N1D	148.49(6)	P1A	O1A	Gd1	161.71(11)
O4B	Gd1	O3B	51.62(6)	C2A	C1A	P1A	116.78(16)
O4B	Gd1	N1B	25.98(6)	O2A	C2A	C1A	119.6(2)
O4B	Gd1	O3C	78.21(7)	O2A	C2A	C3A	121.7(2)
O4B	Gd1	O4C	75.63(7)	C3A	C2A	C1A	118.7(2)
O4B	Gd1	N1C	75.83(6)	C4A	C3A	C2A	122.6(2)
O4B	Gd1	O3D	150.43(7)	C4A	C3A	C8A	119.5(3)
O4B	Gd1	O4D	145.24(6)	C8A	C3A	C2A	117.9(2)
O4B	Gd1	N1D	159.89(6)	C5A	C4A	C3A	119.5(3)
N1B	Gd1	N1C	101.60(6)	C6A	C5A	C4A	121.2(4)
N1B	Gd1	N1D	174.11(6)	C5A	C6A	C7A	119.6(3)
O3C	Gd1	N1B	100.04(7)	C8A	C7A	C6A	120.6(3)
O3C	Gd1	O4C	50.98(6)	C7A	C8A	C3A	119.7(3)
O3C	Gd1	N1C	25.44(6)	C10A	C9A	P1A	118.49(17)
O3C	Gd1	O3D	75.07(7)	C14A	C9A	P1A	121.47(17)
O3C	Gd1	O4D	95.23(7)	C14A	C9A	C10A	120.0(2)
O3C	Gd1	N1D	85.15(7)	C11A	C10A	C9A	119.6(2)
O4C	Gd1	N1B	100.26(7)	C12A	C11A	C10A	120.2(2)
O4C	Gd1	N1C	25.54(6)	C11A	C12A	C13A	120.3(2)
O4C	Gd1	N1D	85.15(7)	C14A	C13A	C12A	120.0(2)
N1C	Gd1	N1D	84.28(6)	C13A	C14A	C9A	119.9(2)
O3D	Gd1	N1B	153.23(6)	C16A	C15A	P1A	117.54(17)
O3D	Gd1	O4C	96.73(7)	C16A	C15A	C20A	119.8(2)

O3D	Gd1	N1C	85.21(6)	C20A	C15A	P1A	122.60(17)
O3D	Gd1	N1D	25.82(6)	C17A	C16A	C15A	119.8(2)
O4D	Gd1	N1B	154.60(6)	C16A	C17A	C18A	120.5(2)
O4D	Gd1	O4C	74.00(7)	C17A	C18A	C19A	120.2(2)
O4D	Gd1	N1C	83.85(6)	C18A	C19A	C20A	120.1(2)
O4D	Gd1	O3D	51.07(5)	C19A	C20A	C15A	119.5(2)
O4D	Gd1	N1D	25.25(6)	N1B	O3B	Gd1	95.95(13)
O1W	Gd1	O3B	73.14(6)	N1B	O4B	Gd1	96.41(13)
O1W	Gd1	O4B	85.36(6)	O3B	N1B	Gd1	58.39(11)
O1W	Gd1	N1B	78.67(6)	O3B	N1B	O4B	116.0(2)
O1W	Gd1	O3C	72.48(6)	O4B	N1B	Gd1	57.61(12)
O1W	Gd1	O4C	122.65(6)	O5B	N1B	Gd1	177.7(2)
O1W	Gd1	N1C	97.60(6)	O5B	N1B	O3B	121.6(2)
O1W	Gd1	O3D	74.76(6)	O5B	N1B	O4B	122.4(2)
O1W	Gd1	O4D	125.61(6)	N1C	O3C	Gd1	97.28(13)
O1W	Gd1	N1D	100.44(6)	N1C	O4C	Gd1	96.08(13)
O1	P1	C2	111.08(11)	O3C	N1C	Gd1	57.27(11)
O1	P1	C9	112.91(10)	O3C	N1C	O4C	115.64(19)
O1	P1	C15	109.73(10)	O4C	N1C	Gd1	58.38(11)
C9	P1	C2	109.13(11)	O5C	N1C	Gd1	178.77(17)
C15	P1	C2	105.33(10)	O5C	N1C	O3C	121.6(2)
C15	P1	C9	108.33(11)	O5C	N1C	O4C	122.7(2)
P1	O1	Gd1	156.31(10)	N1D	O3D	Gd1	96.32(13)
O2	C1	C2	119.4(2)	N1D	O4D	Gd1	97.47(13)
O2	C1	C3	119.6(2)	O3D	N1D	Gd1	57.86(11)
C3	C1	C2	121.0(2)	O4D	N1D	Gd1	57.28(11)
C1	C2	P1	110.19(15)	O4D	N1D	O3D	115.13(19)
C4	C3	C1	117.7(2)	O5D	N1D	Gd1	178.19(18)
C8	C3	C1	123.3(2)	O5D	N1D	O3D	121.5(2)
C8	C3	C4	118.9(2)	O5D	N1D	O4D	123.4(2)

Table 6 Hydrogen Bonds for $Gd(NO_3)_3(4)_2(H_2O)$.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1W	H1WA	O2	0.90	1.84	2.730(2)	175.4
O1W	H1WB	O3D[1]	0.82(4)	1.93(4)	2.752(2)	172(4)

[1]2-X,1-Y,1-Z

Table 7 Torsion Angles for $Gd(NO_3)_3(4)_2(H_2O)$.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Gd1	O3B	N1B	O4B	2.4(2)	C15	C16	C17	C18	-0.1(4)
Gd1	O3B	N1B	O5B	-177.3(3)	C16	C15	C20	C19	-0.6(4)
Gd1	O4B	N1B	O3B	-2.4(2)	C16	C17	C18	C19	-0.8(4)
Gd1	O4B	N1B	O5B	177.3(3)	C17	C18	C19	C20	1.0(4)
Gd1	O3C	N1C	O4C	-1.4(2)	C18	C19	C20	C15	-0.3(4)
Gd1	O3C	N1C	O5C	179.3(2)	C20	C15	C16	C17	0.8(3)
Gd1	O4C	N1C	O3C	1.3(2)	P1A	C1A	C2A	O2A	-77.5(3)
Gd1	O4C	N1C	O5C	-179.4(2)	P1A	C1A	C2A	C3A	104.0(2)
Gd1	O3D	N1D	O4D	-1.4(2)	P1A	C9A	C10A	C11A	-178.8(2)

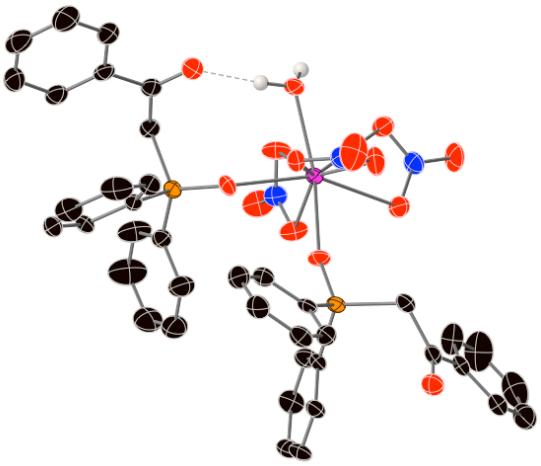
Gd1	O3D	N1D	O5D	178.0(2)	P1A	C9A	C14A	C13A	178.89(18)
Gd1	O4D	N1D	O3D	1.4(2)	P1A	C15A	C16A	C17A	178.2(2)
Gd1	O4D	N1D	O5D	-178.0(2)	P1A	C15A	C20A	C19A	-177.84(18)
P1	C9	C10	C11	180.0(3)	O1A	P1A	C1A	C2A	-140.17(17)
P1	C9	C14	C13	179.2(3)	O1A	P1A	C9A	C10A	18.6(2)
P1	C15	C16	C17	-171.09(18)	O1A	P1A	C9A	C14A	-161.00(18)
P1	C15	C20	C19	171.5(2)	O1A	P1A	C15A	C16A	19.8(2)
O1	P1	C2	C1	-63.50(19)	O1A	P1A	C15A	C20A	-161.80(18)
O1	P1	C9	C10	-131.8(2)	O2A	C2A	C3A	C4A	162.9(3)
O1	P1	C9	C14	49.4(2)	O2A	C2A	C3A	C8A	-16.4(3)
O1	P1	C15	C16	-158.68(17)	C1A	P1A	O1A	Gd1	-34.3(3)
O1	P1	C15	C20	29.2(2)	C1A	P1A	C9A	C10A	-101.0(2)
O2	C1	C2	P1	76.3(3)	C1A	P1A	C9A	C14A	79.4(2)
O2	C1	C3	C4	3.3(3)	C1A	P1A	C15A	C16A	140.62(18)
O2	C1	C3	C8	-173.9(2)	C1A	P1A	C15A	C20A	-41.0(2)
C1	C3	C4	C5	-177.5(3)	C1A	C2A	C3A	C4A	-18.5(4)
C1	C3	C8	C7	177.2(2)	C1A	C2A	C3A	C8A	162.2(2)
C2	P1	O1	Gd1	-66.3(3)	C2A	C3A	C4A	C5A	-178.7(3)
C2	P1	C9	C10	-7.8(3)	C2A	C3A	C8A	C7A	179.6(2)
C2	P1	C9	C14	173.5(2)	C3A	C4A	C5A	C6A	-0.8(6)
C2	P1	C15	C16	81.7(2)	C4A	C3A	C8A	C7A	0.3(4)
C2	P1	C15	C20	-90.4(2)	C4A	C5A	C6A	C7A	0.2(6)
C2	C1	C3	C4	-178.5(2)	C5A	C6A	C7A	C8A	0.6(5)
C2	C1	C3	C8	4.2(3)	C6A	C7A	C8A	C3A	-0.9(5)
C3	C1	C2	P1	-101.9(2)	C8A	C3A	C4A	C5A	0.5(5)
C3	C4	C5	C6	0.2(5)	C9A	P1A	O1A	Gd1	-153.4(3)
C4	C3	C8	C7	0.0(4)	C9A	P1A	C1A	C2A	-20.3(2)
C4	C5	C6	C7	-0.1(5)	C9A	P1A	C15A	C16A	-101.01(19)
C5	C6	C7	C8	0.0(5)	C9A	P1A	C15A	C20A	77.4(2)
C6	C7	C8	C3	0.1(4)	C9A	C10A	C11A	C12A	0.3(4)
C8	C3	C4	C5	-0.1(4)	C10A	C9A	C14A	C13A	-0.7(4)
C9	P1	O1	Gd1	56.7(3)	C10A	C11A	C12A	C13A	-1.5(4)
C9	P1	C2	C1	171.38(17)	C11A	C12A	C13A	C14A	1.6(4)
C9	P1	C15	C16	-35.0(2)	C12A	C13A	C14A	C9A	-0.5(4)
C9	P1	C15	C20	152.93(18)	C14A	C9A	C10A	C11A	0.8(4)
C9	C10	C11	C12	1.2(6)	C15A	P1A	O1A	Gd1	86.6(3)
C10	C9	C14	C13	0.4(5)	C15A	P1A	C1A	C2A	98.00(19)
C10	C11	C12	C13	-0.2(6)	C15A	P1A	C9A	C10A	140.13(19)
C11	C12	C13	C14	-0.7(6)	C15A	P1A	C9A	C14A	-39.5(2)
C12	C13	C14	C9	0.6(5)	C15A	C16A	C17A	C18A	0.0(4)
C14	C9	C10	C11	-1.3(5)	C16A	C15A	C20A	C19A	0.5(3)
C15	P1	O1	Gd1	177.6(2)	C16A	C17A	C18A	C19A	0.1(4)
C15	P1	C2	C1	55.2(2)	C17A	C18A	C19A	C20A	0.2(4)
C15	P1	C9	C10	106.4(3)	C18A	C19A	C20A	C15A	-0.5(4)
C15	P1	C9	C14	-72.4(2)	C20A	C15A	C16A	C17A	-0.3(4)

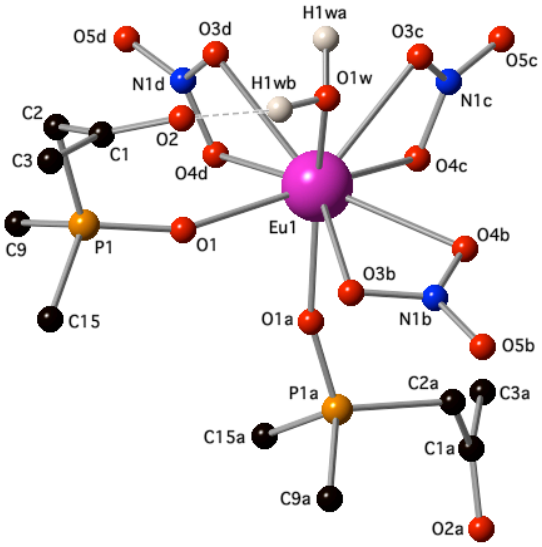
Table 8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for $Gd(NO_3)_3(4)_2(H_2O)$.

Atom	***x***	***y***	***z***	**U(eq)**
H2A	9713	2437	4643	30
H2B	9799	1206	4388	30

H4	14110	353	4063	45
H5	15461	-1664	3867	57
H6	14573	-3083	3745	58
H7	12313	-2481	3824	51
H8	10941	-456	4026	38
H10	7496	2134	4424	55
H11	5268	2702	4424	68
H12	4273	4188	3391	57
H13	5515	5134	2345	62
H14	7734	4611	2357	51
H16	9112	1099	2816	37
H17	10416	-314	2031	55
H18	12440	-212	1403	63
H19	13180	1314	1515	56
H20	11915	2735	2299	36
H1AA	8879	9385	1607	31
H1AB	9883	9168	843	31
H4A	6913	10092	2114	58
H5A	5102	11553	2680	82
H6A	4026	13565	1959	76
H7A	4746	14146	649	63
H8A	6519	12698	55	46
H10A	6527	7512	2240	35
H11A	4441	7762	2063	42
H12A	3948	8232	828	38
H13A	5500	8548	-240	34
H14A	7589	8296	-74	29
H16A	10518	5066	1356	34
H17A	12030	3890	505	43
H18A	12475	4898	-780	43
H19A	11407	7102	-1226	38
H20A	9892	8314	-380	30
H1WA	11663	3951	4038	38
H1WB	11450(40)	4840(30)	4450(20)	55(11)

D. $Eu(NO_3)_3$4$_2$(H_2O)





Experimental

Single crystals of $C_{40}H_{36}EuN_3O_{14}P_2$ were grown at 4 °C by diffusion of hexane into a solution of the 1:3 $Eu(NO_3)_3$-4 complex in chloroform and used as received. A suitable crystal was selected and mounted using a small amount of paratone oil on a nylon loop on a Bruker APEX-II CCD diffractometer. The crystal was kept at 173(2) K during data collection. Using Olex2 [1], the structure was solved with the ShelXS [2] structure solution program using Structure Expansion and refined with the ShelXL [3] refinement package using Least Squares minimization.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of $Eu(NO_3)_3$(4)$_2$(H_2O)

Crystal Data for $C_{40}H_{36}EuN_3O_{14}P_2$ (M =996.62 g/mol): triclinic, space group P-1 (no. 2), a = 11.2311(19) Å, b = 11.6325(19) Å, c = 18.480(3) Å, α = 72.083(2)°, β = 75.706(2)°, γ = 66.718(2)°, V = 2088.3(6) Å^3, Z = 2, T = 173.15 K, μ(MoKα) = 1.649 mm^{-1}, *Dcalc* = 1.585 g/cm^3, 21495 reflections measured (3.922° ≤ 2Θ ≤ 50.86°), 7660 unique (R_{int} = 0.0483, R_{sigma} = 0.0523) which were used in all calculations. The final R_1 was 0.0452 (I > 2σ(I)) and wR_2 was 0.1246 (all data).

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups
 At 1.5 times of:
  All O(H,H) groups
2.a Rotating group:
 O1W(H1WA,H1WB)
2.b Secondary CH2 refined with riding coordinates:
 C2(H2A,H2B), C2A(H2AA,H2AB)
2.c Aromatic/amide H refined with riding coordinates:
 C4(H4), C5(H5), C6(H6), C7(H7), C8(H8), C10(H10), C11(H11), C12(H12),
 C13(H13), C14(H14), C16(H16), C17(H17), C18(H18), C19(H19), C20(H20), C4A(H4A),
  C5A(H5A), C6A(H6A), C7A(H7A), C8A(H8A), C10A(H10A), C11A(H11A), C12A(H12A),
 C13A(H13A), C14A(H14A), C16A(H16A), C17A(H17A), C18A(H18A), C19A(H19A),
 C20A(H20A)

Table 1 Crystal data and structure refinement for $Eu(NO_3)_3(4)_2(H_2O)$

Structure Number	**5**
CCDC Number	1484663
Empirical formula	$C_{40}H_{36}EuN_3O_{14}P_2$
Formula weight	996.62
Temperature/K	173(2)
Crystal system	triclinic
Space group	P-1
a/Å	11.2311(19)
b/Å	11.6325(19)
c/Å	18.480(3)
α/°	72.083(2)
β/°	75.706(2)
γ/°	66.718(2)
Volume/Å^3	2088.3(6)
Z	2
ϱ_{calc}g/cm^3	1.585
μ/mm^{-1}	1.649
F(000)	1004.0
Crystal size/mm^3	0.288 × 0.231 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.922 to 50.86
Index ranges	-13 ≤ h ≤ 13, -14 ≤ k ≤ 13, -22 ≤ l ≤ 22
Reflections collected	21495
Independent reflections	7660 [R_{int} = 0.0483, R_{sigma} = 0.0523]
Data/restraints/parameters	7660/0/542
Goodness-of-fit on F^2	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0452, wR_2 = 0.1178
Final R indexes [all data]	R_1 = 0.0511, wR_2 = 0.1246
Largest diff. peak/hole / e Å^{-3}	2.82/-1.62

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $Eu(NO_3)_3(4)_2(H_2O)$. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Eu1	5166.2(2)	8887.1(2)	6778.0(2)	22.47(10)
P1	5437.8(10)	12021(1)	6671.8(6)	23.1(2)
O1	5080(3)	10840(3)	6889.3(18)	29.8(7)
O2	2884(3)	12790(3)	5842(2)	42.3(9)
C1	3412(4)	13524(4)	5843(3)	30.5(10)
C2	4902(4)	13049(4)	5764(2)	28.5(10)
C3	2617(4)	14837(4)	5938(2)	29.7(10)
C4	1260(5)	15218(5)	5987(3)	40.8(12)
C5	468(5)	16416(6)	6101(4)	54.3(15)
C6	988(6)	17255(6)	6174(3)	53.9(16)
C7	2319(6)	16902(5)	6124(3)	46.8(13)
C8	3133(5)	15698(5)	6010(3)	35.7(11)
C9	7162(4)	11668(4)	6605(3)	28.7(10)

C10	7895(5)	12230(6)	5997(3)	51.5(15)
C11	9219(5)	11908(7)	6000(4)	68(2)
C12	9813(5)	11021(6)	6614(4)	53.7(15)
C13	9071(5)	10473(6)	7228(4)	56.2(17)
C14	7760(5)	10791(6)	7217(3)	47.1(14)
C15	4598(4)	12960(4)	7362(2)	25.3(9)
C16	5057(5)	13859(4)	7446(3)	34.1(11)
C17	4278(6)	14699(5)	7903(3)	48.7(15)
C18	3098(6)	14627(6)	8289(3)	56.6(17)
C19	2641(5)	13740(6)	8214(3)	50.7(15)
C20	3386(5)	12895(5)	7750(3)	33(1)
P1A	6137.1(10)	7358.5(11)	8750.6(6)	22.6(2)
O1A	5934(3)	8097(3)	7942.6(16)	28.9(7)
O2A	6798(3)	4481(3)	10068.8(19)	36.0(8)
C1A	6976(4)	4653(4)	9376(3)	27.5(10)
C2A	6002(4)	5790(4)	8904(3)	28.7(10)
C3A	8098(4)	3759(4)	8975(3)	30.9(10)
C4A	8525(6)	4083(5)	8192(3)	51.1(14)
C5A	9590(7)	3221(7)	7850(4)	73(2)
C6A	10226(6)	2021(7)	8284(5)	69(2)
C7A	9811(6)	1684(6)	9058(4)	57.1(17)
C8A	8758(5)	2544(5)	9405(3)	42.6(12)
C9A	4943(4)	8193(4)	9435(2)	24.4(9)
C10A	4677(4)	7600(5)	10191(3)	30.8(10)
C11A	3787(4)	8308(5)	10701(3)	34.5(11)
C12A	3141(5)	9600(5)	10437(3)	38.0(11)
C13A	3419(5)	10204(5)	9667(3)	39.9(12)
C14A	4314(4)	9499(5)	9172(3)	31.4(10)
C15A	7740(4)	7131(4)	8907(2)	24.0(9)
C16A	8668(4)	7291(5)	8267(3)	33.4(11)
C17A	9911(5)	7136(5)	8372(3)	39.1(12)
C18A	10199(4)	6849(5)	9106(3)	34.5(11)
C19A	9281(4)	6681(5)	9733(3)	32.9(10)
C20A	8050(4)	6821(4)	9638(3)	28.7(10)
O3B	3126(3)	9732(3)	7648.8(18)	30.3(7)
O4B	3563(3)	7832(3)	7522(2)	46.0(9)
O5B	1866(4)	8662(4)	8305(3)	68.1(14)
N1B	2821(4)	8738(4)	7841(3)	37(1)
O3C	5209(4)	7641(3)	5891(2)	43.9(9)
O4C	6373(4)	6543(3)	6798(2)	44.1(9)
O5C	6311(4)	5619(3)	5950(2)	47.4(9)
N1C	5981(4)	6564(4)	6197(2)	35.2(9)
O3D	6357(3)	9756(4)	5528.6(18)	39.7(8)
O4D	7539(3)	8624(3)	6426.6(19)	39.4(8)
O5D	8433(3)	9486(4)	5321(2)	51.6(10)
N1D	7495(4)	9289(4)	5742(2)	32.8(9)
O1W	3508(3)	10226(3)	5979.6(17)	29.2(7)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $Eu(NO_3)_3(4)_2(H_2O)$. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**

Eu1	28.74(14)	21.87(15)	19.01(15)	-8.56(10)	-7.96(9)	-5.55(10)
P1	28.7(5)	23.4(6)	19.4(6)	-7.3(5)	-5.1(4)	-8.6(4)
O1	38.1(16)	27.2(17)	31.8(17)	-14.1(14)	-8.1(14)	-12.1(13)
O2	42.6(18)	32.4(19)	55(2)	-12.9(17)	-17.6(17)	-8.3(16)
C1	39(2)	30(3)	22(2)	-5(2)	-9.4(19)	-10(2)
C2	35(2)	28(2)	19(2)	-7.8(19)	-4.0(18)	-6.9(19)
C3	36(2)	27(2)	21(2)	-4.4(19)	-10.3(18)	-2.6(19)
C4	44(3)	31(3)	45(3)	-9(2)	-15(2)	-6(2)
C5	42(3)	44(3)	67(4)	-16(3)	-14(3)	2(3)
C6	63(4)	37(3)	50(3)	-18(3)	-22(3)	10(3)
C7	65(4)	33(3)	45(3)	-13(2)	-18(3)	-12(3)
C8	44(3)	33(3)	26(2)	-4(2)	-11(2)	-8(2)
C9	33(2)	28(2)	25(2)	-9.1(19)	-7.5(18)	-6.5(19)
C10	36(3)	75(4)	32(3)	0(3)	-4(2)	-18(3)
C11	38(3)	104(6)	50(4)	-7(4)	2(3)	-28(3)
C12	30(2)	62(4)	70(4)	-20(3)	-10(3)	-11(3)
C13	45(3)	50(4)	72(4)	5(3)	-29(3)	-17(3)
C14	43(3)	49(3)	47(3)	9(3)	-18(2)	-23(3)
C15	38(2)	22(2)	18(2)	-4.3(18)	-9.9(18)	-9.2(18)
C16	48(3)	30(3)	32(3)	-9(2)	-19(2)	-13(2)
C17	77(4)	27(3)	52(3)	-20(2)	-39(3)	-2(3)
C18	72(4)	52(4)	44(3)	-38(3)	-26(3)	12(3)
C19	44(3)	66(4)	32(3)	-26(3)	-3(2)	1(3)
C20	41(2)	35(3)	23(2)	-11(2)	-2.6(19)	-12(2)
P1A	26.3(5)	25.4(6)	19.2(5)	-7.3(5)	-7.4(4)	-8.0(4)
O1A	34.1(15)	34.7(18)	16.6(15)	-5.9(13)	-9.5(12)	-7.3(13)
O2A	42.9(18)	39(2)	29.2(19)	-9.2(15)	-6.6(14)	-15.9(15)
C1A	30(2)	28(2)	31(3)	-8(2)	-4.9(18)	-16.0(19)
C2A	33(2)	32(2)	28(2)	-13(2)	-8.1(18)	-10.5(19)
C3A	34(2)	26(2)	41(3)	-13(2)	-11(2)	-11.6(19)
C4A	55(3)	39(3)	54(4)	-18(3)	7(3)	-14(3)
C5A	78(4)	68(5)	68(5)	-35(4)	28(4)	-29(4)
C6A	50(3)	55(4)	112(6)	-54(4)	6(4)	-13(3)
C7A	45(3)	37(3)	97(5)	-31(3)	-27(3)	-1(3)
C8A	48(3)	33(3)	56(3)	-13(2)	-23(3)	-13(2)
C9A	26.0(19)	29(2)	23(2)	-11.5(19)	-9.5(17)	-7.1(18)
C10A	33(2)	31(3)	29(2)	-5(2)	-4.4(19)	-13(2)
C11A	39(2)	45(3)	25(2)	-14(2)	-1.7(19)	-18(2)
C12A	38(2)	45(3)	36(3)	-24(2)	-2(2)	-10(2)
C13A	46(3)	34(3)	40(3)	-17(2)	-10(2)	-5(2)
C14A	38(2)	35(3)	25(2)	-9(2)	-7.6(19)	-13(2)
C15A	28(2)	23(2)	27(2)	-7.1(18)	-8.3(18)	-10.6(17)
C16A	37(2)	42(3)	24(2)	-7(2)	-5.9(19)	-16(2)
C17A	33(2)	52(3)	33(3)	-11(2)	3(2)	-20(2)
C18A	27(2)	42(3)	40(3)	-14(2)	-9(2)	-12(2)
C19A	36(2)	41(3)	28(2)	-14(2)	-12(2)	-12(2)
C20A	32(2)	32(3)	27(2)	-9(2)	-7.3(18)	-13.9(19)
O3B	34.4(16)	28.3(17)	32.4(18)	-10.7(14)	-2.4(13)	-14.0(14)
O4B	48(2)	32(2)	64(3)	-16.3(19)	-4.2(18)	-18.1(17)
O5B	49(2)	63(3)	84(3)	-14(3)	20(2)	-31(2)
N1B	31(2)	42(3)	40(2)	-6(2)	-4.4(18)	-17.1(19)
O3C	67(2)	28.8(19)	37(2)	-16.6(16)	-26.4(18)	0.5(17)

O4C	58(2)	28.6(18)	46(2)	-17.2(16)	-24.6(18)	0.4(16)
O5C	71(2)	30.0(19)	45(2)	-23.4(17)	-3.8(19)	-13.3(18)
N1C	47(2)	33(2)	30(2)	-15.2(19)	-5.8(18)	-12.7(19)
O3D	32.0(16)	59(2)	23.9(17)	-9.9(16)	-7.7(13)	-9.6(16)
O4D	33.4(17)	43(2)	29.1(19)	-0.9(16)	-6.4(14)	-4.7(15)
O5D	36.3(19)	69(3)	39(2)	-11(2)	7.1(17)	-16.8(19)
N1D	31(2)	37(2)	27(2)	-13.6(19)	-1.6(17)	-6.1(17)
O1W	36.3(16)	30.3(17)	23.4(16)	-12.5(14)	-11.4(13)	-5.2(14)

Table 4 Bond Lengths for $Eu(NO_3)_3(4)_2(H_2O)$

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Eu1	O1	2.306(3)	C19	C20	1.385(7)
Eu1	O1A	2.301(3)	P1A	O1A	1.498(3)
Eu1	O3B	2.486(3)	P1A	C2A	1.820(5)
Eu1	O4B	2.475(4)	P1A	C9A	1.797(4)
Eu1	N1B	2.902(4)	P1A	C15A	1.796(4)
Eu1	O3C	2.482(3)	O2A	C1A	1.210(5)
Eu1	O4C	2.513(3)	C1A	C2A	1.525(6)
Eu1	N1C	2.939(4)	C1A	C3A	1.482(6)
Eu1	O3D	2.500(3)	C3A	C4A	1.390(7)
Eu1	O4D	2.498(3)	C3A	C8A	1.397(7)
Eu1	N1D	2.944(4)	C4A	C5A	1.380(8)
Eu1	O1W	2.392(3)	C5A	C6A	1.381(10)
P1	O1	1.492(3)	C6A	C7A	1.374(10)
P1	C2	1.816(4)	C7A	C8A	1.376(8)
P1	C9	1.794(4)	C9A	C10A	1.372(6)
P1	C15	1.777(4)	C9A	C14A	1.382(6)
O2	C1	1.218(6)	C10A	C11A	1.388(6)
C1	C2	1.525(6)	C11A	C12A	1.373(7)
C1	C3	1.474(6)	C12A	C13A	1.399(7)
C3	C4	1.396(7)	C13A	C14A	1.369(7)
C3	C8	1.390(7)	C15A	C16A	1.388(6)
C4	C5	1.374(7)	C15A	C20A	1.382(6)
C5	C6	1.372(9)	C16A	C17A	1.389(7)
C6	C7	1.372(8)	C17A	C18A	1.382(7)
C7	C8	1.384(7)	C18A	C19A	1.369(7)
C9	C10	1.373(7)	C19A	C20A	1.376(6)
C9	C14	1.377(7)	O3B	N1B	1.257(5)
C10	C11	1.383(8)	O4B	N1B	1.264(5)
C11	C12	1.380(9)	O5B	N1B	1.211(5)
C12	C13	1.378(8)	O3C	N1C	1.261(5)
C13	C14	1.373(7)	O4C	N1C	1.282(5)
C15	C16	1.396(6)	O5C	N1C	1.208(5)
C15	C20	1.393(7)	O3D	N1D	1.285(5)
C16	C17	1.379(7)	O4D	N1D	1.265(5)
C17	C18	1.362(9)	O5D	N1D	1.201(5)
C18	C19	1.374(9)			

Table 5 Bond Angles for $Eu(NO_3)_3(4)_2(H_2O)$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Eu1	O3B	72.52(10)	C5	C4	C3	120.2(5)
O1	Eu1	O4B	123.42(11)	C6	C5	C4	121.0(5)
O1	Eu1	N1B	97.84(12)	C7	C6	C5	119.7(5)
O1	Eu1	O3C	145.77(12)	C6	C7	C8	120.1(5)
O1	Eu1	O4C	151.16(12)	C7	C8	C3	120.7(5)
O1	Eu1	N1C	160.10(12)	C10	C9	P1	124.2(4)
O1	Eu1	O3D	75.64(12)	C10	C9	C14	119.2(4)
O1	Eu1	O4D	80.04(12)	C14	C9	P1	116.6(4)
O1	Eu1	N1D	76.22(11)	C9	C10	C11	120.2(5)
O1	Eu1	O1W	82.81(11)	C12	C11	C10	120.4(6)
O1A	Eu1	O1	84.39(11)	C13	C12	C11	119.3(5)
O1A	Eu1	O3B	79.20(10)	C14	C13	C12	119.9(5)
O1A	Eu1	O4B	80.86(12)	C13	C14	C9	121.1(5)
O1A	Eu1	N1B	78.22(11)	C16	C15	P1	120.9(4)
O1A	Eu1	O3C	127.63(11)	C20	C15	P1	118.3(3)
O1A	Eu1	O4C	77.56(11)	C20	C15	C16	120.3(4)
O1A	Eu1	N1C	102.98(11)	C17	C16	C15	119.0(5)
O1A	Eu1	O3D	125.55(11)	C18	C17	C16	120.7(5)
O1A	Eu1	O4D	76.23(11)	C17	C18	C19	120.8(5)
O1A	Eu1	N1D	100.66(11)	C18	C19	C20	120.2(5)
O1A	Eu1	O1W	152.05(11)	C19	C20	C15	119.0(5)
O3B	Eu1	N1B	25.51(11)	O1A	P1A	C2A	109.04(19)
O3B	Eu1	O4C	124.65(12)	O1A	P1A	C9A	111.35(19)
O3B	Eu1	N1C	126.73(11)	O1A	P1A	C15A	109.90(19)
O3B	Eu1	O3D	136.97(11)	C9A	P1A	C2A	109.1(2)
O3B	Eu1	O4D	144.61(11)	C15A	P1A	C2A	109.0(2)
O3B	Eu1	N1D	148.61(11)	C15A	P1A	C9A	108.51(19)
O4B	Eu1	O3B	51.14(11)	P1A	O1A	Eu1	161.7(2)
O4B	Eu1	N1B	25.65(11)	O2A	C1A	C2A	119.5(4)
O4B	Eu1	O3C	78.76(13)	O2A	C1A	C3A	121.6(4)
O4B	Eu1	O4C	75.89(13)	C3A	C1A	C2A	118.9(4)
O4B	Eu1	N1C	76.31(12)	C1A	C2A	P1A	116.2(3)
O4B	Eu1	O3D	151.02(13)	C4A	C3A	C1A	122.8(4)
O4B	Eu1	O4D	145.28(12)	C4A	C3A	C8A	118.7(5)
O4B	Eu1	N1D	160.24(12)	C8A	C3A	C1A	118.5(5)
N1B	Eu1	N1C	101.74(12)	C5A	C4A	C3A	120.4(6)
N1B	Eu1	N1D	174.05(11)	C4A	C5A	C6A	120.0(7)
O3C	Eu1	O3B	120.25(12)	C7A	C6A	C5A	120.3(6)
O3C	Eu1	N1B	100.31(13)	C6A	C7A	C8A	120.0(6)
O3C	Eu1	O4C	50.83(11)	C7A	C8A	C3A	120.5(6)
O3C	Eu1	N1C	25.13(11)	C10A	C9A	P1A	123.0(3)
O3C	Eu1	O3D	75.18(13)	C10A	C9A	C14A	120.2(4)
O3C	Eu1	O4D	94.98(12)	C14A	C9A	P1A	116.8(3)
O3C	Eu1	N1D	85.03(13)	C9A	C10A	C11A	120.3(4)
O4C	Eu1	N1B	100.22(13)	C12A	C11A	C10A	119.5(4)
O4C	Eu1	N1C	25.71(11)	C11A	C12A	C13A	120.0(4)
O4C	Eu1	N1D	85.16(13)	C14A	C13A	C12A	119.9(5)
N1C	Eu1	N1D	84.21(12)	C13A	C14A	C9A	120.0(4)
O3D	Eu1	N1B	153.53(11)	C16A	C15A	P1A	118.0(3)
O3D	Eu1	O4C	96.78(12)	C20A	C15A	P1A	121.6(3)

O3D	Eu1	N1C	85.18(12)	C20A	C15A	C16A	120.3(4)
O3D	Eu1	N1D	25.68(10)	C15A	C16A	C17A	119.2(4)
O4D	Eu1	N1B	154.44(12)	C18A	C17A	C16A	119.8(4)
O4D	Eu1	O4C	73.96(13)	C19A	C18A	C17A	120.6(4)
O4D	Eu1	N1C	83.78(12)	C18A	C19A	C20A	120.2(4)
O4D	Eu1	O3D	50.89(10)	C19A	C20A	C15A	119.9(4)
O4D	Eu1	N1D	25.21(11)	N1B	O3B	Eu1	96.1(3)
O1W	Eu1	O3B	73.29(10)	N1B	O4B	Eu1	96.4(3)
O1W	Eu1	O4B	85.66(12)	O3B	N1B	Eu1	58.4(2)
O1W	Eu1	N1B	79.06(11)	O3B	N1B	O4B	116.3(4)
O1W	Eu1	O3C	72.57(11)	O4B	N1B	Eu1	58.0(2)
O1W	Eu1	O4C	122.60(11)	O5B	N1B	Eu1	177.9(4)
O1W	Eu1	N1C	97.38(11)	O5B	N1B	O3B	121.4(5)
O1W	Eu1	O3D	74.70(10)	O5B	N1B	O4B	122.3(4)
O1W	Eu1	O4D	125.39(11)	N1C	O3C	Eu1	98.2(2)
O1W	Eu1	N1D	100.25(11)	N1C	O4C	Eu1	96.1(3)
O1	P1	C2	111.1(2)	O3C	N1C	Eu1	56.7(2)
O1	P1	C9	113.0(2)	O3C	N1C	O4C	114.9(4)
O1	P1	C15	109.7(2)	O4C	N1C	Eu1	58.2(2)
C9	P1	C2	108.9(2)	O5C	N1C	Eu1	179.2(3)
C15	P1	C2	105.5(2)	O5C	N1C	O3C	122.6(4)
C15	P1	C9	108.4(2)	O5C	N1C	O4C	122.5(4)
P1	O1	Eu1	156.0(2)	N1D	O3D	Eu1	96.9(3)
O2	C1	C2	118.9(4)	N1D	O4D	Eu1	97.5(2)
O2	C1	C3	120.2(4)	O3D	N1D	Eu1	57.5(2)
C3	C1	C2	120.8(4)	O4D	N1D	Eu1	57.2(2)
C1	C2	P1	109.9(3)	O4D	N1D	O3D	114.7(4)
C4	C3	C1	117.7(4)	O5D	N1D	Eu1	178.3(4)
C8	C3	C1	123.9(4)	O5D	N1D	O3D	122.1(4)
C8	C3	C4	118.3(4)	O5D	N1D	O4D	123.2(4)

Table 6 Hydrogen Bonds for $Eu(NO_3)_3(4)_2(H_2O)$

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1W	H1WA	O3D[1]	0.90	1.90	2.748(4)	156.8
O1W	H1WB	O2	0.90	1.83	2.725(5)	172.9

[1]1-X,2-Y,1-Z

Table 7 Torsion Angles for $Eu(NO_3)_3(4)_2(H_2O)$.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Eu1	O3B	N1B	O4B	-2.8(4)	C15	C16	C17	C18	2.2(7)
Eu1	O3B	N1B	O5B	177.5(4)	C16	C15	C20	C19	0.4(7)
Eu1	O4B	N1B	O3B	2.8(4)	C16	C17	C18	C19	-1.9(8)
Eu1	O4B	N1B	O5B	-177.5(4)	C17	C18	C19	C20	0.7(8)
Eu1	O3C	N1C	O4C	1.4(4)	C18	C19	C20	C15	0.0(8)
Eu1	O3C	N1C	O5C	-179.7(4)	C20	C15	C16	C17	-1.5(7)
Eu1	O4C	N1C	O3C	-1.4(4)	P1A	C9A	C10A	C11A	177.0(3)
Eu1	O4C	N1C	O5C	179.8(4)	P1A	C9A	C14A	C13A	-178.2(4)

Eu1	O3D	N1D	O4D	1.3(4)	P1A	C15A	C16A	C17A	179.3(4)
Eu1	O3D	N1D	O5D	-178.1(4)	P1A	C15A	C20A	C19A	-178.6(4)
Eu1	O4D	N1D	O3D	-1.3(4)	O1A	P1A	C2A	C1A	140.0(3)
Eu1	O4D	N1D	O5D	178.1(4)	O1A	P1A	C9A	C10A	161.8(4)
P1	C9	C10	C11	179.2(5)	O1A	P1A	C9A	C14A	-20.2(4)
P1	C9	C14	C13	-178.8(5)	O1A	P1A	C15A	C16A	-18.1(4)
P1	C15	C16	C17	170.4(4)	O1A	P1A	C15A	C20A	161.2(4)
P1	C15	C20	C19	-171.7(4)	O2A	C1A	C2A	P1A	77.9(5)
O1	P1	C2	C1	63.3(4)	O2A	C1A	C3A	C4A	-163.3(5)
O1	P1	C9	C10	131.4(5)	O2A	C1A	C3A	C8A	16.2(6)
O1	P1	C9	C14	-49.7(5)	C1A	C3A	C4A	C5A	178.9(5)
O1	P1	C15	C16	158.7(3)	C1A	C3A	C8A	C7A	-179.5(5)
O1	P1	C15	C20	-29.3(4)	C2A	P1A	O1A	Eu1	35.0(7)
O2	C1	C2	P1	-76.8(5)	C2A	P1A	C9A	C10A	41.4(4)
O2	C1	C3	C4	-3.2(7)	C2A	P1A	C9A	C14A	-140.6(3)
O2	C1	C3	C8	174.5(4)	C2A	P1A	C15A	C16A	101.3(4)
C1	C3	C4	C5	177.9(5)	C2A	P1A	C15A	C20A	-79.4(4)
C1	C3	C8	C7	-177.7(5)	C2A	C1A	C3A	C4A	18.8(7)
C2	P1	O1	Eu1	67.1(5)	C2A	C1A	C3A	C8A	-161.7(4)
C2	P1	C9	C10	7.5(5)	C3A	C1A	C2A	P1A	-104.1(4)
C2	P1	C9	C14	-173.6(4)	C3A	C4A	C5A	C6A	0.9(10)
C2	P1	C15	C16	-81.6(4)	C4A	C3A	C8A	C7A	0.0(7)
C2	P1	C15	C20	90.5(4)	C4A	C5A	C6A	C7A	-0.6(11)
C2	C1	C3	C4	178.4(4)	C5A	C6A	C7A	C8A	-0.1(10)
C2	C1	C3	C8	-3.9(7)	C6A	C7A	C8A	C3A	0.4(8)
C3	C1	C2	P1	101.6(4)	C8A	C3A	C4A	C5A	-0.6(9)
C3	C4	C5	C6	-0.4(9)	C9A	P1A	O1A	Eu1	-85.4(6)
C4	C3	C8	C7	-0.1(7)	C9A	P1A	C2A	C1A	-98.2(4)
C4	C5	C6	C7	0.7(10)	C9A	P1A	C15A	C16A	-140.1(4)
C5	C6	C7	C8	-0.7(9)	C9A	P1A	C15A	C20A	39.2(4)
C6	C7	C8	C3	0.4(8)	C9A	C10A	C11A	C12A	2.2(7)
C8	C3	C4	C5	0.1(7)	C10A	C9A	C14A	C13A	-0.1(7)
C9	P1	O1	Eu1	-55.6(5)	C10A	C11A	C12A	C13A	-2.5(7)
C9	P1	C2	C1	-171.7(3)	C11A	C12A	C13A	C14A	1.5(8)
C9	P1	C15	C16	34.9(4)	C12A	C13A	C14A	C9A	-0.2(7)
C9	P1	C15	C20	-153.1(3)	C14A	C9A	C10A	C11A	-0.9(7)
C9	C10	C11	C12	0.0(11)	C15A	P1A	O1A	Eu1	154.4(6)
C10	C9	C14	C13	0.1(9)	C15A	P1A	C2A	C1A	20.0(4)
C10	C11	C12	C13	-0.9(11)	C15A	P1A	C9A	C10A	-77.1(4)
C11	C12	C13	C14	1.4(10)	C15A	P1A	C9A	C14A	100.8(3)
C12	C13	C14	C9	-1.1(10)	C15A	C16A	C17A	C18A	-1.2(8)
C14	C9	C10	C11	0.4(9)	C16A	C15A	C20A	C19A	0.6(7)
C15	P1	O1	Eu1	-176.6(4)	C16A	C17A	C18A	C19A	1.8(8)
C15	P1	C2	C1	-55.6(4)	C17A	C18A	C19A	C20A	-1.2(8)
C15	P1	C9	C10	-106.8(5)	C18A	C19A	C20A	C15A	0.0(7)
C15	P1	C9	C14	72.1(4)	C20A	C15A	C16A	C17A	0.0(7)

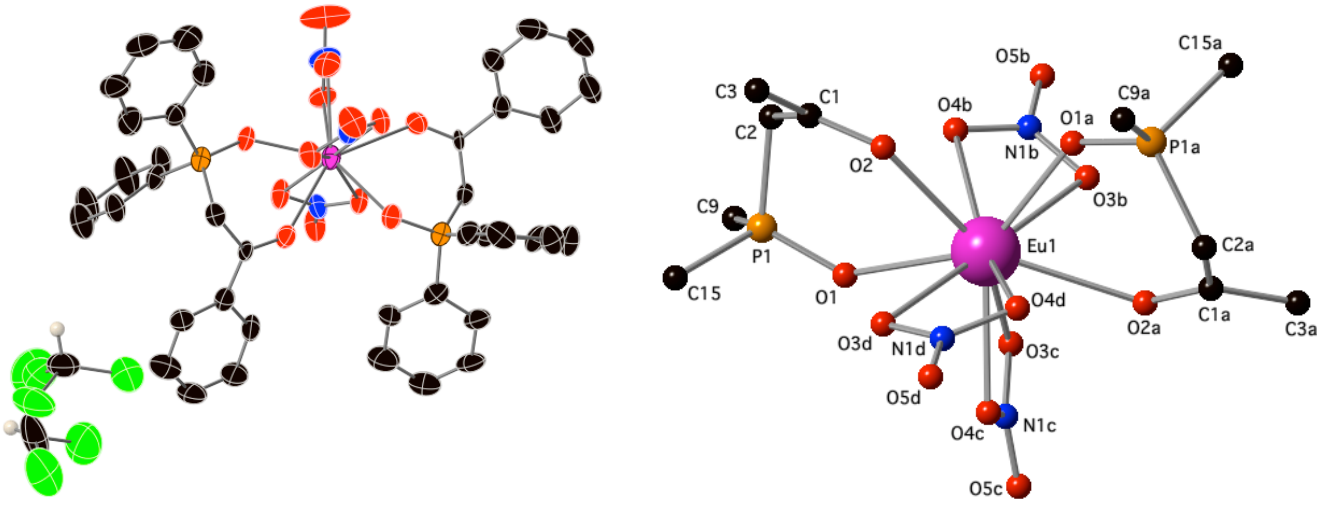
Table 8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for $Eu(NO_3)_3(4)_2(H_2O)$.

Atom	***x***	***y***	***z***	**U(eq)**
H2A	5203	13794	5614	34

H2B	5291	12561	5358	34
H4	884	14646	5941	49
H5	-454	16668	6130	65
H6	429	18077	6259	65
H7	2683	17484	6169	56
H8	4053	15457	5979	43
H10	7493	12841	5572	62
H11	9722	12299	5577	81
H12	10725	10791	6612	64
H13	9466	9877	7659	67
H14	7257	10398	7639	56
H16	5892	13892	7192	41
H17	4567	15335	7950	58
H18	2585	15196	8614	68
H19	1812	13707	8482	61
H20	3074	12281	7696	40
H2AA	5106	5835	9162	34
H2AB	6107	5617	8396	34
H4A	8081	4902	7890	61
H5A	9886	3452	7315	87
H6A	10954	1426	8047	83
H7A	10252	858	9355	68
H8A	8478	2308	9941	51
H10A	5103	6700	10366	37
H11A	3626	7901	11228	41
H12A	2505	10084	10778	46
H13A	2988	11103	9487	48
H14A	4503	9908	8648	38
H16A	8456	7505	7764	40
H17A	10561	7226	7940	47
H18A	11041	6768	9176	41
H19A	9494	6468	10236	39
H20A	7414	6704	10074	34
H1WA	3789	10142	5495	44
H1WB	3296	11054	5977	44

E. $Eu(NO_3)_3$**4**$_2$•$(CHCl_3)_2$

For this structure, only one orientation of the disordered $CHCl_3$ molecule is shown.



Experimental

Single crystals of $C_{42}H_{36}Cl_6EuN_3O_{13}P_2$ were grown at 4 °C from slow diffusion of hexane into a solution of the 3:1 $Eu(NO_3)_3$-4 complex in chloroform and used as received. A suitable crystal was selected and mounted using a small amount of paratone oil on a nylon loop on a Bruker APEX-II CCD diffractometer. The crystal was kept at 173(2) K during data collection. Using Olex2 [1], the structure was solved with the olex2.solve [2] structure solution program using Charge Flipping and refined with the ShelXL [3] refinement package using Least Squares minimization.

The disordered $CHCl_3$ molecule was modeled over two positions with 50% occupancy each. Severely disordered electron density located on a symmetry center with coordinates of [0.000, 0.000, 0.500] and likely corresponding to another $CHCl_3$ molecule was removed using the BYPASS [4] instructions as implemented in Olex2. [1] This space has a volume of 147.9 Å^3 and contains 57.7 electrons.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Bourhis, L.J., Dolomanov, O.V., Gildea, R.J., Howard, J.A.K., Puschmann, H. (2015). Acta Cryst. A71, 59-75.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.
4. van der Sluis, P.; Spek, A. L. (1990). Acta Cryst. A*46*, 194-201.

Crystal structure determination of $Eu(NO_3)_3$**4**$_2$•$(CHCl_3)_2$

Crystal Data for $C_{42}H_{36}Cl_6EuN_3O_{13}P_2$ (M =1217.34 g/mol): triclinic, space group P-1 (no. 2), a = 12.5305(12) Å, b = 14.0929(14) Å, c = 16.2116(16) Å, α = 71.5480(10)°, β = 80.1730(10)°, γ = 72.0490(10)°, V = 2575.0(4) Å^3, Z = 2, T = 173.15 K, μ(MoKα) = 1.652 mm^{-1}, *Dcalc* = 1.570 g/cm^3, 51489 reflections measured (2.658° ≤ 2Θ ≤ 51.478°), 9820 unique (R_{int} = 0.1507, R_{sigma} = 0.1278) which were used in all calculations. The final R_1 was 0.0730 (I > 2σ(I)) and wR_2 was 0.1769 (all data).

Refinement model description

Number of restraints - 39, number of constraints - unknown.
Details:
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups
2. Rigid bond restraints
 Cl1X, Cl2X, Cl3X, C1X
 with sigma for 1-2 distances of 0.005 and sigma for 1-3 distances of 0.005
 Cl1Y, Cl2Y, Cl3Y, C1Y
 with sigma for 1-2 distances of 0.005 and sigma for 1-3 distances of 0.005

3. Uiso/Uaniso restraints and constraints
Cl1X ≈ Cl2X ≈ Cl3X ≈ C1X: within 1.8A with sigma of 0.01 and sigma
for terminal atoms of 0.02
Cl1Y ≈ Cl2Y ≈ Cl3Y ≈ C1Y: within 1.8A with sigma of 0.01 and sigma
for terminal atoms of 0.02
4. Same fragment restrains
{Cl1S, C1S} sigma for 1-2: 0.02, 1-3: 0.04
as
{Cl1X, C1X}
{Cl1S, C1S} sigma for 1-2: 0.02, 1-3: 0.04
as
{Cl1Y, C1Y}
5. Others
Fixed Sof: Cl1X(0.5) C1X(0.5) H1X(0.5) Cl2X(0.5) Cl3X(0.5) Cl1Y(0.5) C1Y(0.5)
H1Y(0.5) Cl2Y(0.5) Cl3Y(0.5)
6.a Ternary CH refined with riding coordinates:
C1X(H1X), C1Y(H1Y), C1S(H1S)
6.b Secondary CH2 refined with riding coordinates:
C2(H2A,H2B), C2A(H2AA,H2AB)
6.c Aromatic/amide H refined with riding coordinates:
C4(H4), C5(H5), C6(H6), C7(H7), C8(H8), C10(H10), C11(H11), C12(H12),
C13(H13), C14(H14), C16(H16), C17(H17), C18(H18), C19(H19), C20(H20), C4A(H4A),
C5A(H5A), C6A(H6A), C7A(H7A), C8A(H8A), C10A(H10A), C11A(H11A), C12A(H12A),
C13A(H13A), C14A(H14A), C16A(H16A), C17A(H17A), C18A(H18A), C19A(H19A),
C20A(H20A)

Table 1 Crystal data and structure refinement for $Eu(NO_3)_3L_2 \bullet (CHCl_3)_2$.

Structure number	**9**
CCDC number	1484661
Empirical formula	$C_{42}H_{36}Cl_6EuN_3O_{13}P_2$
Formula weight	1217.34
Temperature/K	173(2)
Crystal system	triclinic
Space group	P-1
a/Å	12.5305(12)
b/Å	14.0929(14)
c/Å	16.2116(16)
α/°	71.5480(10)
β/°	80.1730(10)
γ/°	72.0490(10)
Volume/Å^3	2575.0(4)
Z	2
ϱ_{calc}g/cm^3	1.570
μ/mm^{-1}	1.652
F(000)	1216.0
Crystal size/mm^3	0.19 × 0.119 × 0.073
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.658 to 51.478
Index ranges	-15 ≤ h ≤ 15, -17 ≤ k ≤ 17, -19 ≤ l ≤ 19
Reflections collected	51489
Independent reflections	9820 [R_{int} = 0.1507, R_{sigma} = 0.1278]
Data/restraints/parameters	9820/39/640
Goodness-of-fit on F^2	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0730, wR_2 = 0.1540
Final R indexes [all data]	R_1 = 0.1287, wR_2 = 0.1769

Largest diff. peak/hole / e Å^{-3} 1.86/-0.92

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $Eu(NO_3)_3 4_2 \bullet (CHCl_3)_2$. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Eu1	3823.6(4)	2844.1(3)	7590.0(3)	33.14(16)
P1	3910(2)	2162.7(17)	9916.7(14)	36.2(6)
O1	3378(5)	2689(4)	9083(3)	36.7(14)
O2	5621(5)	2344(4)	8287(4)	40.6(14)
O4D	4418(5)	4415(4)	6652(3)	37.3(14)
O3D	4218(5)	4342(4)	8000(4)	45.8(16)
O5D	4597(6)	5688(5)	7035(4)	52.9(18)
O3B	3437(5)	1313(4)	7209(4)	39.1(14)
O4B	4204(5)	927(4)	8399(4)	43.8(15)
O5B	3812(6)	-269(4)	8047(4)	55.1(18)
O3C	1806(5)	2835(5)	7856(4)	52.1(17)
O4C	2149(5)	4332(4)	7508(4)	43.0(15)
O5C	429(7)	4247(7)	7663(7)	111(3)
N1D	4403(6)	4836(5)	7231(5)	37.3(17)
N1B	3801(6)	644(5)	7882(5)	36.0(17)
N1C	1439(7)	3805(7)	7684(6)	59(2)
C1	5984(7)	1972(6)	9014(5)	33(2)
C2	5315(7)	1381(6)	9734(5)	34(2)
C3	6948(7)	2261(6)	9189(5)	39(2)
C4	7430(8)	2961(7)	8523(6)	45(2)
C5	8367(9)	3201(9)	8637(8)	67(3)
C6	8842(9)	2762(9)	9408(8)	65(3)
C7	8416(9)	2055(8)	10076(8)	64(3)
C8	7477(8)	1811(7)	9958(6)	47(2)
C9	3120(7)	1308(7)	10636(6)	40(2)
C10	2287(8)	1134(7)	10302(6)	51(3)
C11	1677(9)	466(8)	10804(8)	63(3)
C12	1897(9)	-11(8)	11654(8)	64(3)
C13	2732(10)	124(9)	11984(7)	76(4)
C14	3338(9)	813(8)	11499(6)	61(3)
C15	4049(7)	3079(6)	10412(5)	36(2)
C16	3453(8)	4124(7)	10107(6)	49(2)
C17	3583(10)	4815(7)	10485(7)	70(3)
C18	4252(10)	4533(8)	11141(7)	68(3)
C19	4831(10)	3530(8)	11435(7)	64(3)
C20	4741(8)	2787(7)	11088(6)	45(2)
P1A	5632.8(19)	2628.3(17)	5640.6(14)	34.5(5)
O1A	5302(5)	2251(4)	6592(3)	36.8(14)
O2A	3038(5)	3320(4)	6126(4)	37.9(14)
C1A	3413(7)	3459(6)	5355(5)	32.1(19)
C2A	4539(6)	3672(6)	5081(5)	31.4(19)
C3A	2763(7)	3292(6)	4751(5)	36(2)
C4A	1834(8)	2906(7)	5083(6)	46(2)
C5A	1231(8)	2748(8)	4545(8)	61(3)
C6A	1511(10)	2972(10)	3658(8)	79(4)
C7A	2422(10)	3350(9)	3311(7)	75(4)
C8A	3036(9)	3510(8)	3855(6)	56(3)

C9A	6796(7)	3160(6)	5464(6)	40(2)
C10A	7295(7)	3553(7)	4631(6)	48(2)
C11A	8118(7)	4022(7)	4531(6)	52(3)
C12A	8517(8)	4110(8)	5232(8)	60(3)
C13A	8034(9)	3716(9)	6067(8)	73(3)
C14A	7208(8)	3240(8)	6172(6)	50(3)
C15A	5944(7)	1607(6)	5139(5)	37(2)
C16A	6130(8)	584(7)	5666(6)	47(2)
C17A	6384(8)	-235(7)	5313(7)	55(3)
C18A	6486(8)	-52(8)	4412(7)	53(3)
C19A	6289(8)	952(8)	3883(6)	54(3)
C20A	6023(8)	1767(7)	4248(6)	47(2)
Cl1X	-614(8)	4679(8)	647(6)	151(3)
C1X	-600(30)	3830(30)	1678(17)	106(5)
Cl2X	454(12)	2676(11)	1719(9)	128(4)
Cl3X	-1933(13)	3501(11)	1926(9)	144(4)
Cl1Y	-980(9)	2661(9)	2924(7)	148(3)
C1Y	-820(50)	3530(40)	1910(20)	161(7)
Cl2Y	-1889(19)	3619(16)	1406(12)	220(7)
Cl3Y	580(20)	3093(14)	1420(12)	220(9)
Cl1S	784(3)	736(2)	8643(2)	82.8(9)
C1S	1052(10)	734(11)	7561(7)	88(4)
Cl2S	1163(3)	-497(4)	7480(3)	112.2(13)
Cl3S	41(3)	1686(3)	6929(2)	124.9(16)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $Eu(NO_3)_3 4_2 \bullet (CHCl_3)_2$. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Eu1	46.4(3)	30.0(2)	25.3(2)	-6.57(17)	0.26(18)	-16.45(19)
P1	46.6(14)	35.4(13)	28.1(12)	-10.6(10)	1.6(10)	-13.9(11)
O1	48(4)	37(3)	23(3)	-8(3)	3(3)	-13(3)
O2	47(4)	48(4)	30(3)	-11(3)	5(3)	-22(3)
O4D	58(4)	35(3)	25(3)	-10(3)	4(3)	-25(3)
O3D	75(5)	42(4)	25(3)	-8(3)	3(3)	-27(3)
O5D	99(5)	38(4)	34(4)	-5(3)	-7(3)	-41(4)
O3B	58(4)	34(3)	28(3)	-5(3)	-9(3)	-17(3)
O4B	64(4)	35(3)	40(4)	-11(3)	-7(3)	-24(3)
O5B	80(5)	26(3)	66(5)	-12(3)	-19(4)	-18(3)
O3C	62(4)	47(4)	51(4)	-8(3)	7(3)	-33(3)
O4C	38(4)	34(3)	55(4)	-9(3)	5(3)	-16(3)
O5C	45(5)	89(6)	185(10)	-28(6)	10(6)	-22(5)
N1D	50(5)	38(4)	30(4)	-11(4)	-7(3)	-17(4)
N1B	51(5)	30(4)	33(4)	-11(3)	0(4)	-20(4)
N1C	43(6)	58(6)	76(6)	-18(5)	10(5)	-21(5)
C1	39(5)	52(5)	15(4)	-5(4)	5(4)	-30(4)
C2	43(5)	25(4)	32(5)	-5(4)	-9(4)	-6(4)
C3	43(5)	39(5)	33(5)	-12(4)	0(4)	-7(4)
C4	64(7)	54(6)	28(5)	-15(4)	5(4)	-33(5)
C5	64(7)	95(9)	68(8)	-37(7)	8(6)	-53(7)
C6	48(7)	89(9)	80(8)	-36(7)	-1(6)	-38(6)

C7	49(7)	63(7)	86(8)	-24(6)	-15(6)	-13(6)
C8	46(6)	56(6)	44(6)	-11(5)	1(5)	-27(5)
C9	40(5)	41(5)	37(5)	-16(4)	1(4)	-7(4)
C10	60(7)	58(6)	42(6)	-15(5)	0(5)	-26(5)
C11	66(7)	62(7)	72(8)	-22(6)	11(6)	-41(6)
C12	49(7)	62(7)	74(8)	-9(6)	10(6)	-24(6)
C13	73(8)	91(9)	47(7)	24(6)	-8(6)	-39(7)
C14	66(7)	77(8)	41(6)	-5(5)	0(5)	-34(6)
C15	49(5)	33(5)	32(5)	-16(4)	6(4)	-14(4)
C16	66(7)	42(6)	39(6)	-20(4)	-15(5)	1(5)
C17	116(10)	32(6)	67(8)	-25(5)	-36(7)	-2(6)
C18	108(10)	50(7)	59(7)	-28(6)	-27(7)	-17(6)
C19	92(9)	51(7)	54(7)	-20(5)	-23(6)	-13(6)
C20	59(6)	39(5)	43(6)	-22(4)	-13(5)	-4(5)
P1A	40.3(13)	33.0(12)	28.2(12)	-8.4(10)	0.6(10)	-9.4(10)
O1A	47(4)	30(3)	30(3)	-6(2)	-3(3)	-8(3)
O2A	41(4)	36(3)	38(4)	-9(3)	-6(3)	-13(3)
C1A	34(5)	49(5)	12(4)	-9(4)	-6(4)	-8(4)
C2A	44(5)	34(5)	24(4)	-11(4)	4(4)	-21(4)
C3A	41(5)	32(5)	28(5)	-8(4)	-8(4)	1(4)
C4A	50(6)	56(6)	45(6)	-21(5)	-1(5)	-25(5)
C5A	36(6)	66(7)	86(9)	-32(6)	-7(6)	-11(5)
C6A	66(8)	114(11)	66(8)	-26(8)	-30(7)	-23(7)
C7A	90(9)	107(10)	44(7)	-15(6)	-18(6)	-50(8)
C8A	65(7)	69(7)	42(6)	-16(5)	-14(5)	-23(6)
C9A	36(5)	29(5)	45(6)	-6(4)	0(4)	1(4)
C10A	36(5)	53(6)	47(6)	-2(5)	2(4)	-16(5)
C11A	37(6)	56(6)	49(6)	9(5)	3(5)	-21(5)
C12A	47(6)	55(7)	78(8)	-12(6)	-9(6)	-19(5)
C13A	61(7)	89(9)	89(9)	-34(7)	-4(7)	-38(7)
C14A	46(6)	75(7)	43(6)	-18(5)	0(5)	-37(5)
C15A	39(5)	35(5)	32(5)	-11(4)	-2(4)	-4(4)
C16A	51(6)	49(6)	39(5)	-8(5)	3(4)	-19(5)
C17A	61(7)	38(6)	71(8)	-17(5)	-15(6)	-14(5)
C18A	57(7)	54(6)	57(7)	-32(5)	-8(5)	-9(5)
C19A	70(7)	54(6)	38(6)	-23(5)	3(5)	-12(5)
C20A	55(6)	42(5)	44(6)	-23(5)	12(5)	-9(5)
Cl1X	131(7)	177(8)	99(6)	-28(5)	-33(5)	26(6)
C1X	104(9)	113(12)	92(9)	-54(8)	-71(10)	45(7)
Cl2X	137(7)	98(6)	155(10)	-90(6)	-51(8)	34(6)
Cl3X	144(7)	110(8)	179(11)	-92(9)	11(9)	3(6)
Cl1Y	157(8)	179(9)	135(7)	-65(6)	-32(6)	-53(7)
C1Y	186(12)	143(15)	122(12)	-65(10)	-42(9)	45(13)
Cl2Y	281(13)	144(10)	219(12)	-88(11)	-145(12)	72(10)
Cl3Y	253(11)	180(18)	153(12)	-71(11)	46(9)	35(12)
Cl1S	106(3)	66.9(19)	82(2)	-10.1(16)	-14.2(18)	-40.1(18)
C1S	56(8)	134(12)	69(8)	-2(8)	-7(6)	-43(8)
Cl2S	87(3)	151(4)	116(3)	-80(3)	5(2)	-20(2)
Cl3S	101(3)	155(4)	98(3)	51(3)	-42(2)	-77(3)

Table 4 Bond Lengths for $Eu(NO_3)_3 4_2 \bullet (CHCl_3)_2$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Eu1	O1	2.345(5)	C15	C16	1.400(11)
Eu1	O2	2.496(6)	C15	C20	1.392(12)
Eu1	O4D	2.504(5)	C16	C17	1.364(12)
Eu1	O3D	2.605(6)	C17	C18	1.350(14)
Eu1	O3B	2.620(5)	C18	C19	1.346(13)
Eu1	O4B	2.535(5)	C19	C20	1.376(12)
Eu1	O3C	2.494(6)	P1A	O1A	1.493(5)
Eu1	O4C	2.454(6)	P1A	C2A	1.789(8)
Eu1	N1D	2.970(7)	P1A	C9A	1.778(9)
Eu1	N1C	2.875(9)	P1A	C15A	1.781(8)
Eu1	O1A	2.372(5)	O2A	C1A	1.234(9)
Eu1	O2A	2.536(6)	C1A	C2A	1.497(11)
P1	O1	1.480(6)	C1A	C3A	1.489(11)
P1	C2	1.798(8)	C3A	C4A	1.390(11)
P1	C9	1.801(9)	C3A	C8A	1.391(12)
P1	C15	1.785(8)	C4A	C5A	1.355(13)
O2	C1	1.231(9)	C5A	C6A	1.378(15)
O4D	N1D	1.255(8)	C6A	C7A	1.367(15)
O3D	N1D	1.241(8)	C7A	C8A	1.373(13)
O5D	N1D	1.231(8)	C9A	C10A	1.404(11)
O3B	N1B	1.241(8)	C9A	C14A	1.385(12)
O4B	N1B	1.263(8)	C10A	C11A	1.350(12)
O5B	N1B	1.225(8)	C11A	C12A	1.369(13)
O3C	N1C	1.254(9)	C12A	C13A	1.399(15)
O4C	N1C	1.270(9)	C13A	C14A	1.359(12)
O5C	N1C	1.228(10)	C15A	C16A	1.394(11)
C1	C2	1.498(10)	C15A	C20A	1.380(11)
C1	C3	1.482(11)	C16A	C17A	1.377(12)
C3	C4	1.404(11)	C17A	C18A	1.390(13)
C3	C8	1.386(12)	C18A	C19A	1.373(13)
C4	C5	1.373(13)	C19A	C20A	1.382(12)
C5	C6	1.355(15)	Cl1X	C1X	1.72(2)
C6	C7	1.377(14)	C1X	Cl2X	1.74(4)
C7	C8	1.381(12)	C1X	Cl3X	1.82(4)
C9	C10	1.370(12)	Cl1Y	C1Y	1.73(2)
C9	C14	1.383(12)	C1Y	Cl2Y	1.64(7)
C10	C11	1.372(12)	C1Y	Cl3Y	1.81(6)
C11	C12	1.362(14)	Cl1S	C1S	1.729(12)
C12	C13	1.340(14)	C1S	Cl2S	1.743(14)
C13	C14	1.381(13)	C1S	Cl3S	1.726(12)

Table 5 Bond Angles for $Eu(NO_3)_3 4_2 \bullet (CHCl_3)_2$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Eu1	O2	72.03(18)	O3B	N1B	Eu1	60.7(4)
O1	Eu1	O4D	118.02(18)	O3B	N1B	O4B	117.6(6)
O1	Eu1	O3D	69.02(17)	O4B	N1B	Eu1	56.9(4)
O1	Eu1	O3B	110.00(18)	O5B	N1B	Eu1	176.4(6)
O1	Eu1	O4B	71.94(18)	O5B	N1B	O3B	122.8(7)

O1	Eu1	O3C	75.1(2)	O5B	N1B	O4B	119.6(7)
O1	Eu1	O4C	80.65(19)	O3C	N1C	Eu1	59.9(4)
O1	Eu1	N1D	93.38(19)	O3C	N1C	O4C	118.0(8)
O1	Eu1	N1C	77.2(2)	O4C	N1C	Eu1	58.2(4)
O1	Eu1	O1A	141.61(19)	O5C	N1C	Eu1	175.5(8)
O1	Eu1	O2A	145.35(19)	O5C	N1C	O3C	122.0(8)
O2	Eu1	O4D	85.75(18)	O5C	N1C	O4C	120.0(9)
O2	Eu1	O3D	65.55(19)	O2	C1	C2	118.0(7)
O2	Eu1	O3B	113.69(18)	O2	C1	C3	119.6(7)
O2	Eu1	O4B	73.31(19)	C3	C1	C2	121.6(7)
O2	Eu1	N1D	75.62(19)	C1	C2	P1	112.0(6)
O2	Eu1	N1C	146.6(2)	C4	C3	C1	119.5(8)
O2	Eu1	O2A	142.53(18)	C8	C3	C1	123.6(8)
O4D	Eu1	O3D	49.22(17)	C8	C3	C4	116.7(8)
O4D	Eu1	O3B	131.81(17)	C5	C4	C3	121.5(9)
O4D	Eu1	O4B	153.02(19)	C6	C5	C4	119.9(10)
O4D	Eu1	N1D	24.66(16)	C5	C6	C7	120.9(10)
O4D	Eu1	N1C	97.5(2)	C6	C7	C8	119.1(10)
O4D	Eu1	O2A	73.41(17)	C7	C8	C3	121.8(9)
O3D	Eu1	O3B	178.85(18)	C10	C9	P1	118.0(7)
O3D	Eu1	N1D	24.63(16)	C10	C9	C14	119.5(9)
O3D	Eu1	N1C	91.5(2)	C14	C9	P1	122.5(7)
O3B	Eu1	N1D	156.43(18)	C9	C10	C11	121.2(10)
O3B	Eu1	N1C	88.8(2)	C12	C11	C10	118.6(10)
O4B	Eu1	O3D	129.80(19)	C13	C12	C11	121.0(10)
O4B	Eu1	O3B	49.07(18)	C12	C13	C14	121.3(10)
O4B	Eu1	N1D	148.44(19)	C13	C14	C9	118.2(10)
O4B	Eu1	N1C	109.4(2)	C16	C15	P1	119.0(7)
O4B	Eu1	O2A	113.69(18)	C20	C15	P1	122.0(7)
O3C	Eu1	O2	144.66(19)	C20	C15	C16	119.0(8)
O3C	Eu1	O4D	121.6(2)	C17	C16	C15	118.2(9)
O3C	Eu1	O3D	113.6(2)	C18	C17	C16	122.9(10)
O3C	Eu1	O3B	66.4(2)	C19	C18	C17	119.3(10)
O3C	Eu1	O4B	84.6(2)	C18	C19	C20	121.2(10)
O3C	Eu1	N1D	119.3(2)	C19	C20	C15	119.5(9)
O3C	Eu1	N1C	25.79(19)	O1A	P1A	Eu1	27.2(2)
O3C	Eu1	O2A	71.66(19)	O1A	P1A	C2A	112.0(3)
O4C	Eu1	O2	132.22(19)	O1A	P1A	C9A	111.2(4)
O4C	Eu1	O4D	73.37(18)	O1A	P1A	C15A	110.6(4)
O4C	Eu1	O3D	68.34(19)	C2A	P1A	Eu1	85.3(3)
O4C	Eu1	O3B	112.21(19)	C9A	P1A	Eu1	115.5(3)
O4C	Eu1	O4B	133.49(18)	C9A	P1A	C2A	104.5(4)
O4C	Eu1	O3C	51.8(2)	C9A	P1A	C15A	110.7(4)
O4C	Eu1	N1D	67.56(19)	C15A	P1A	Eu1	126.8(3)
O4C	Eu1	N1C	26.1(2)	C15A	P1A	C2A	107.6(4)
O4C	Eu1	O2A	71.38(19)	P1A	O1A	Eu1	136.0(3)
N1C	Eu1	N1D	93.6(2)	C1A	O2A	Eu1	136.7(5)
O1A	Eu1	O2	72.86(18)	O2A	C1A	C2A	120.0(7)
O1A	Eu1	O4D	73.93(18)	O2A	C1A	C3A	117.2(7)
O1A	Eu1	O3D	109.18(18)	C3A	C1A	C2A	122.4(7)
O1A	Eu1	O3B	71.19(18)	C1A	C2A	P1A	111.5(5)
O1A	Eu1	O4B	83.58(18)	C4A	C3A	C1A	119.4(7)

O1A	Eu1	O3C	132.5(2)	C4A	C3A	C8A	117.5(8)
O1A	Eu1	O4C	135.98(18)	C8A	C3A	C1A	123.0(8)
O1A	Eu1	N1D	92.55(19)	C5A	C4A	C3A	120.4(9)
O1A	Eu1	N1C	140.1(2)	C4A	C5A	C6A	121.2(10)
O1A	Eu1	O2A	71.60(18)	C7A	C6A	C5A	119.7(10)
O2A	Eu1	O3D	116.42(17)	C6A	C7A	C8A	119.2(10)
O2A	Eu1	O3B	64.72(17)	C7A	C8A	C3A	121.9(10)
O2A	Eu1	N1D	94.41(18)	C10A	C9A	P1A	123.3(7)
O2A	Eu1	N1C	68.6(2)	C14A	C9A	P1A	119.2(6)
O1	P1	Eu1	25.2(2)	C14A	C9A	C10A	117.5(8)
O1	P1	C2	110.6(3)	C11A	C10A	C9A	120.7(9)
O1	P1	C9	109.8(4)	C10A	C11A	C12A	121.7(9)
O1	P1	C15	111.4(4)	C11A	C12A	C13A	118.3(9)
C2	P1	Eu1	85.4(3)	C14A	C13A	C12A	120.2(11)
C2	P1	C9	107.5(4)	C13A	C14A	C9A	121.5(9)
C9	P1	Eu1	120.6(3)	C16A	C15A	P1A	118.9(7)
C15	P1	Eu1	120.1(3)	C20A	C15A	P1A	123.6(7)
C15	P1	C2	105.9(4)	C20A	C15A	C16A	117.5(8)
C15	P1	C9	111.5(4)	C17A	C16A	C15A	121.3(9)
P1	O1	Eu1	139.2(3)	C16A	C17A	C18A	119.9(9)
C1	O2	Eu1	140.0(5)	C19A	C18A	C17A	119.6(9)
N1D	O4D	Eu1	99.0(4)	C18A	C19A	C20A	119.8(9)
N1D	O3D	Eu1	94.4(4)	C15A	C20A	C19A	121.9(9)
N1B	O3B	Eu1	94.9(4)	Cl1X	C1X	Cl2X	111(2)
N1B	O4B	Eu1	98.4(4)	Cl1X	C1X	Cl3X	107.3(19)
N1C	O3C	Eu1	94.3(5)	Cl2X	C1X	Cl3X	107(2)
N1C	O4C	Eu1	95.8(5)	Cl1Y	C1Y	Cl3Y	109(3)
O4D	N1D	Eu1	56.4(3)	Cl2Y	C1Y	Cl1Y	104(3)
O3D	N1D	Eu1	61.0(4)	Cl2Y	C1Y	Cl3Y	118(3)
O3D	N1D	O4D	117.1(6)	Cl1S	C1S	Cl2S	109.7(7)
O5D	N1D	Eu1	175.6(6)	Cl3S	C1S	Cl1S	111.3(8)
O5D	N1D	O4D	120.5(7)	Cl3S	C1S	Cl2S	111.9(7)
O5D	N1D	O3D	122.4(7)				

Table 6 Torsion Angles for $Eu(NO_3)_3 4_2 \bullet (CHCl_3)_2$.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Eu1	P1	C2	C1	48.5(5)	C11	C12	C13	C14	5.3(19)
Eu1	P1	C9	C10	-15.8(8)	C12	C13	C14	C9	-4.7(18)
Eu1	P1	C9	C14	163.0(7)	C14	C9	C10	C11	-1.0(14)
Eu1	P1	C15	C16	40.4(8)	C15	P1	O1	Eu1	115.7(5)
Eu1	P1	C15	C20	-139.0(6)	C15	P1	C2	C1	-71.6(6)
Eu1	O2	C1	C2	19.7(13)	C15	P1	C9	C10	133.6(7)
Eu1	O2	C1	C3	-150.3(6)	C15	P1	C9	C14	-47.7(9)
Eu1	O4D	N1D	O3D	5.7(7)	C15	C16	C17	C18	-0.5(17)
Eu1	O4D	N1D	O5D	-176.3(7)	C16	C15	C20	C19	-0.5(13)
Eu1	O3D	N1D	O4D	-5.4(7)	C16	C17	C18	C19	0.8(19)
Eu1	O3D	N1D	O5D	176.7(7)	C17	C18	C19	C20	-1.0(18)
Eu1	O3B	N1B	O4B	-2.5(7)	C18	C19	C20	C15	0.8(16)
Eu1	O3B	N1B	O5B	179.5(7)	C20	C15	C16	C17	0.3(14)
Eu1	O4B	N1B	O3B	2.6(7)	P1A	C9A	C10A	C11A	174.7(7)

Eu1	O4B	N1B	O5B	-179.4(6)	P1A	C9A	C14A	C13A	-174.6(8)
Eu1	O3C	N1C	O4C	-3.0(8)	P1A	C15A	C16A	C17A	-179.3(7)
Eu1	O3C	N1C	O5C	175.3(10)	P1A	C15A	C20A	C19A	178.6(7)
Eu1	O4C	N1C	O3C	3.1(9)	O1A	P1A	C2A	C1A	-44.1(6)
Eu1	O4C	N1C	O5C	-175.3(9)	O1A	P1A	C9A	C10A	178.7(7)
Eu1	P1A	C2A	C1A	-49.6(5)	O1A	P1A	C9A	C14A	-4.4(8)
Eu1	P1A	C9A	C10A	-151.9(6)	O1A	P1A	C15A	C16A	-15.9(8)
Eu1	P1A	C9A	C14A	25.0(8)	O1A	P1A	C15A	C20A	164.7(7)
Eu1	P1A	C15A	C16A	-41.1(8)	O2A	C1A	C2A	P1A	59.8(9)
Eu1	P1A	C15A	C20A	139.6(7)	O2A	C1A	C3A	C4A	-5.6(12)
Eu1	O2A	C1A	C2A	-19.1(12)	O2A	C1A	C3A	C8A	174.1(8)
Eu1	O2A	C1A	C3A	154.6(5)	C1A	C3A	C4A	C5A	-180.0(8)
P1	C9	C10	C11	177.8(8)	C1A	C3A	C8A	C7A	-179.9(9)
P1	C9	C14	C13	-176.2(8)	C2A	P1A	O1A	Eu1	-11.9(6)
P1	C15	C16	C17	-179.0(8)	C2A	P1A	C9A	C10A	-60.2(8)
P1	C15	C20	C19	178.9(8)	C2A	P1A	C9A	C14A	116.7(7)
O1	P1	C2	C1	49.2(7)	C2A	P1A	C15A	C16A	-138.6(7)
O1	P1	C9	C10	9.5(8)	C2A	P1A	C15A	C20A	42.1(9)
O1	P1	C9	C14	-171.8(8)	C2A	C1A	C3A	C4A	167.9(8)
O1	P1	C15	C16	14.1(8)	C2A	C1A	C3A	C8A	-12.4(13)
O1	P1	C15	C20	-165.3(7)	C3A	C1A	C2A	P1A	-113.5(7)
O2	C1	C2	P1	-58.4(9)	C3A	C4A	C5A	C6A	-0.6(15)
O2	C1	C3	C4	0.4(13)	C4A	C3A	C8A	C7A	-0.2(14)
O2	C1	C3	C8	-173.9(8)	C4A	C5A	C6A	C7A	0.7(18)
C1	C3	C4	C5	-175.9(9)	C5A	C6A	C7A	C8A	-0.6(19)
C1	C3	C8	C7	176.0(9)	C6A	C7A	C8A	C3A	0.3(18)
C2	P1	O1	Eu1	-1.8(6)	C8A	C3A	C4A	C5A	0.3(13)
C2	P1	C9	C10	-110.8(7)	C9A	P1A	O1A	Eu1	104.6(5)
C2	P1	C9	C14	67.9(9)	C9A	P1A	C2A	C1A	-164.7(6)
C2	P1	C15	C16	134.4(7)	C9A	P1A	C15A	C16A	107.8(7)
C2	P1	C15	C20	-45.0(8)	C9A	P1A	C15A	C20A	-71.5(9)
C2	C1	C3	C4	-169.3(8)	C9A	C10A	C11A	C12A	1.7(15)
C2	C1	C3	C8	16.4(13)	C10A	C9A	C14A	C13A	2.5(14)
C3	C1	C2	P1	111.4(8)	C10A	C11A	C12A	C13A	-1.3(15)
C3	C4	C5	C6	-0.3(16)	C11A	C12A	C13A	C14A	1.5(17)
C4	C3	C8	C7	1.5(14)	C12A	C13A	C14A	C9A	-2.2(17)
C4	C5	C6	C7	1.6(17)	C14A	C9A	C10A	C11A	-2.3(13)
C5	C6	C7	C8	-1.3(17)	C15A	P1A	O1A	Eu1	-132.0(5)
C6	C7	C8	C3	-0.4(15)	C15A	P1A	C2A	C1A	77.6(6)
C8	C3	C4	C5	-1.2(13)	C15A	P1A	C9A	C10A	55.3(8)
C9	P1	O1	Eu1	-120.2(5)	C15A	P1A	C9A	C14A	-127.7(7)
C9	P1	C2	C1	169.1(6)	C15A	C16A	C17A	C18A	1.6(14)
C9	P1	C15	C16	-109.0(7)	C16A	C15A	C20A	C19A	-0.7(14)
C9	P1	C15	C20	71.6(8)	C16A	C17A	C18A	C19A	-2.5(15)
C9	C10	C11	C12	1.4(16)	C17A	C18A	C19A	C20A	1.8(15)
C10	C9	C14	C13	2.5(15)	C18A	C19A	C20A	C15A	-0.2(15)
C10	C11	C12	C13	-3.5(17)	C20A	C15A	C16A	C17A	0.1(13)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for $Eu(NO_3)_3L_2$•$(CHCl_3)_2$

Atom	*x*	*y*	*z*	U(eq)
H2A	5700	1134	10278	41
H2B	5277	763	9586	41
H4	7100	3276	7982	54
H5	8681	3673	8177	80
H6	9479	2944	9489	78
H7	8763	1740	10610	77
H8	7186	1320	10418	57
H10	2130	1483	9712	61
H11	1112	338	10564	75
H12	1452	-445	12017	77
H13	2910	-262	12564	92
H14	3891	944	11751	73
H16	2972	4346	9649	59
H17	3186	5527	10277	84
H18	4313	5036	11392	81
H19	5311	3331	11890	76
H20	5147	2081	11307	55
H2AA	4522	4322	5204	38
H2AB	4703	3773	4444	38
H4A	1622	2752	5692	56
H5A	602	2477	4784	73
H6A	1073	2864	3289	95
H7A	2626	3501	2701	90
H8A	3666	3776	3612	67
H10A	7051	3489	4133	58
H11A	8429	4299	3960	63
H12A	9107	4429	5154	72
H13A	8283	3783	6562	88
H14A	6906	2955	6744	60
H16A	6080	451	6282	56
H17A	6490	-926	5684	66
H18A	6690	-617	4165	64
H19A	6336	1085	3268	64
H20A	5891	2458	3875	57
H1X	-495	4155	2113	127
H1Y	-909	4223	2001	193
H1S	1794	889	7344	106

Table 8 Atomic Occupancy for $Eu(NO_3)_3L_2$•$(CHCl_3)_2$.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
Cl1X	0.5	C1X	0.5	H1X	0.5
Cl2X	0.5	Cl3X	0.5	Cl1Y	0.5
C1Y	0.5	H1Y	0.5	Cl2Y	0.5
Cl3Y	0.5				

Table 9 Solvent masks information for $Eu(NO_3)_3L_2$•$(CHCl_3)_2$.

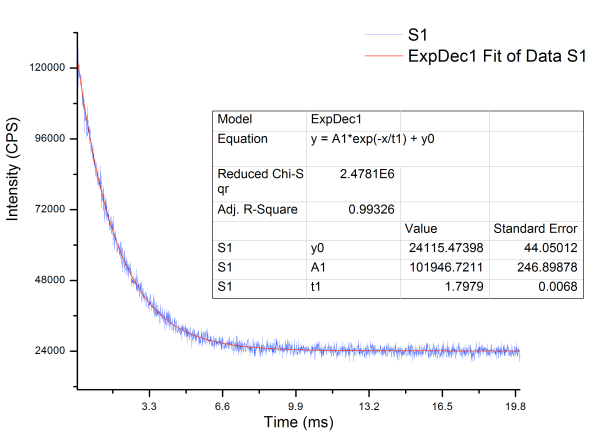
Number	X	Y	Z	Volume	Electron count
1	0.000	0.000	0.500	147.9	57.7
2	0.428	0.153	0.288	9.2	0.0
3	0.572	0.847	0.712	9.2	0.0

II. Luminescence studies

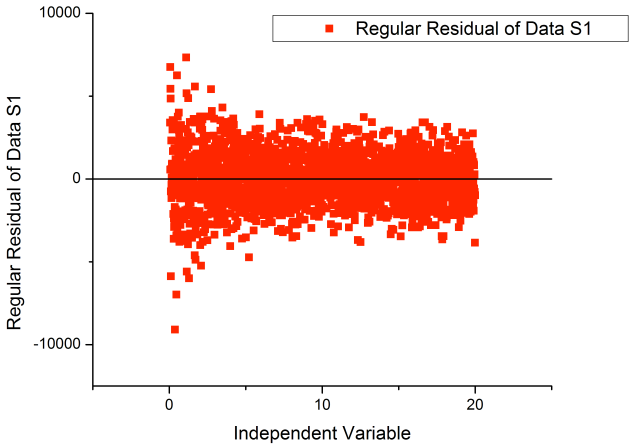
A. Lifetime decay curves and fitting residuals. All lifetimes were measured in CH_3CN with a complex concentration of 2.0 mM and three equivalents of ligand relative to the metal. For all sets of data below, the blue curve is connected data points and the red curve is the fit. All complexes were excited at 350 nm. Please note for each of the residual plots, the units of the x-axis are time (ms), while the units of the y-axis are intensity (counts).

1. Lifetime decay curves of $Tb(NO_3)_3$ complex, monitored at 545 nm.

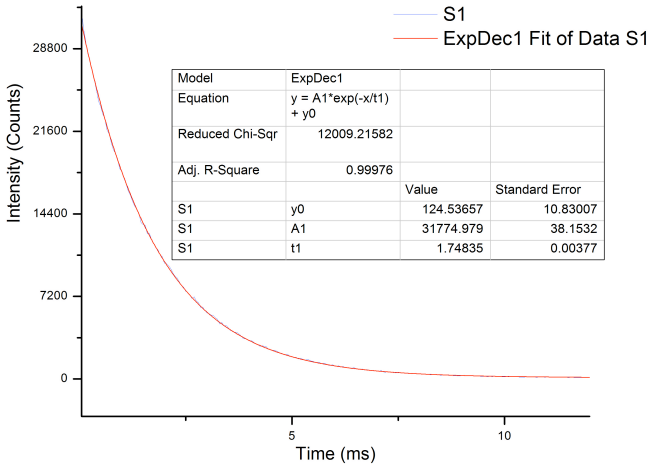
Trial 1 settings: *sample window: 15.00 ms; max delay: 20 ms; averages: 50; slit widths: 0.50 nm both excitation and emission; number of data points: 1996.*



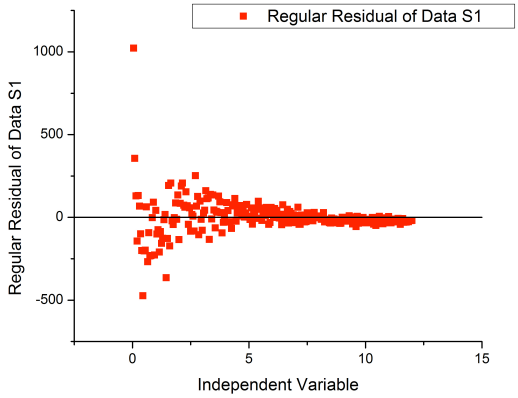
Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	2.4781E6		
Adj. R-Square	0.99326		
		Value	Standard Error
S1	y0	24115.47398	44.05012
S1	A1	101946.7211	246.89878
S1	t1	1.7979	0.0068



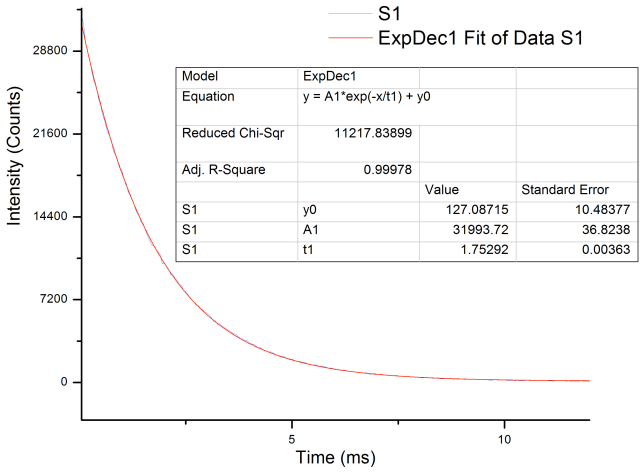
Trial 2 settings: *sample window: 1.80 ms; max delay: 12 ms; averages: 100; slit widths: 1.00 nm both excitation and emission; number or data points: 240.*



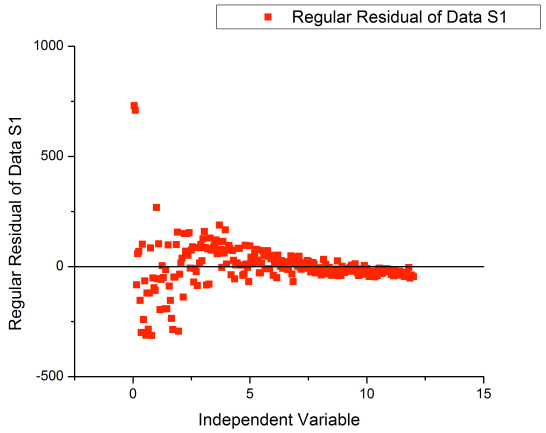
Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	12009.21582		
Adj. R-Square	0.99976		
		Value	Standard Error
S1	y0	124.53657	10.83007
S1	A1	31774.979	38.1532
S1	t1	1.74835	0.00377



Trial 3 settings: *sample window: 1.80 ms; max delay: 12 ms; averages: 100; slit widths: 1.00 nm both excitation and emission; number or data points: 240.*

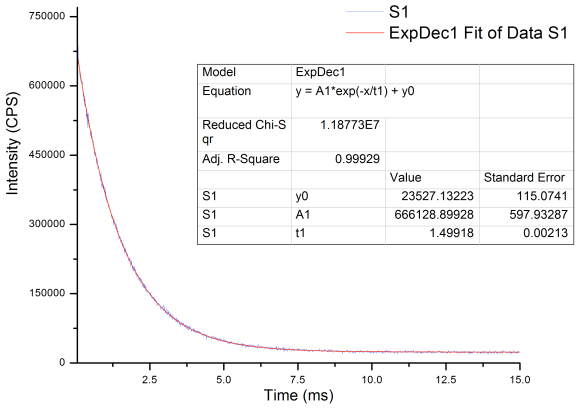


Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	11217.83899		
Adj. R-Square	0.99978		
		Value	Standard Error
S1	y0	127.08715	10.48377
S1	A1	31993.72	36.8238
S1	t1	1.75292	0.00363

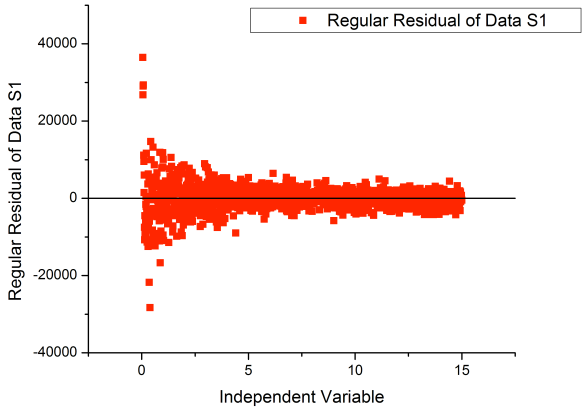


2. Lifetime decay curves of $Eu(NO_3)_3$ complex, monotored at 620 nm.

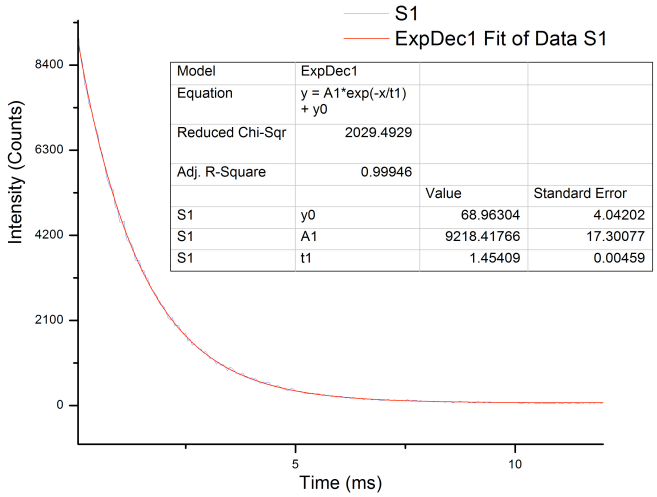
Trial 1 settings: *sample window: 10.00 ms; max delay: 15 ms; averages: 50; slit widths: 1.00 nm both excitation and emission; number of data points: 1496.*



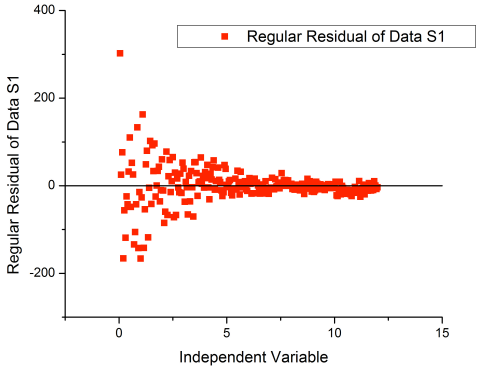
Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	1.18773E7		
Adj. R-Square	0.99929		
		Value	Standard Error
S1	y0	23527.13223	115.0741
S1	A1	666128.89928	597.93287
S1	t1	1.49918	0.00213



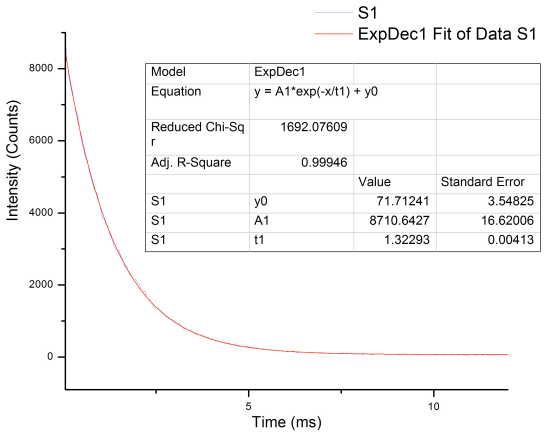
Trial 2 settings: *sample window: 1.50 ms; max delay: 12 ms; averages: 100; slit widths: 1.00 nm both excitation and emission; number of data points: 240.*



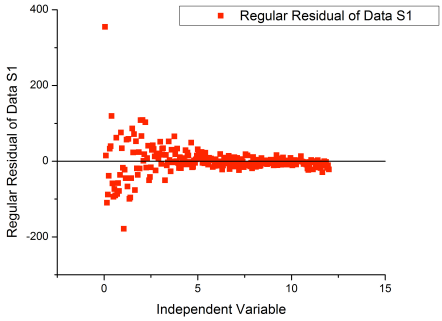
Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	2029.4929		
Adj. R-Square	0.99946		
		Value	Standard Error
S1	y0	68.96304	4.04202
S1	A1	9218.41766	17.30077
S1	t1	1.45409	0.00459



Trial 3 settings: *sample window: 1.50 ms; max delay: 12 ms; averages: 100; slit widths: 1.00 nm both excitation and emission; number of data points: 240.*

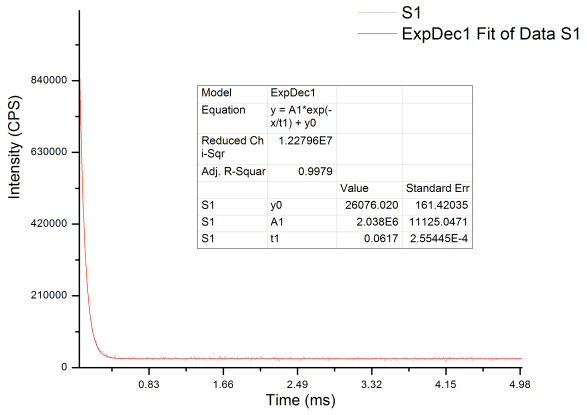


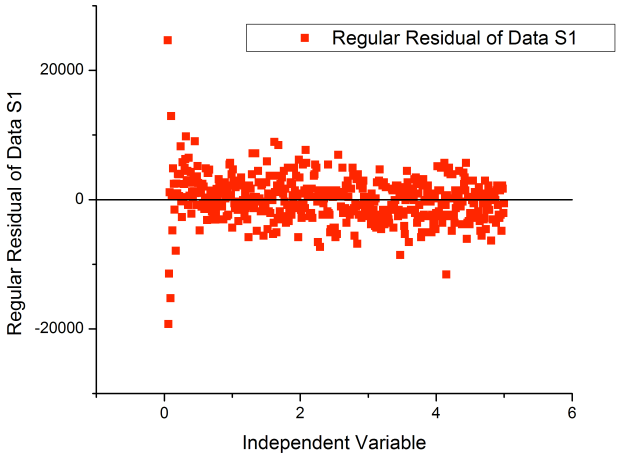
Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	1692.07609		
Adj. R-Square	0.99946		
		Value	Standard Error
S1	y0	71.71241	3.54825
S1	A1	8710.6427	16.62006
S1	t1	1.32293	0.00413



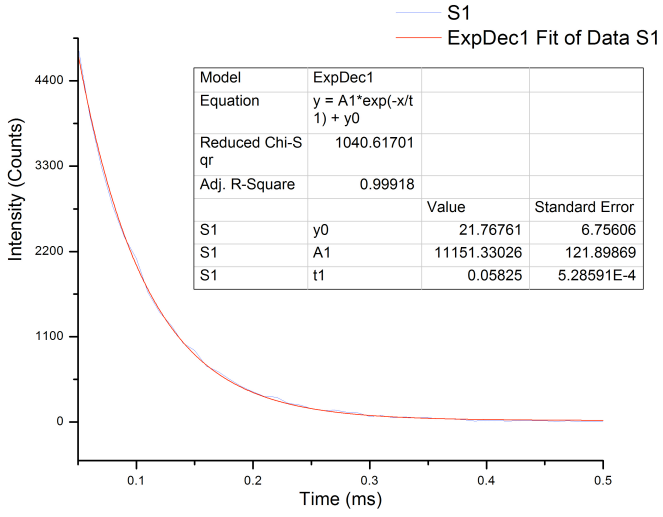
3. Lifetime decay curve of $Dy(NO_3)_3$ complex in CH_3CN, monitored at 580 nm.

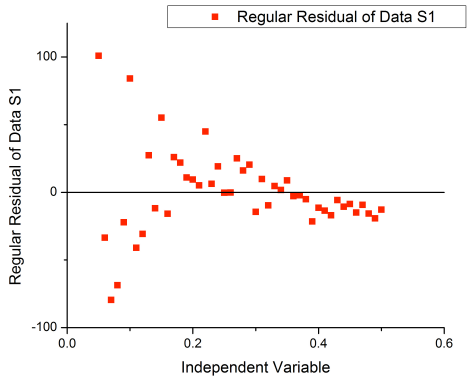
Trial 1 settings: *sample window: 4.00 ms; averages: 50; max delay: 5; slit widths: 2.00 nm both emission and excitation; number of data points: 496.*



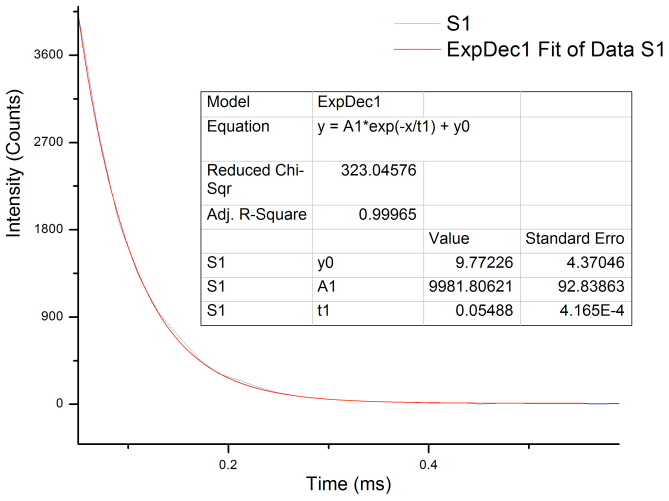


Trial 2 settings: *sample window: 0.06 ms; averages: 100; max delay: 0.5 ms; slit widths: 2.00 nm both emission and excitation; number of data points: 46.*

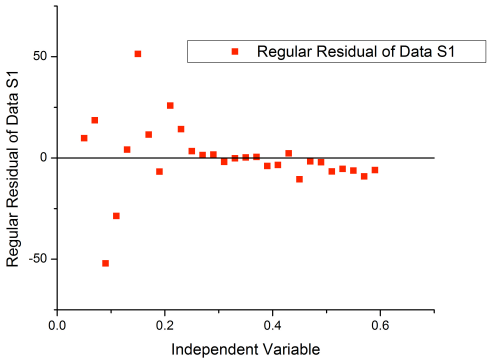




Trial 3 settings: *sample window: 0.06 ms; averages: 100; max delay: 0.5 ms; slit widths: 2.00 nm both emission and excitation; number of data points: 46.*

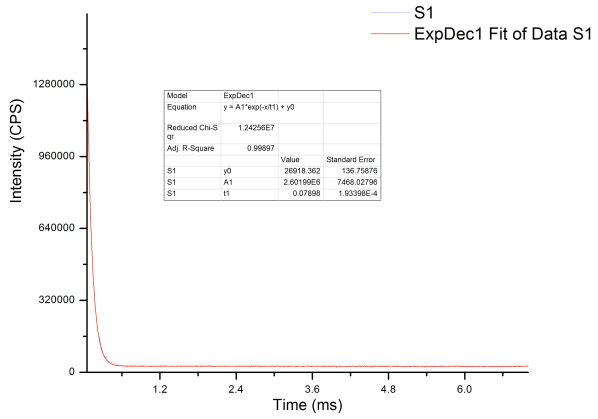


Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	323.04576		
Adj. R-Square	0.99965		
		Value	Standard Erro
S1	y0	9.77226	4.37046
S1	A1	9981.80621	92.83863
S1	t1	0.05488	4.165E-4

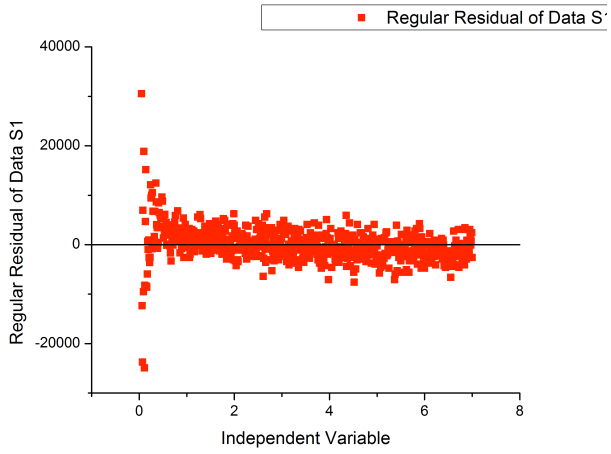


4. Lifetime decay curves of $Sm(NO_3)_3$ complex in CH_3CN, monitored at 600 nm.

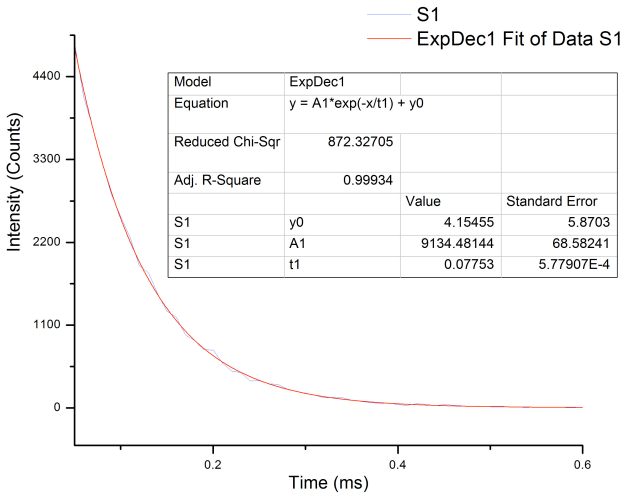
Trial 1 settings: *sample window: 6.00 ms; max delay: 7 ms; averages: 50; slit widths: 3.00 nm both emission and excitation; number of data points: 696.*



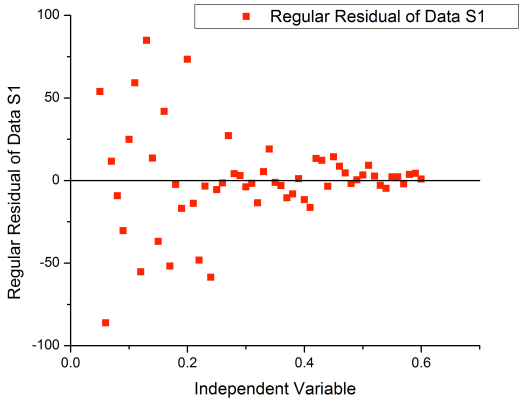
Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	1.24256E7		
Adj. R-Square	0.99897		
		Value	Standard Error
S1	y0	26918.362	136.75876
S1	A1	2.60199E6	7468.02796
S1	t1	0.07898	1.93398E-4



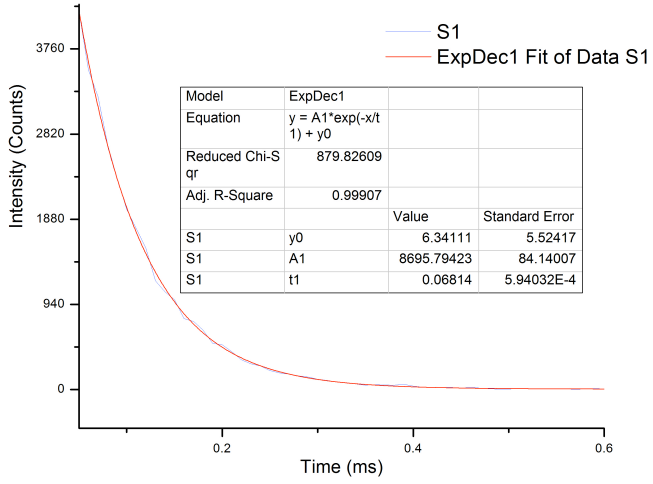
Trial 2 settings: *sample window: 0.08 ms; max delay: 0.6 ms; averages: 100; slit widths: 2.50 nm both emission and excitation; number of data points: 56.*



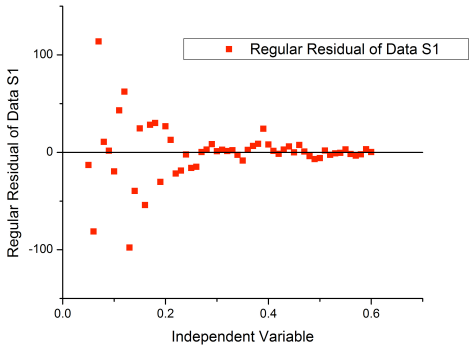
Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	872.32705		
Adj. R-Square	0.99934		
		Value	Standard Error
S1	y0	4.15455	5.8703
S1	A1	9134.48144	68.58241
S1	t1	0.07753	5.77907E-4



Trial 3 settings: *sample window: 0.08 ms; max delay: 0.6 ms; averages: 100; slit widths: 2.50 nm both emission and excitation; number of data points: 56.*

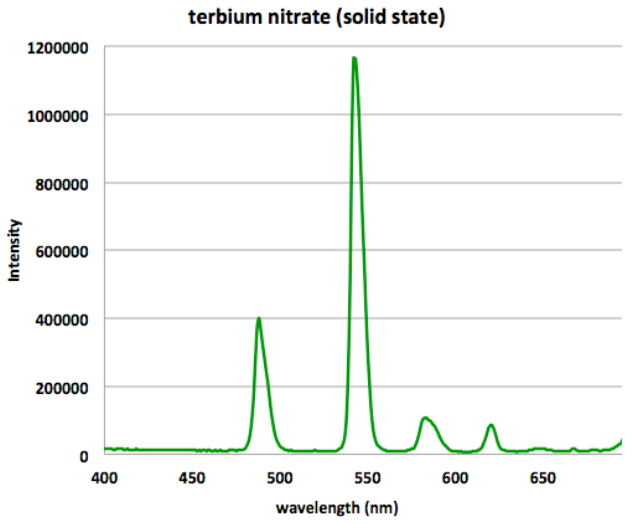


Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	879.82609		
Adj. R-Square	0.99907		
		Value	Standard Error
S1	y0	6.34111	5.52417
S1	A1	8695.79423	84.14007
S1	t1	0.06814	5.94032E-4

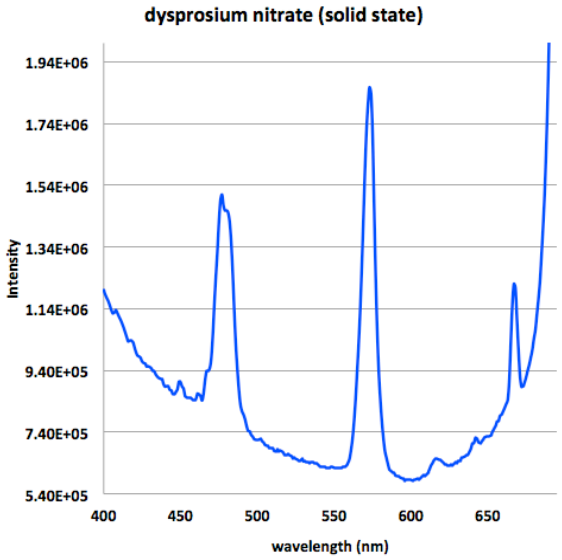


B. Solid state emission spectra

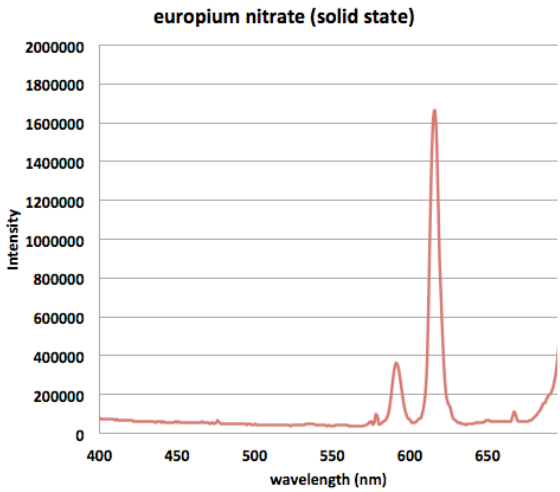
Solid state emission spectra were acquired by placing solid 1:3 $Ln(NO_3)_3$-4 complex into a quartz cuvette and exciting at 350 nm.



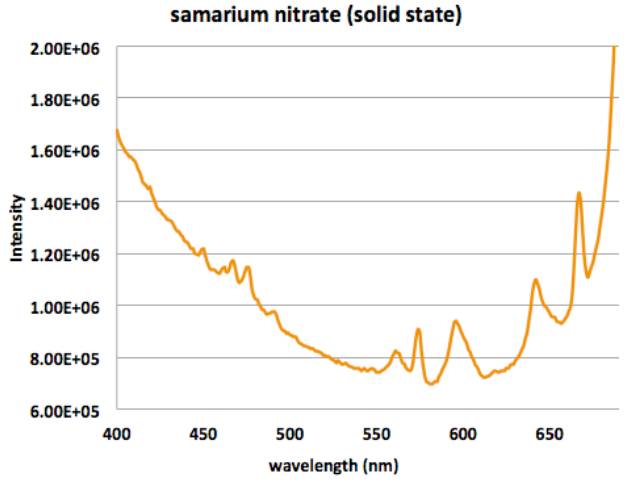
Emission spectrum of 1:3 $Tb(NO_3)_3$-4 in the solid state. Slit widths = 1.0 nm entrance and exit; λ_{ex} = 350 nm.



Emission spectrum of 1:3 $Dy(NO_3)_3$-4 in the solid state. Slit widths = 2.0 nm entrance and exit; λ_{ex} = 350 nm.



Emission spectrum of 1:3 $Eu(NO_3)_3$-4 in the solid state. Slit widths = 1.0 nm entrance and exit; λ_{ex} = 350 nm.

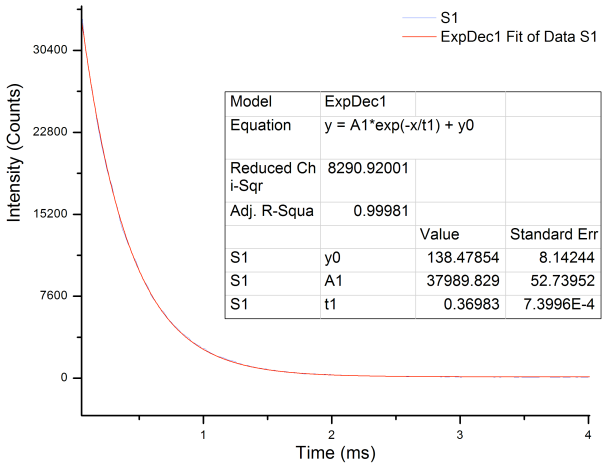


Emission spectrum of 1:3 $Sm(NO_3)_3$-4 in the solid state. Slit widths = 2.0 nm entrance and exit; λ_{ex} = 350 nm.

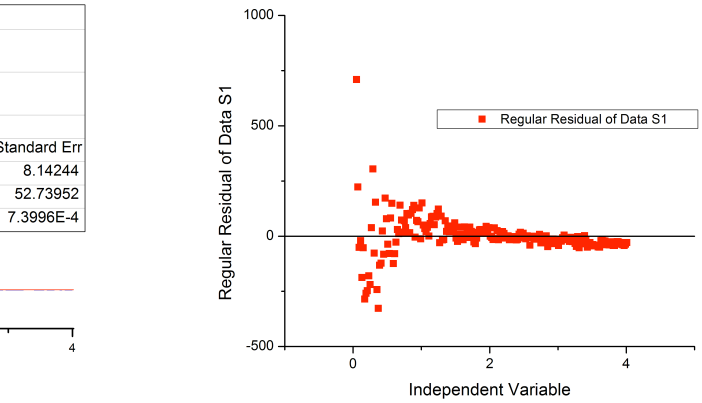
C. Horrocks lifetime decay curves and fitting residuals. Lifetimes were measured in CH_3OH or CH_3OD with a complex concentration of 2.0 mM and three equivalents of ligand relative to $Eu(NO_3)_3$. For all sets of data below, the blue curve is connected data points and the red curve is the fit. All complexes were excited at 350 nm. Please note for each of the residual plots, the units of the x-axis are time (ms), while the units of the y-axis are intensity (counts).

1. Lifetime decay curves in CH_3OH monitored at 591 nm; *Settings for all trials:* *sample window: 0.4 ms; max delay: 4.0 ms; averages: 100; excitation and emission slit widths: 5.00 nm; delay incr.: 0.02 ms.*

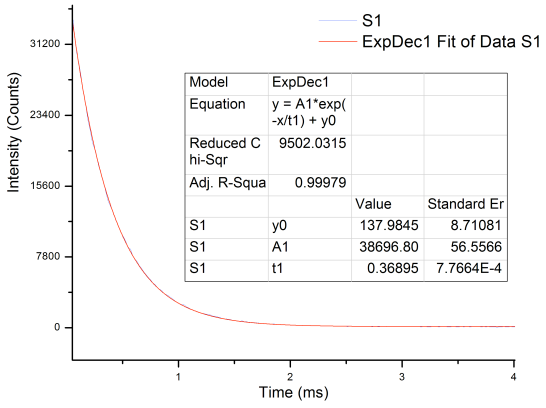
Trial 1



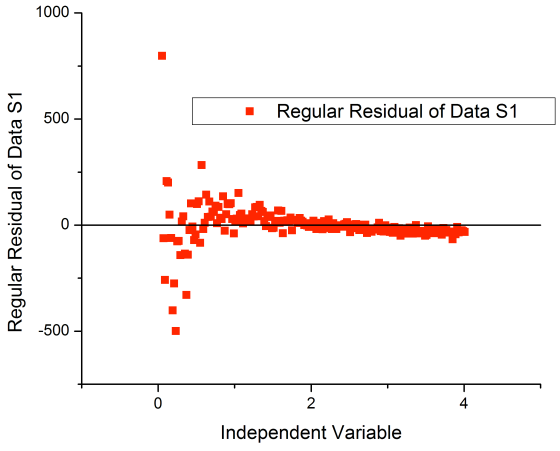
Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	8290.92001		
Adj. R-Squa	0.99981		
		Value	Standard Err
S1	y0	138.47854	8.14244
S1	A1	37989.829	52.73952
S1	t1	0.36983	7.3996E-4



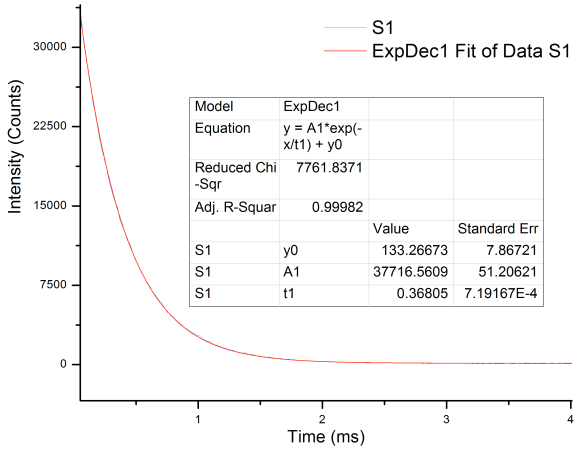
Trial 2



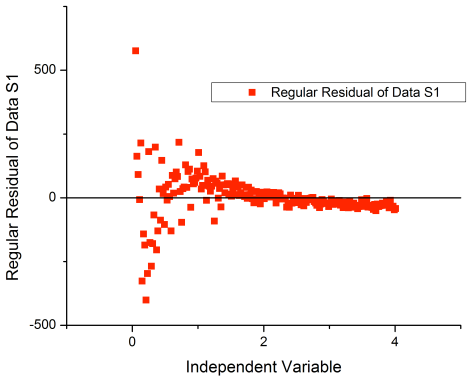
Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	9502.0315		
Adj. R-Squa	0.99979		
		Value	Standard Er
S1	y0	137.9845	8.71081
S1	A1	38696.80	56.5566
S1	t1	0.36895	7.7664E-4



Trial 3

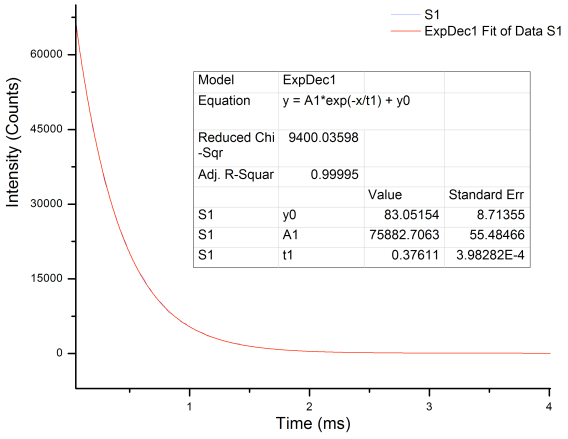


Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	7761.8371		
Adj. R-Squar	0.99982		
		Value	Standard Err
S1	y0	133.26673	7.86721
S1	A1	37716.5609	51.20621
S1	t1	0.36805	7.19167E-4

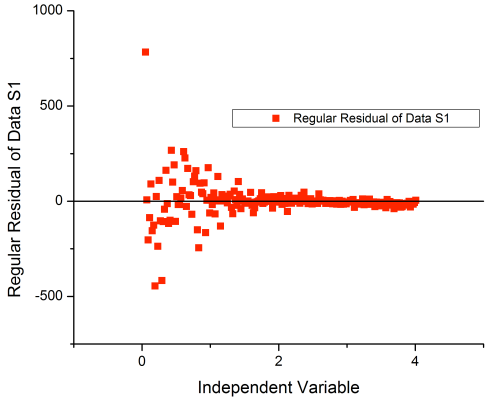


2. Lifetime decay curves in CH_3OH monitored at 619 nm; *Settings for all trials:* *sample window: 0.4 ms; max delay: 4.0 ms; averages: 100; excitation and emission slit widths: 5.00 nm; delay incr.: 0.02 ms.*

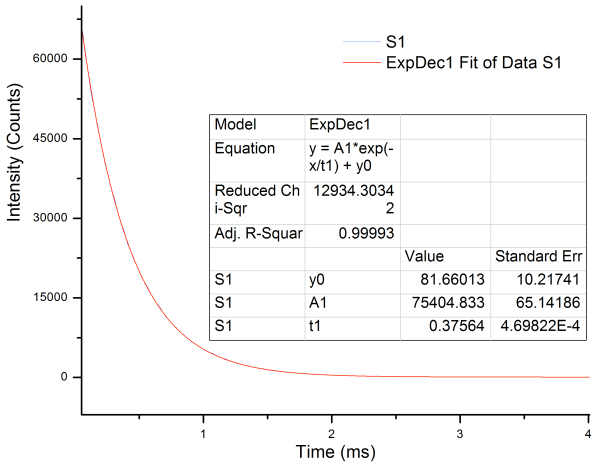
Trial 1



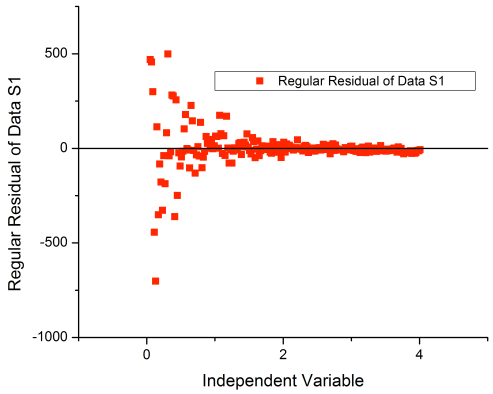
Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	9400.03598		
Adj. R-Squar	0.99995		
		Value	Standard Err
S1	y0	83.05154	8.71355
S1	A1	75882.7063	55.48466
S1	t1	0.37611	3.98282E-4



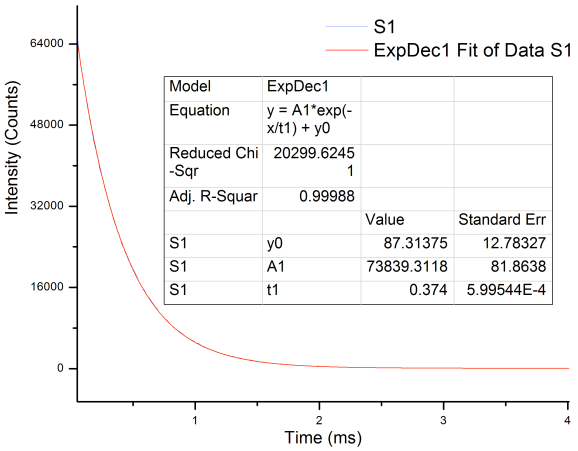
Trial 2



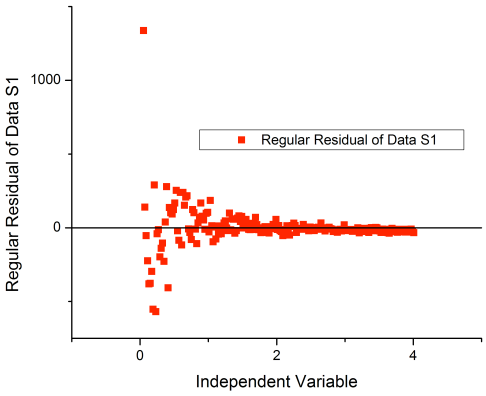
Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	12934.30342		
Adj. R-Squar	0.99993		
		Value	Standard Err
S1	y0	81.66013	10.21741
S1	A1	75404.833	65.14186
S1	t1	0.37564	4.69822E-4



Trial 3

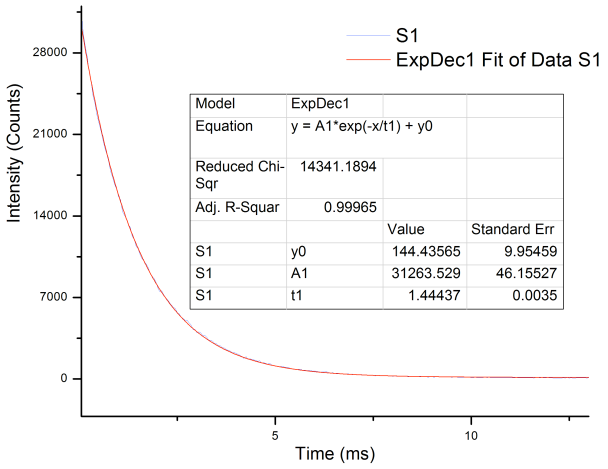


Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	20299.62451		
Adj. R-Squar	0.99988		
		Value	Standard Err
S1	y0	87.31375	12.78327
S1	A1	73839.3118	81.8638
S1	t1	0.374	5.99544E-4

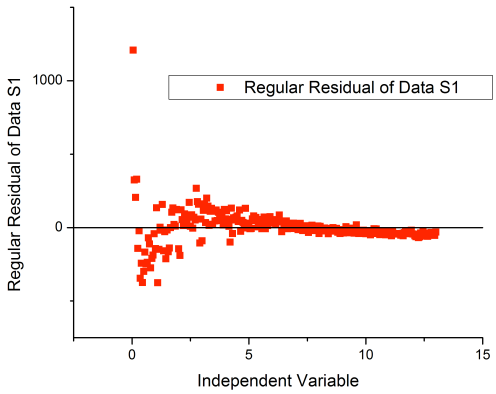


3. Lifetime decay curves in CH_3OD monitored at 591 nm; *Settings for all trials:* *sample window: 1.3 ms; max delay: 13.0 ms; averages: 100; excitation and emission slit widths: 5.00 nm; delay incr.: 0.05 ms.*

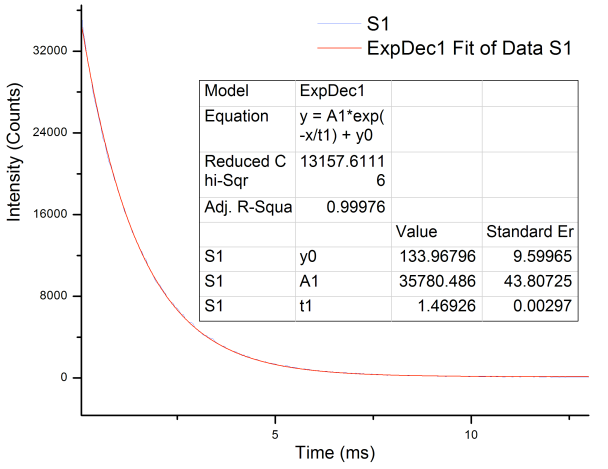
Trial 1



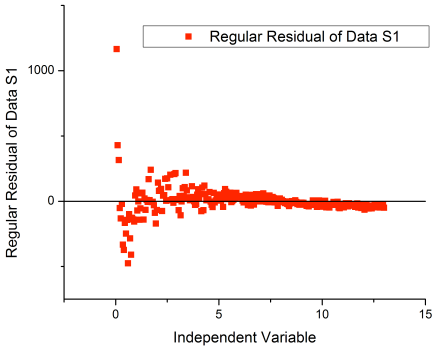
Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	14341.1894		
Adj. R-Squar	0.99965		
		Value	Standard Err
S1	y0	144.43565	9.95459
S1	A1	31263.529	46.15527
S1	t1	1.44437	0.0035



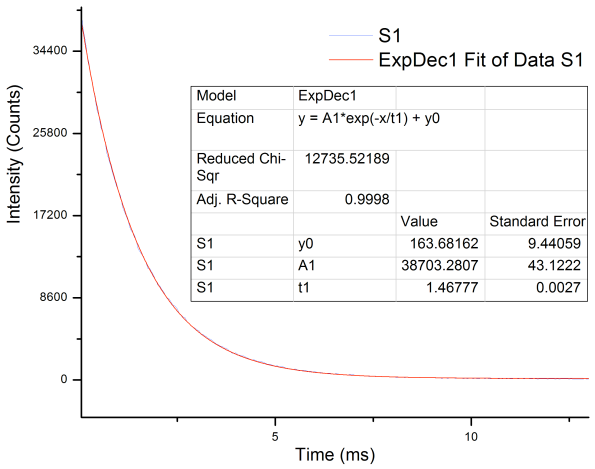
Trial 2



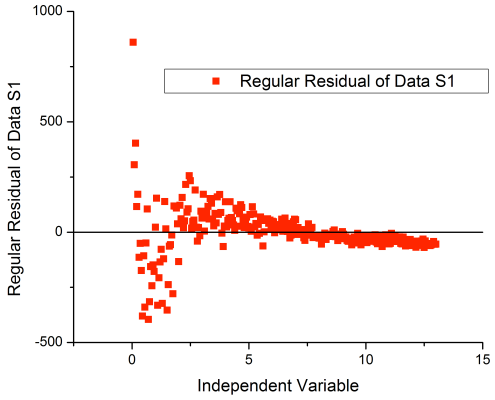
Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	13157.61116		
Adj. R-Squa	0.99976		
		Value	Standard Er
S1	y0	133.96796	9.59965
S1	A1	35780.486	43.80725
S1	t1	1.46926	0.00297



Trial 3

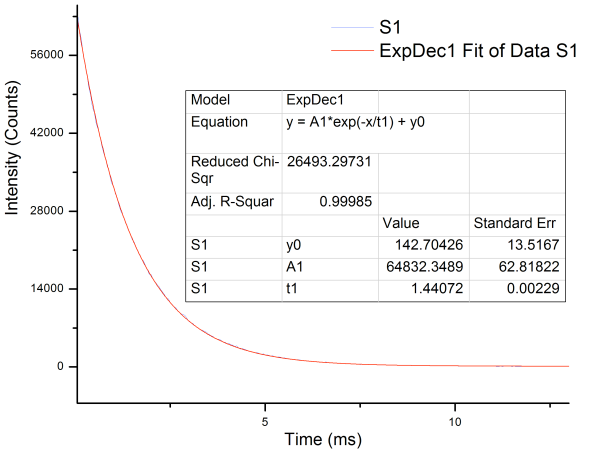


Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	12735.52189		
Adj. R-Square	0.9998		
		Value	Standard Error
S1	y0	163.68162	9.44059
S1	A1	38703.2807	43.1222
S1	t1	1.46777	0.0027

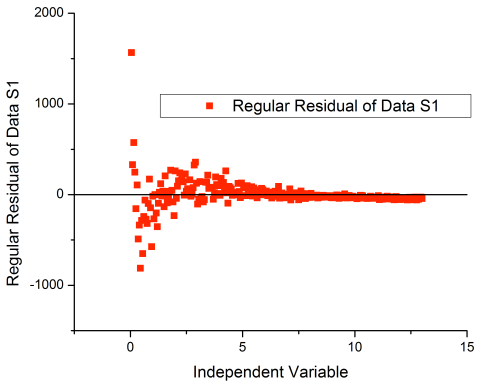


4. Lifetime decay curves in CH_3OD monitored at 619 nm; *Settings for all trials:* *sample window: 1.3 ms; max delay: 13.0 ms; averages: 100; excitation and emission slit widths: 5.00 nm; delay incr.: 0.05 ms.*

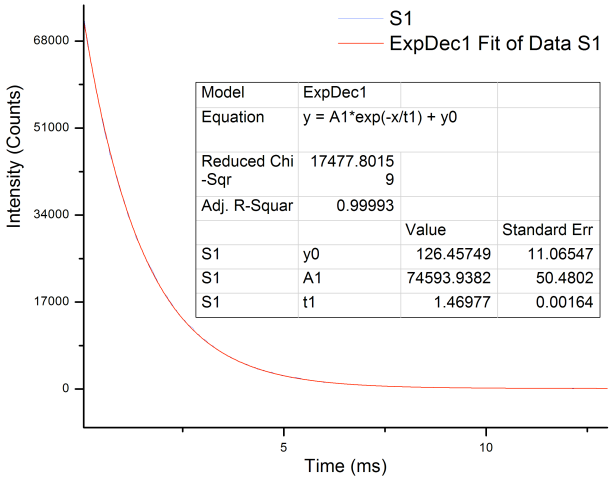
Trial 1



Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	26493.29731		
Adj. R-Squar	0.99985		
		Value	Standard Err
S1	y0	142.70426	13.5167
S1	A1	64832.3489	62.81822
S1	t1	1.44072	0.00229

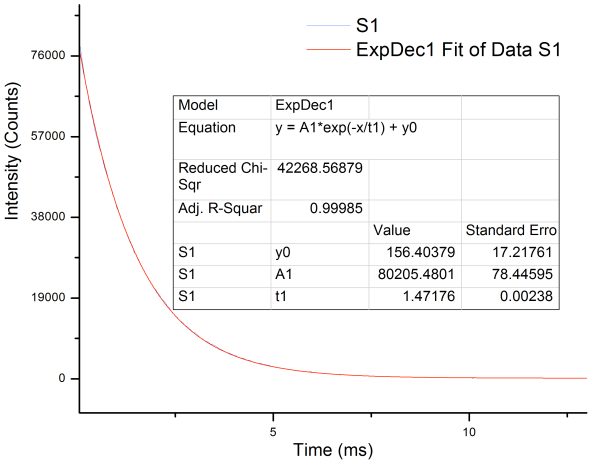


Trial 2

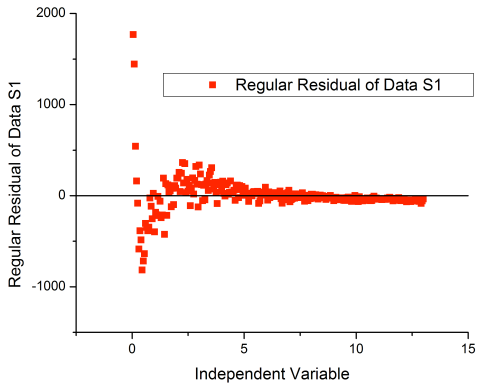


Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	17477.80159		
Adj. R-Squar	0.99993		
		Value	Standard Err
S1	y0	126.45749	11.06547
S1	A1	74593.9382	50.4802
S1	t1	1.46977	0.00164

Trial 3

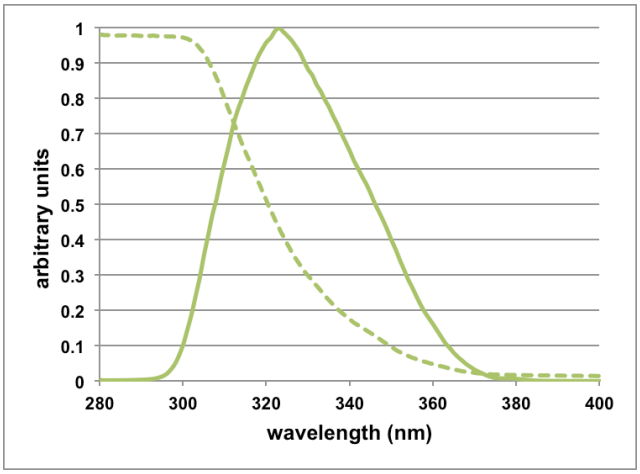


Model	ExpDec1		
Equation	y = A1*exp(-x/t1) + y0		
Reduced Chi-Sqr	42268.56879		
Adj. R-Squar	0.99985		
		Value	Standard Erro
S1	y0	156.40379	17.21761
S1	A1	80205.4801	78.44595
S1	t1	1.47176	0.00238

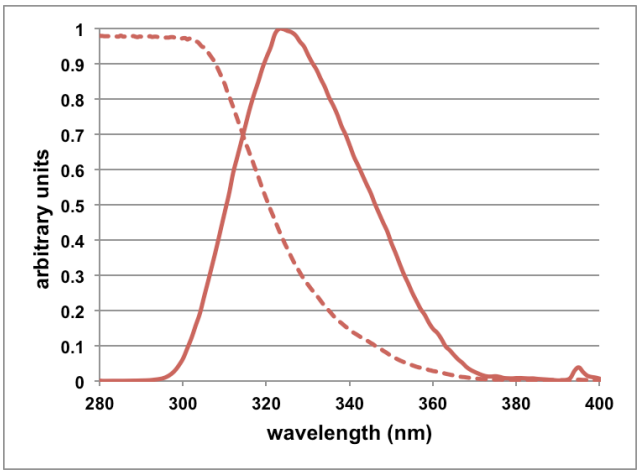


D. Absorption and excitation spectra – Tb, Eu and Sm complexes. Absorption (dashed) and excitation (solid) spectra of the $Ln(NO_3)_3$-**4** complexes with three equivalents of ligand **4** in acetonitrile (2.0 mM complex concentration). Both absorption and excitation spectra have been normalized to have their peaks at 1 arbitrary unit for ease of comparison.

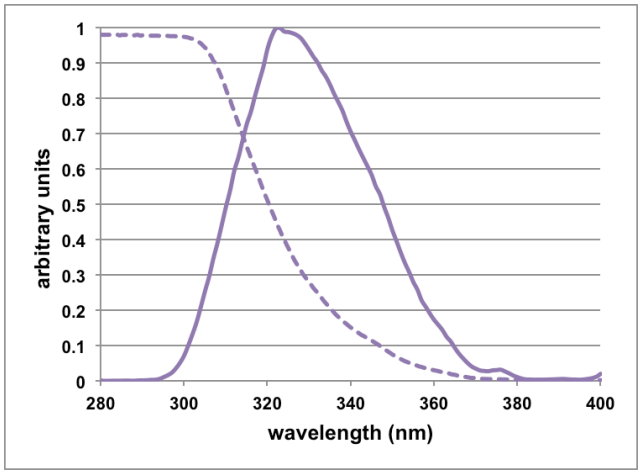
1. $Tb(NO_3)_3$ complex: λ_{em} monitored at 543 nm, 1.0 nm emission and excitation slits).



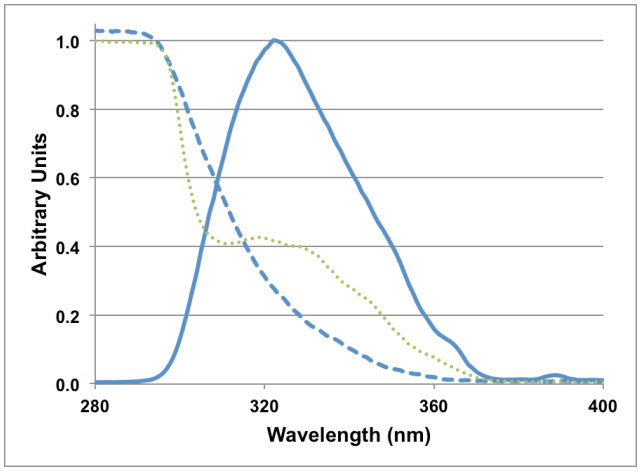
2. $Eu(NO_3)_3$ complex: λ_{em} monitored at 619 nm, 1.0 nm emission and excitation slits).



3. $Sm(NO_3)_3$ complex: λ_{em} monitored at 642 nm, 2.5 nm emission and excitation slits).

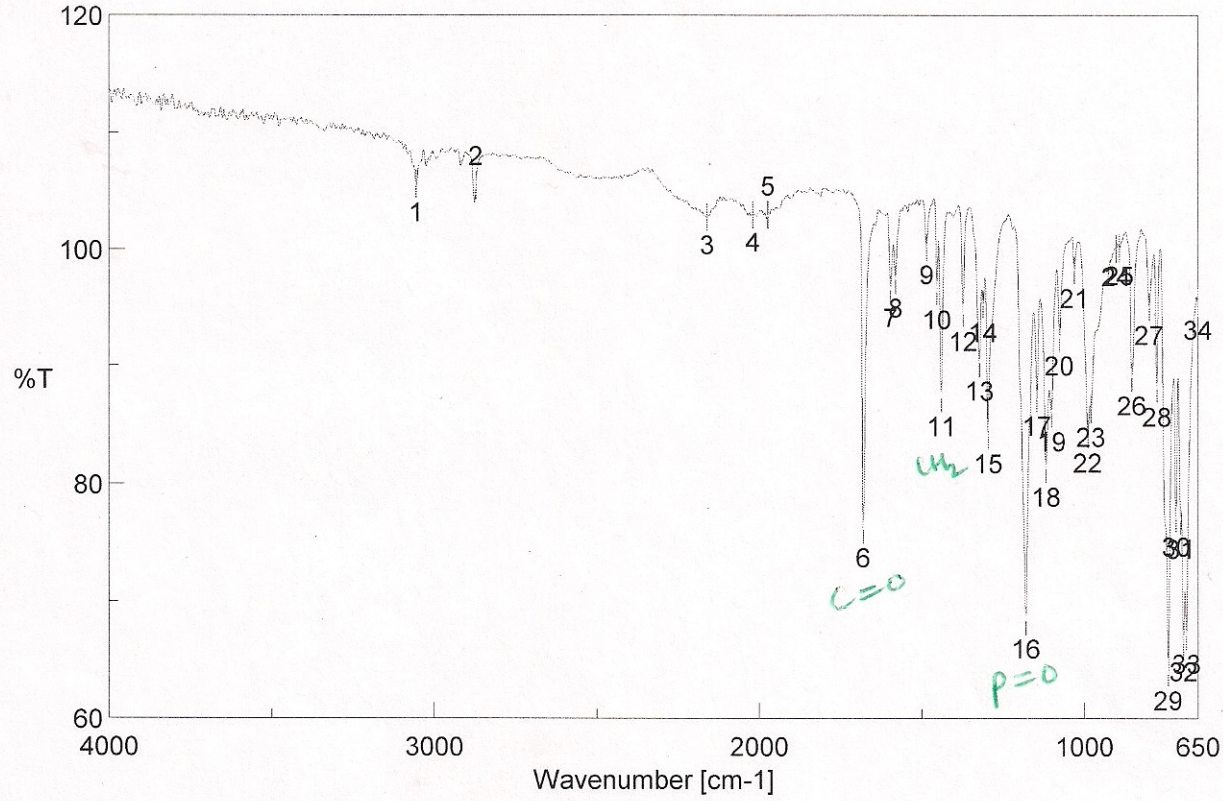


4. $Dy(NO_3)_3$ complex: λ_{em} monitored at 478 nm, 2.0 nm emission and excitation slits). Absorption spectrum of 6.0 mM ligand 4 alone in CH_3CN is also shown here as dotted grey line.



SB2-60-03 FTIR free PhCH2POPh

Peak Find - Memory-1



[Detailed Information]

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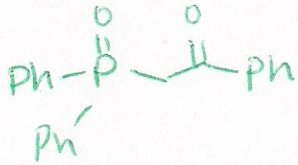
Horizontal axis	Wavenumber [cm-1]
Vertical axis	%T
Start	649.893 cm-1
End	4000.6 cm-1
Data interval	0.964233 cm-1
Data points	3476

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3055.66	105.557	2	2871.49	105.52
3	2160.85	102.777	4	2019.1	103.005
5	1972.82	102.963	6	1679.69	76.1143
7	1595.81	96.5224	8	1580.38	97.3496
9	1484.92	100.197	10	1454.06	96.3512
11	1439.6	87.218	12	1372.1	94.5051
13	1321.96	90.226	14	1311.36	95.2685
15	1295.93	84.094	16	1179.26	68.3544
17	1146.47	87.2427	18	1117.55	81.2567
19	1101.15	85.9478	20	1076.08	92.3742
21	1029.8	98.1853	22	989.304	84.1331
23	978.697	86.3355	24	901.558	100.03
25	891.916	100.127	26	853.347	88.9687
27	800.314	94.9989	28	777.172	88.0239



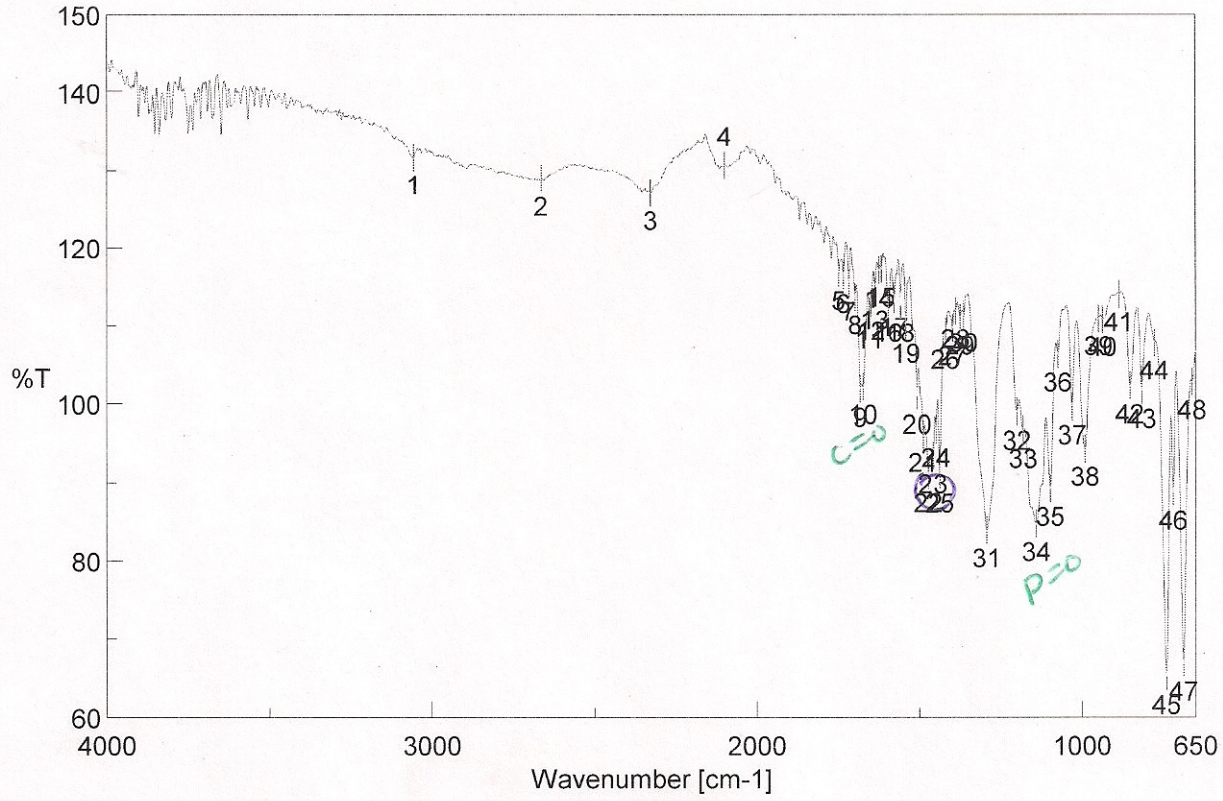
SB 2-60-03 Cpg2

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
29	742.46	63.9233	30	717.39	77.0507
31	703.89	76.8577	32	695.212	66.4142
33	686.534	67.0835	34	650.858	95.4847

SB2-60-05 Tb-PhCAMPOPh complex
1:3 3:1

Peak Find - Memory-2



[Detailed Information]

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Horizontal axis	Wavenumber [cm-1]
Vertical axis	%T
Start	649.893 cm-1
End	4000.6 cm-1
Data interval	0.964233 cm-1
Data points	3476

[Result of Peak Picking]

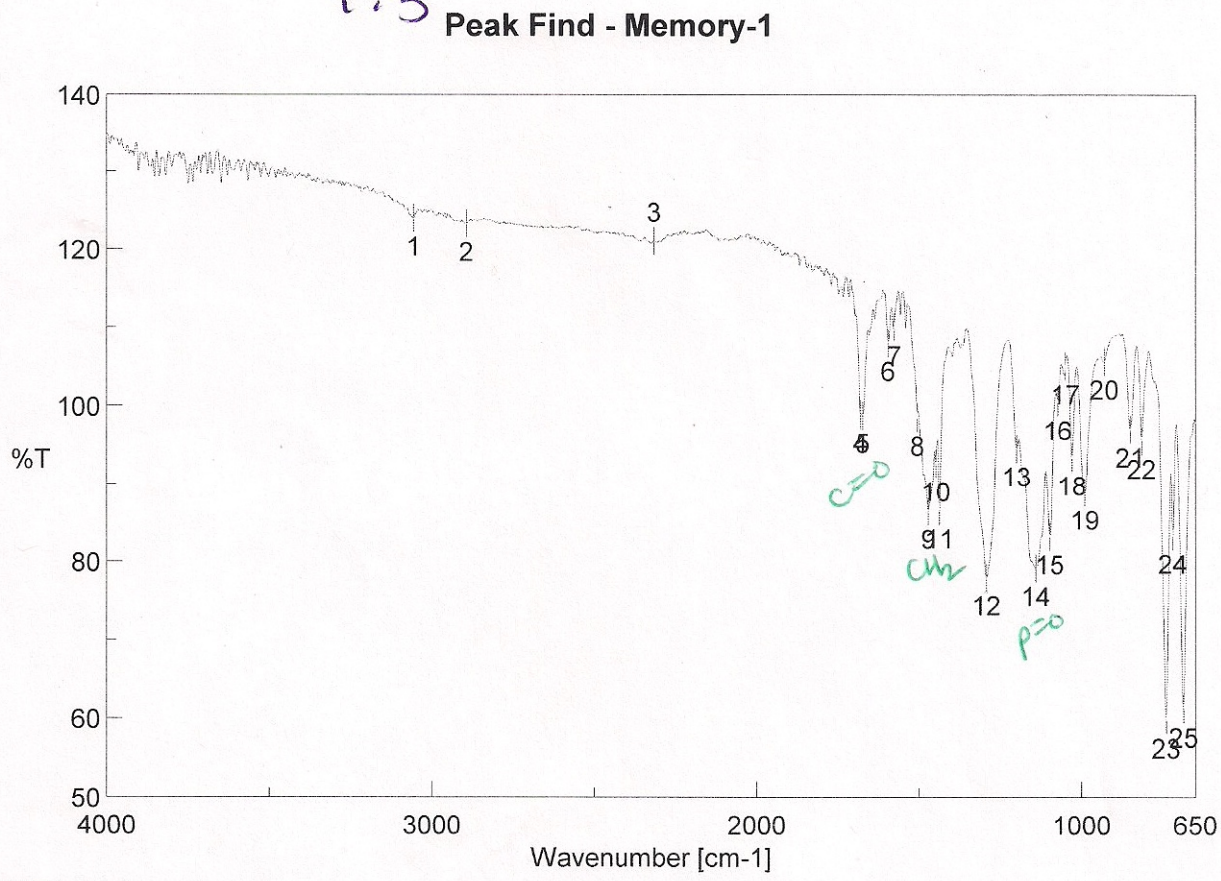
No.	Position	Intensity	No.	Position	Intensity
1	3055.66	131.686	2	2663.21	128.895
3	2326.7	127.043	4	2100.1	130.678
5	1748.16	116.828	6	1732.73	116.394
7	1716.34	115.482	8	1697.05	113.671
9	1681.62	101.825	10	1672.95	102.176
11	1652.7	111.763	12	1647.88	112.887
13	1636.3	114.322	14	1623.77	117.096
15	1617.02	117.254	16	1594.84	112.65
17	1577.49	113.359	18	1558.2	112.637
19	1540.85	109.995	20	1507.1	100.966
21	1487.81	96.1899	22	1472.38	91.0267
23	1457.92	93.4174	24	1448.28	96.7837
25	1436.71	90.9663	26	1419.35	109.185
27	1396.21	109.639	28	1387.53	111.91

SB 2-60-05 (cont pg 2)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
29	1374.03	110.982	30	1363.43	111.359
31	1292.07	83.942	32	1199.51	98.9522
33	1180.22	96.664	34	1140.69	84.7523
35	1097.3	89.2689	36	1073.19	106.3
37	1028.84	99.6492	38	990.268	94.3737
39	948.806	110.907	40	936.271	110.783
41	886.131	114.049	42	851.418	102.227
43	814.777	101.666	44	777.172	107.826
45	740.531	65.1441	46	718.354	88.7708
47	687.498	66.9022	48	660.5	102.759

SB 2-60-04 FT-IR Dy-Phenolpoph 1:3



[Detailed Information]

Creation date	6/12/2015 10:50 AM
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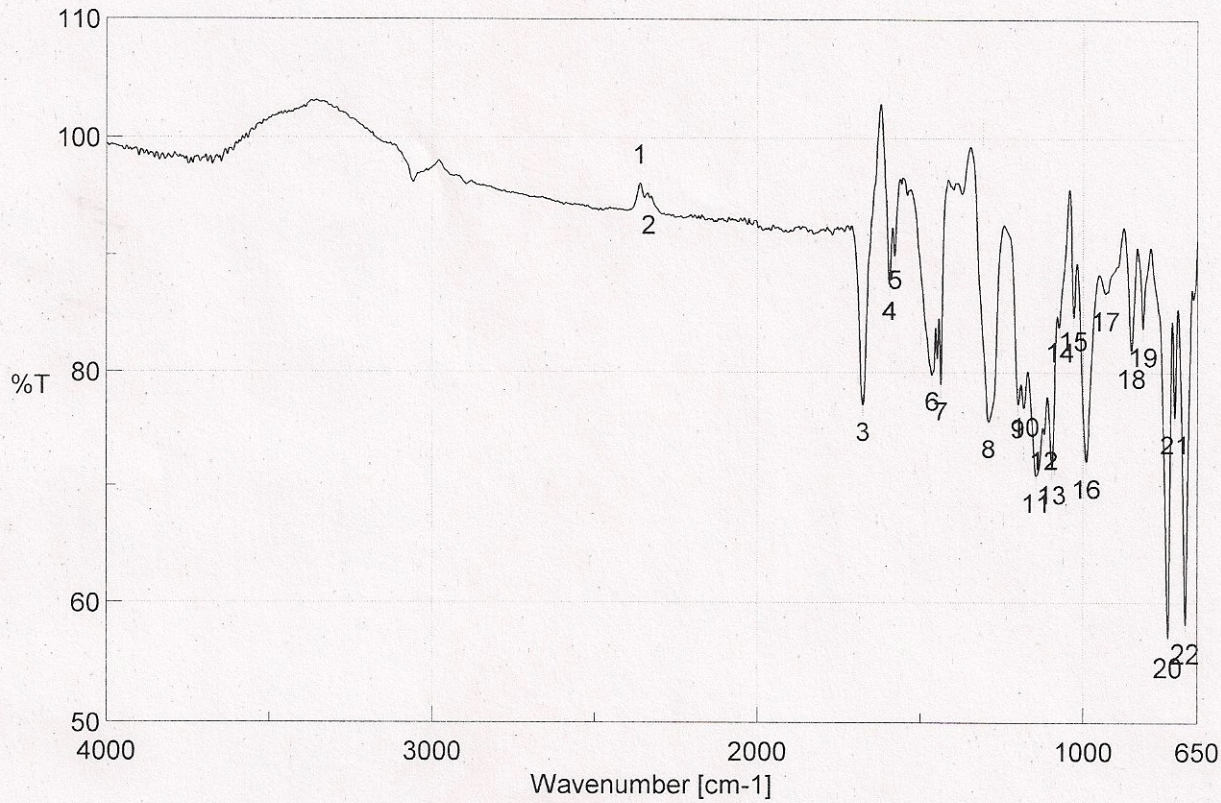
Vertical axis	%T
Start	649.893 cm-1
End	4000.6 cm-1
Data interval	0.964233 cm-1
Data points	3476

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3055.66	123.918	2	2892.7	123.22
3	2316.09	120.977	4	1680.66	98.8873
5	1673.91	98.8136	6	1594.84	107.942
7	1576.52	109.941	8	1506.13	98.4659
9	1472.38	86.4366	10	1448.28	92.549
11	1437.67	86.4538	12	1292.07	77.9521
13	1200.47	94.5156	14	1141.65	79.097
15	1098.26	83.1229	16	1073.19	100.442
17	1050.05	104.962	18	1028.84	93.3269
19	990.268	88.8827	20	929.521	105.572
21	850.454	96.9813	22	814.777	95.5141
23	740.531	59.7747	24	719.318	83.2413
25	686.534	61.1557			

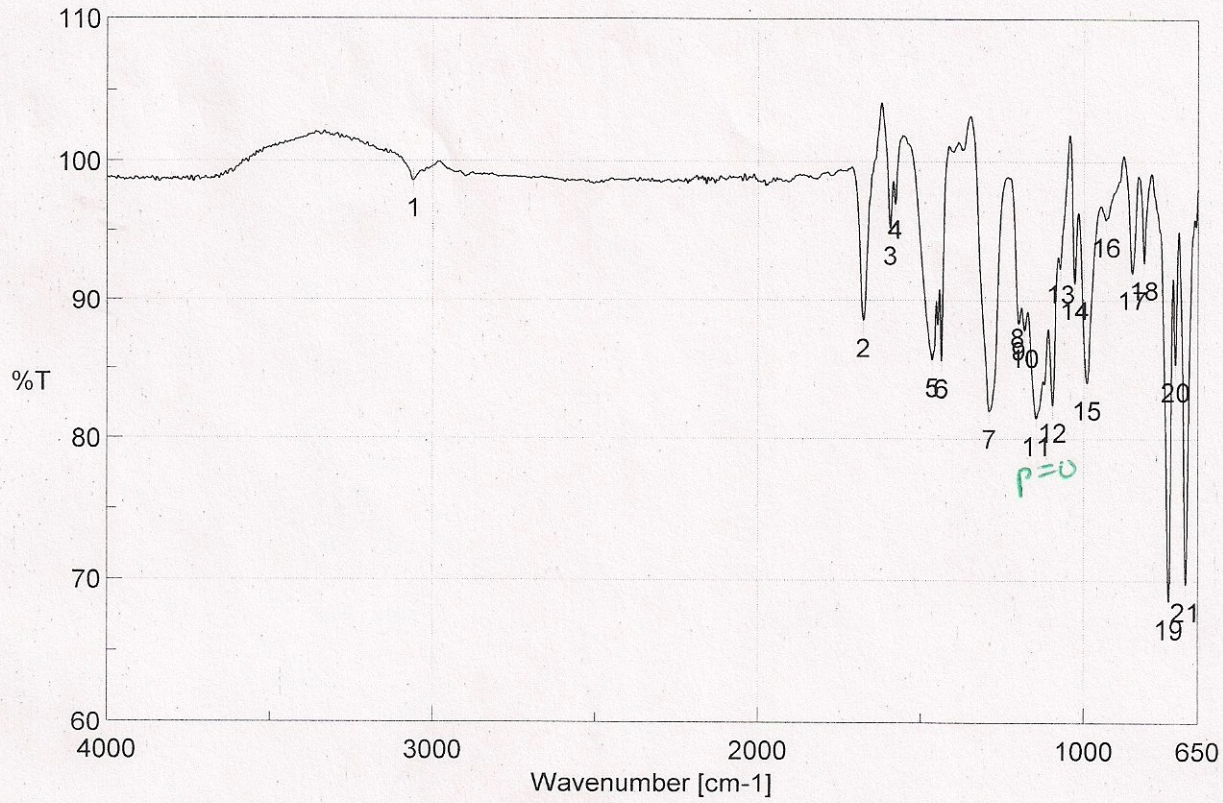
SB2-60-02 FTIR 3:1 $PhCH_2OPh\text{-}Sn(CH_3)_3$



[Result of Peak Picking]

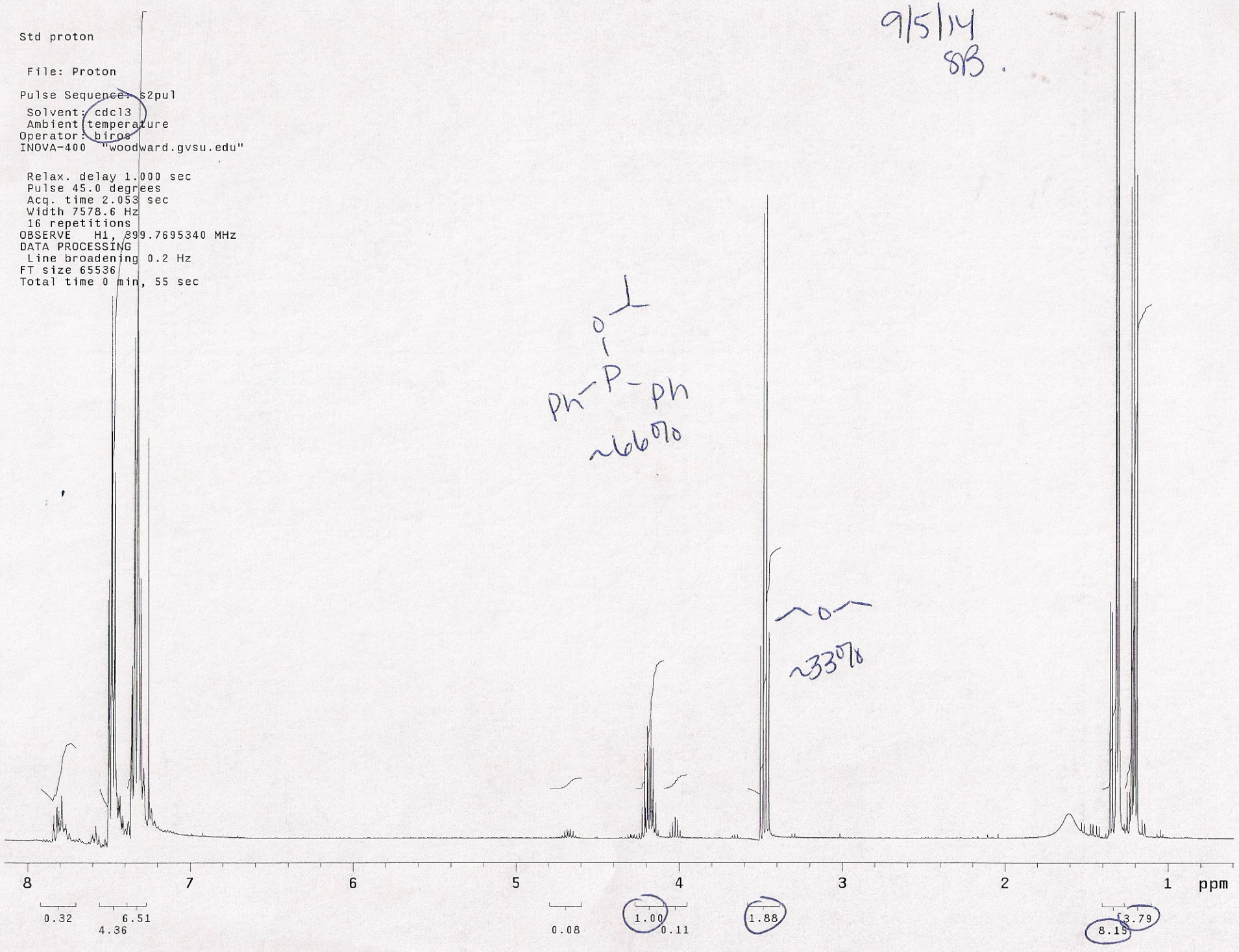
No.	Position	Intensity	No.	Position	Intensity
1	2362.37	96.0866	2	2333.45	94.9927
3	1676.8	77.2041	4	1594.84	87.6516
5	1577.49	90.3771	6	1463.71	79.9014
7	1437.67	79.0377	8	1290.14	75.6922
9	1201.43	77.4917	10	1178.29	77.6755
11	1145.51	70.8827	12	1120.44	74.6647
13	1096.33	71.6272	14	1071.26	84.1375
15	1029.8	85.0865	16	990.268	72.1522
17	932.414	86.7839	18	852.382	81.8908
19	816.706	83.7674	20	740.531	57.0645
21	718.354	76.1039	22	686.534	58.1981

SB2-60-01 FT-IR 3:1 PhenPAPh-$Eu(NO_3)_3$



[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	
1	3059.51	98.5988	2	1676.8	88.5003	C=O
3	1594.84	95.2336	4	1580.38	97.1268	
5	1466.6	85.658	6	1437.67	85.5804	CH_2
7	1290.14	81.9584	8	1204.33	89.2419	
9	1201.43	88.31	10	1182.15	87.7719	
11	1146.47	81.4564	12	1096.33	82.4255	
13	1071.26	92.4483	14	1027.87	91.2243	
15	991.232	84.0176	16	932.414	95.8519	
17	852.382	92.0035	18	815.742	92.7164	
19	739.567	68.5252	20	718.354	85.3427	
21	687.498	69.7481				


Std proton
File: Proton
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: biros
INOVA-400 "woodward.gvsu.edu"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.053 sec
Width 7578.6 Hz
16 repetitions
OBSERVE H1, 899.7695340 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min, 55 sec
9/5/14
SB.
~66%
~33%
8
7
6
5
4
3
2
1
ppm
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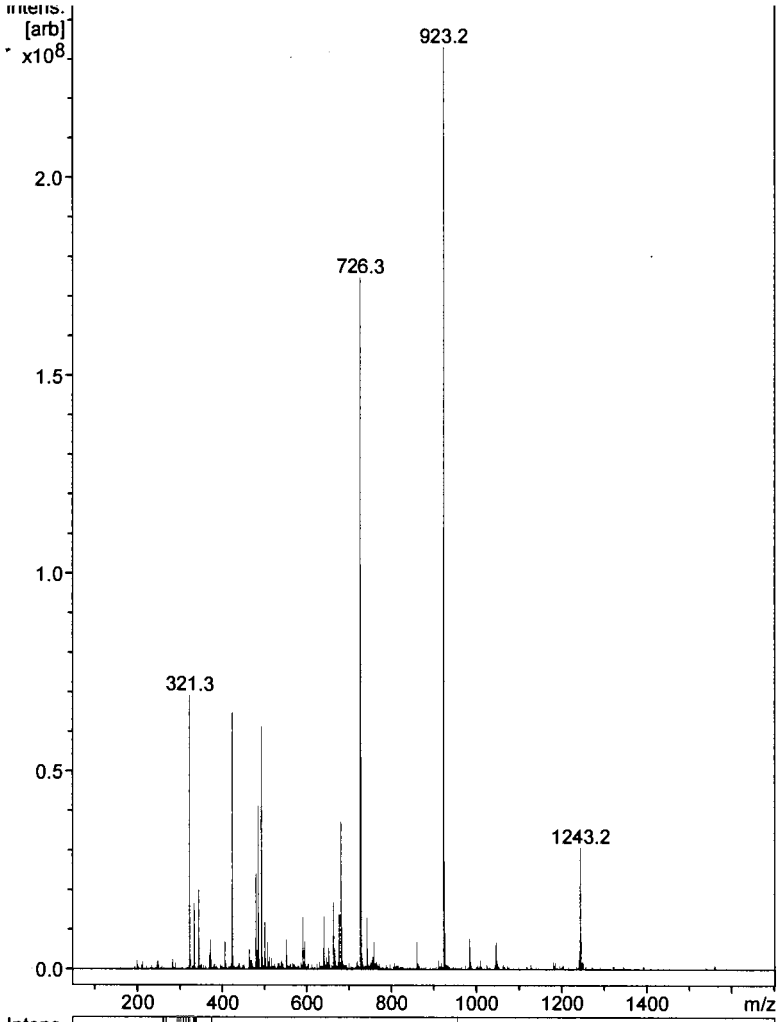
4.36
0.08
1.00
0.11
1.88
8.15
3.79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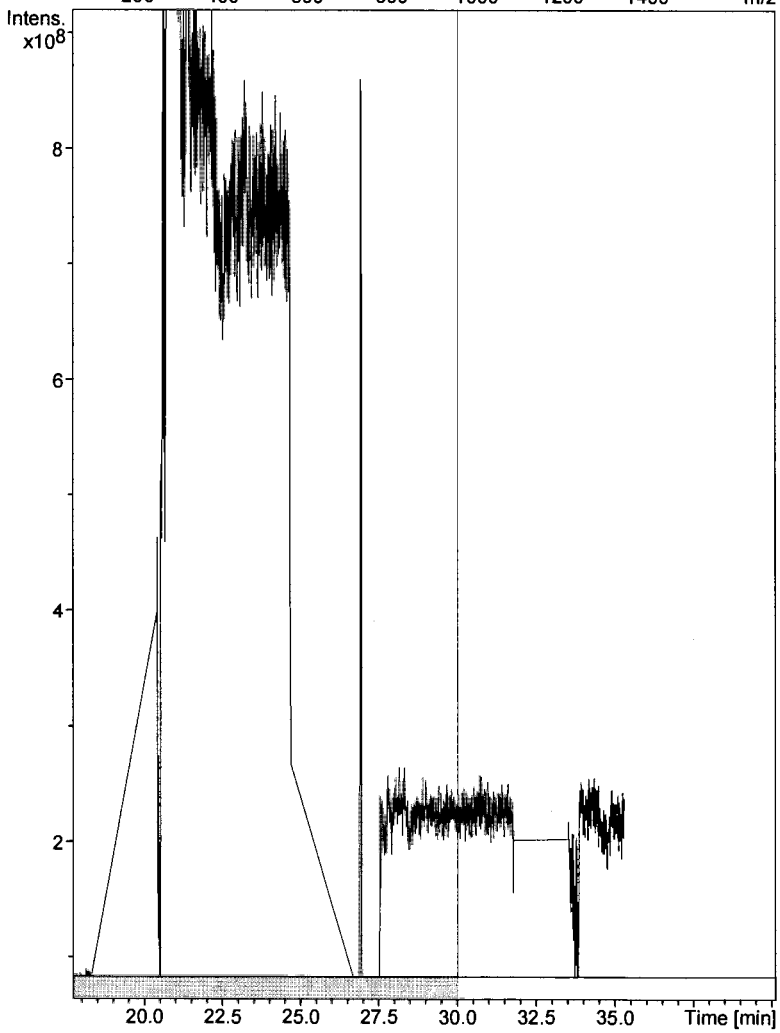
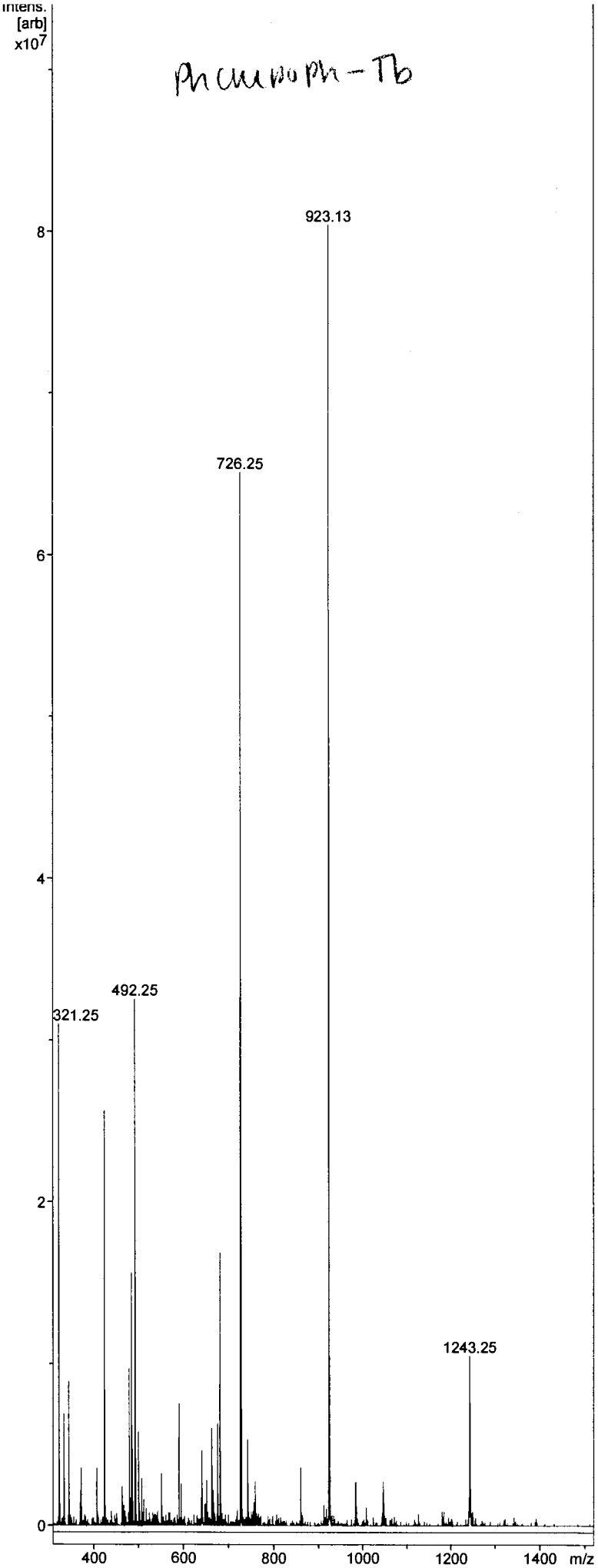
726.3
321.3
1243.2
m/z


Intens.
x10^8
Time [min]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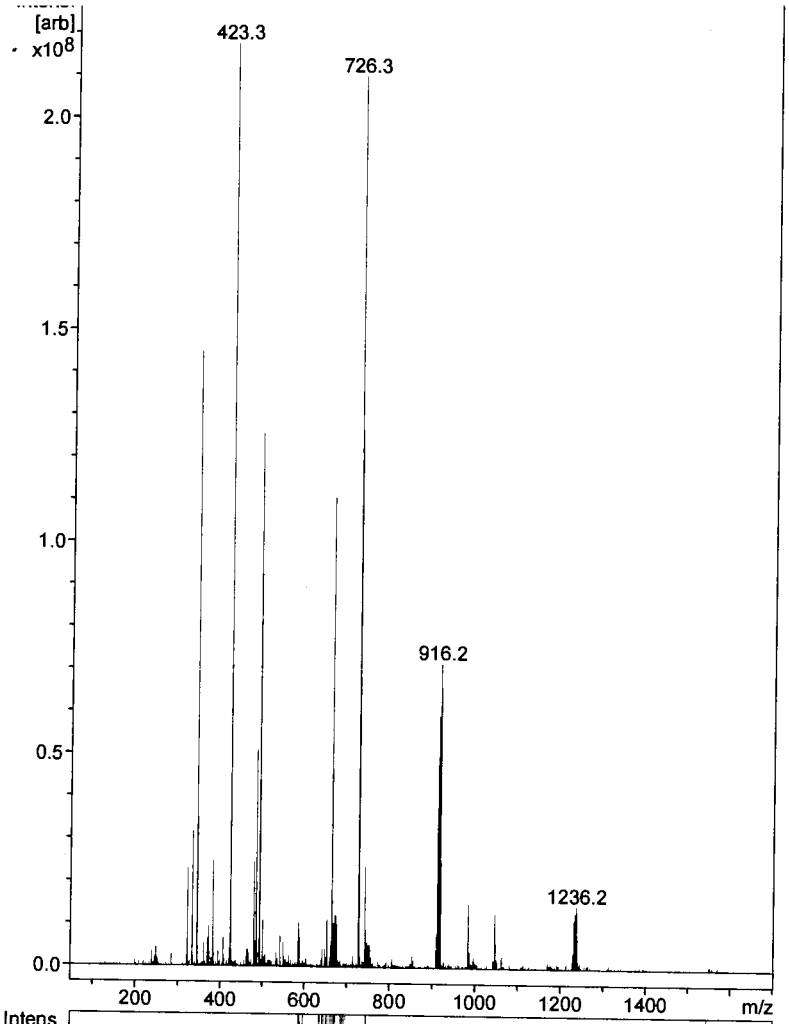
726.25
492.25
321.25
1243.25
m/z

Рисунок – Тб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1236.2
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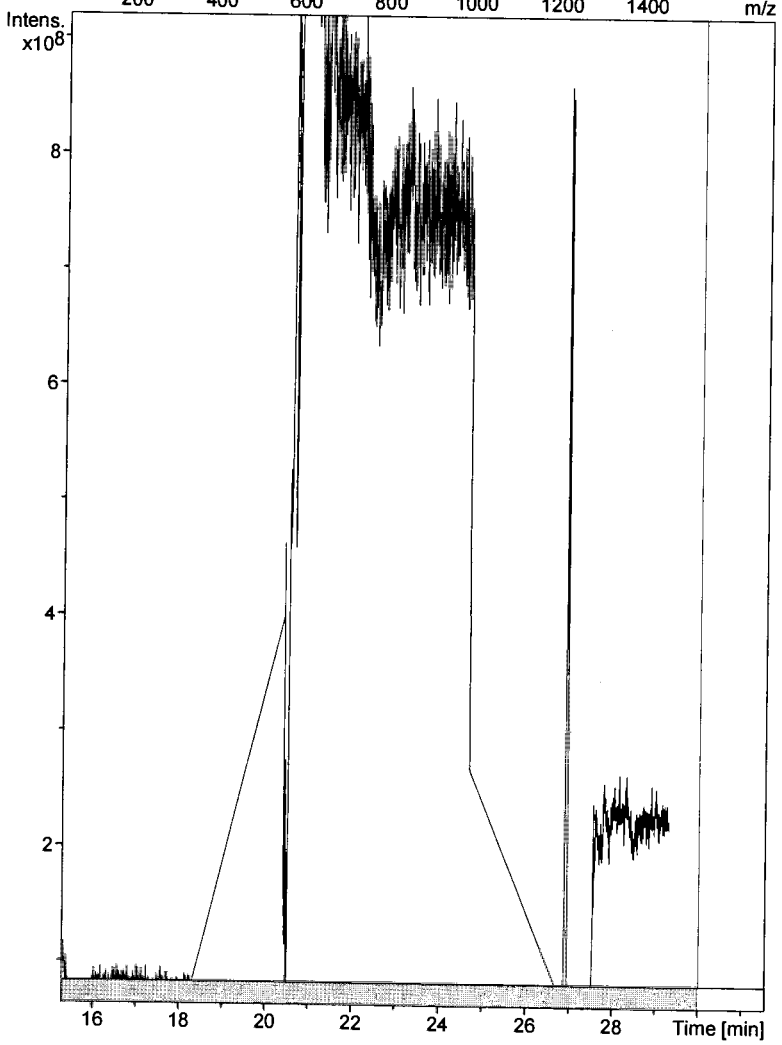
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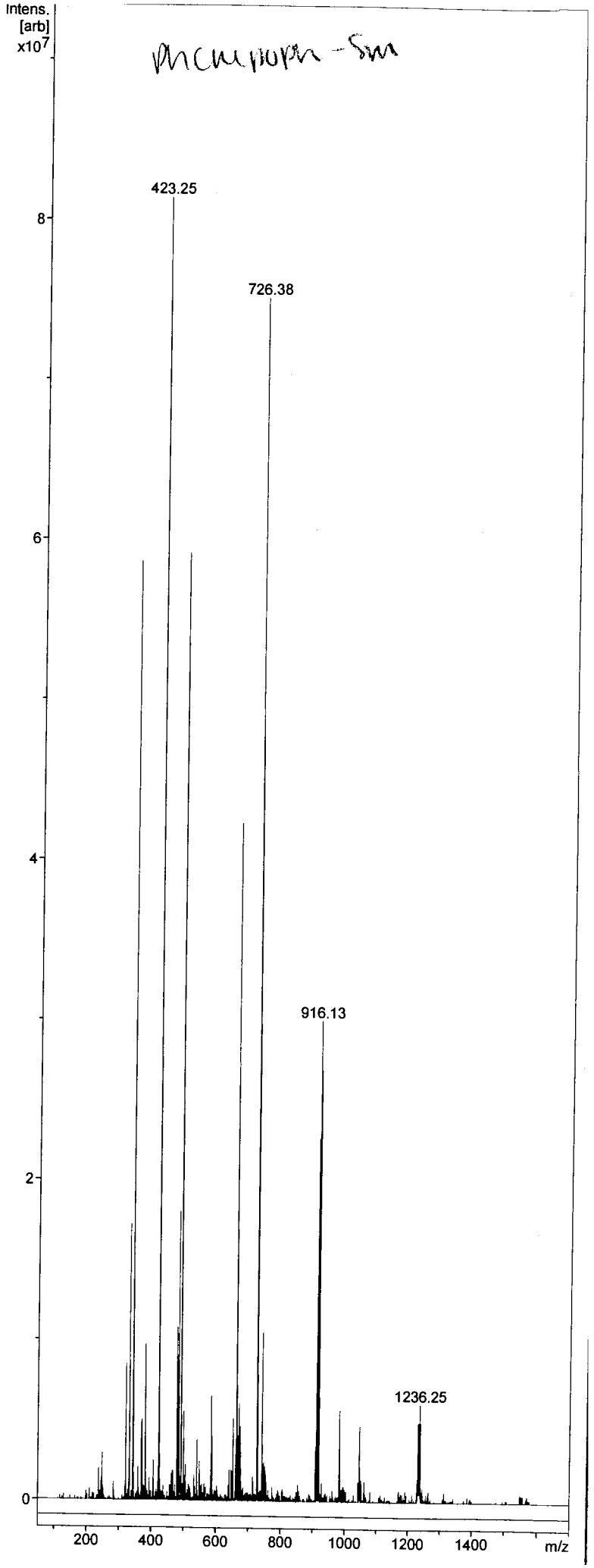
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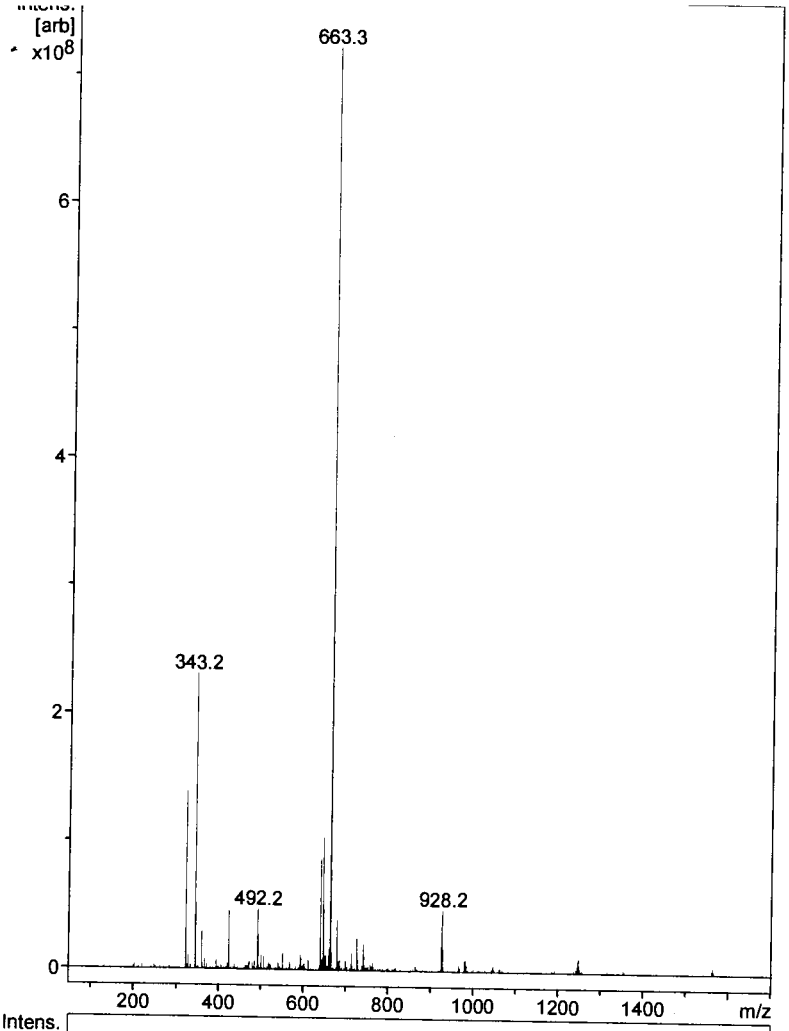
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492.2
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4
2
0
200
400
600
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1200
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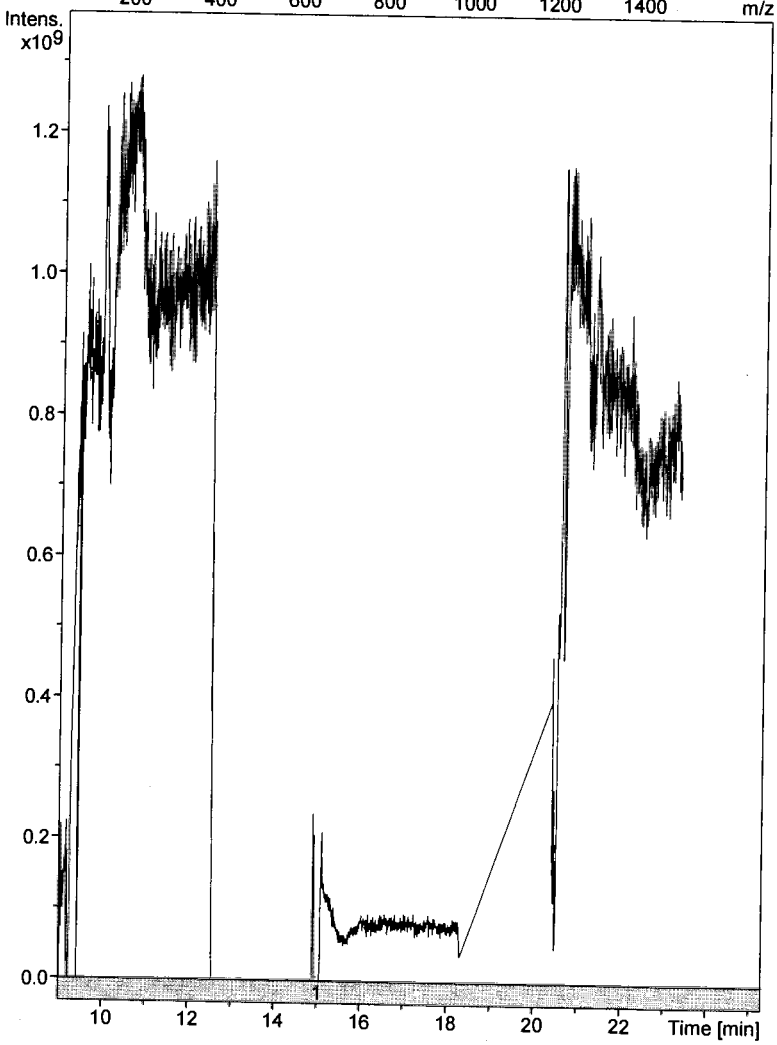
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10
12
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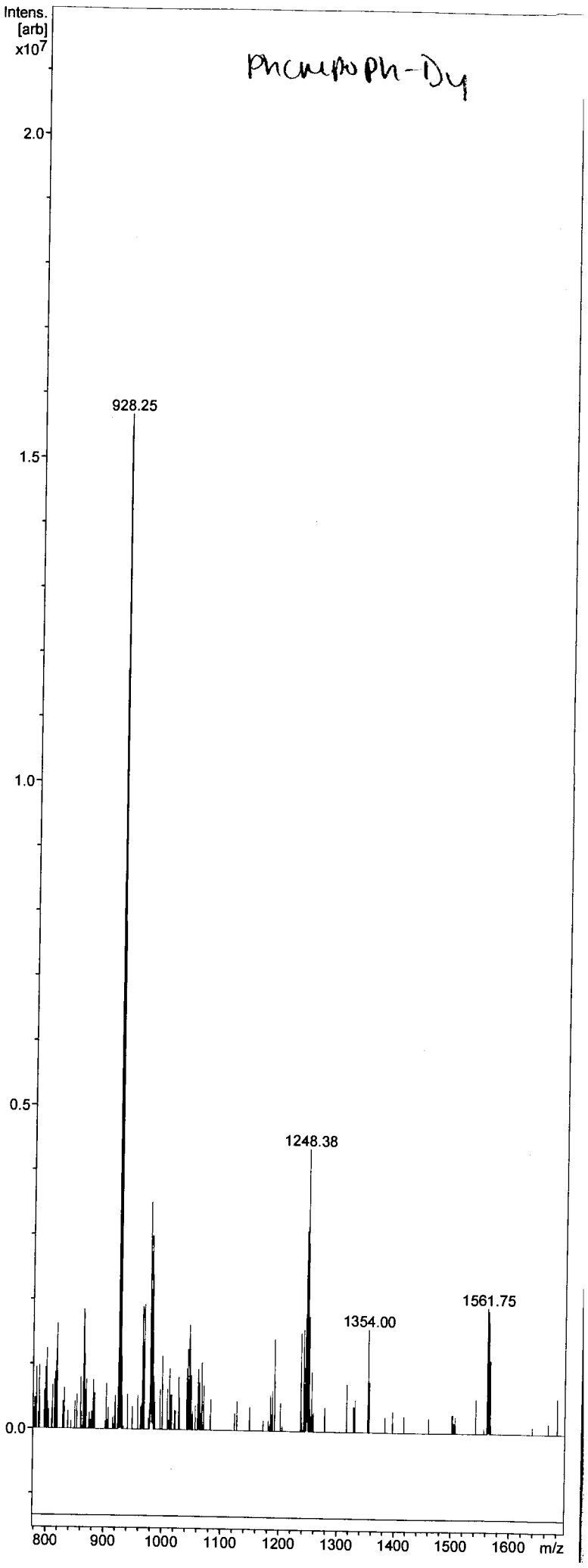
16
18
20
22
Time [min]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1561.75
800
900
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1100
1200
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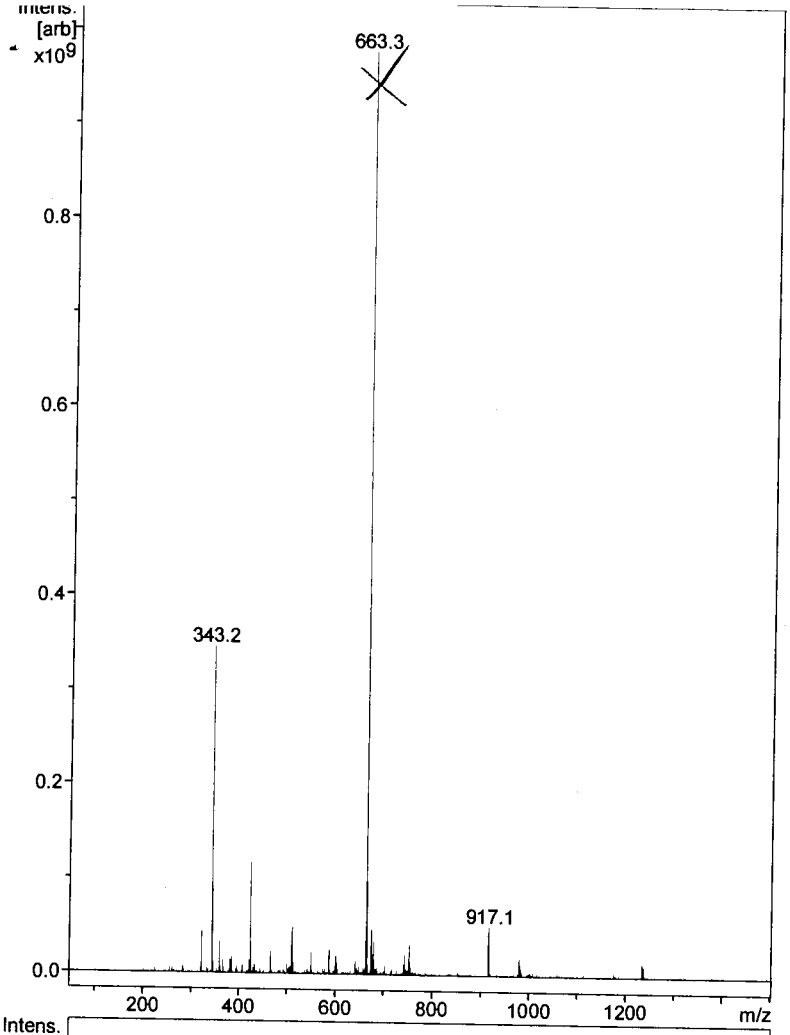
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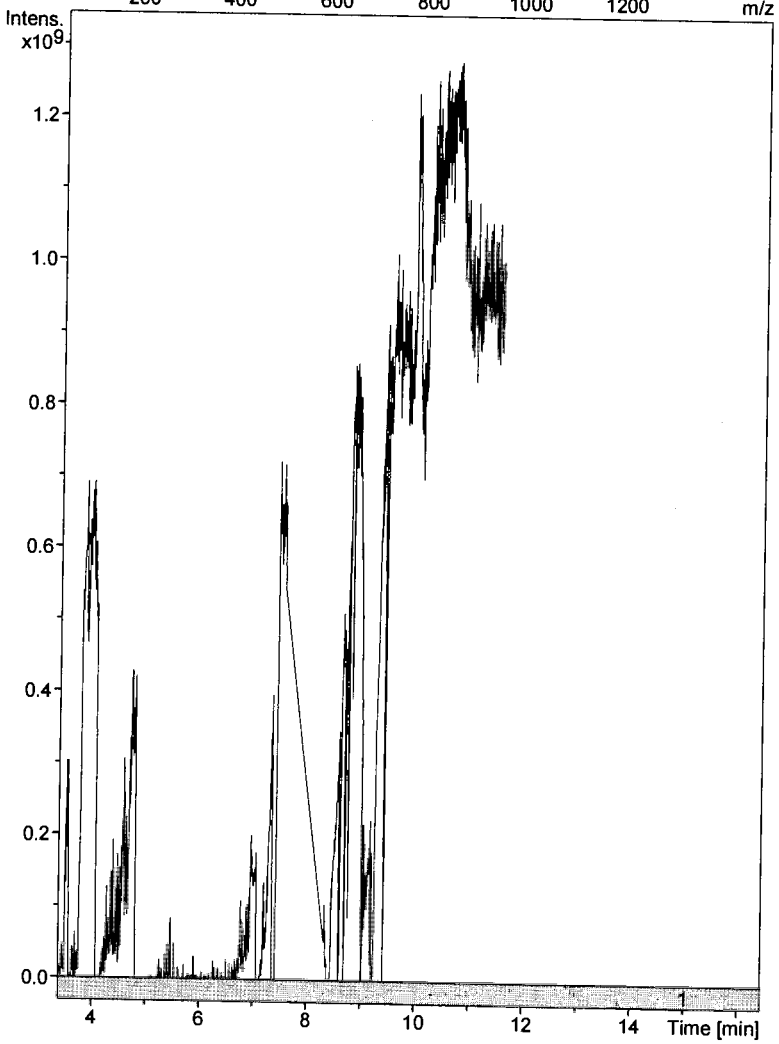
0.2
0.4
0.6
0.8
200
400
600
800
1000
1200
m/z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x10^9
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0.8
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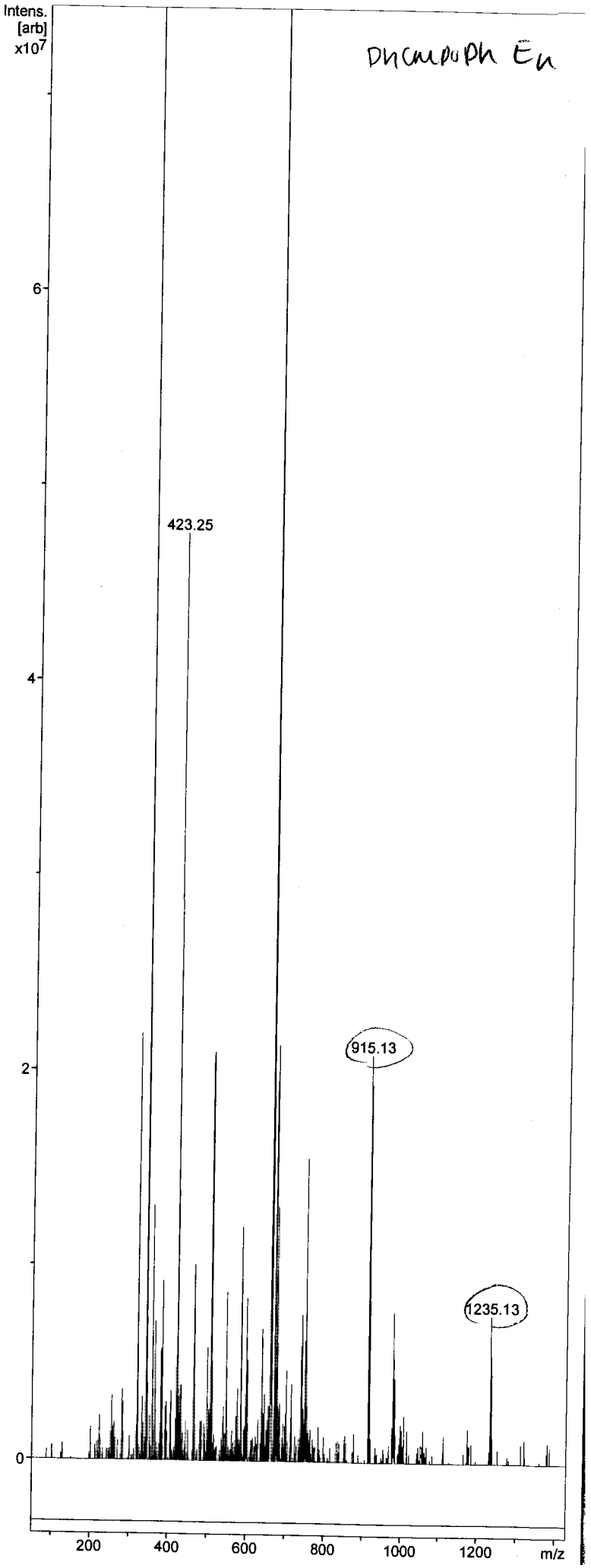
1.2
4
6
8
10
12
14
Time [min]


Intens.
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x10^7
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915.13
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2
4
6
200
400
600
800
1000
1200
m/z