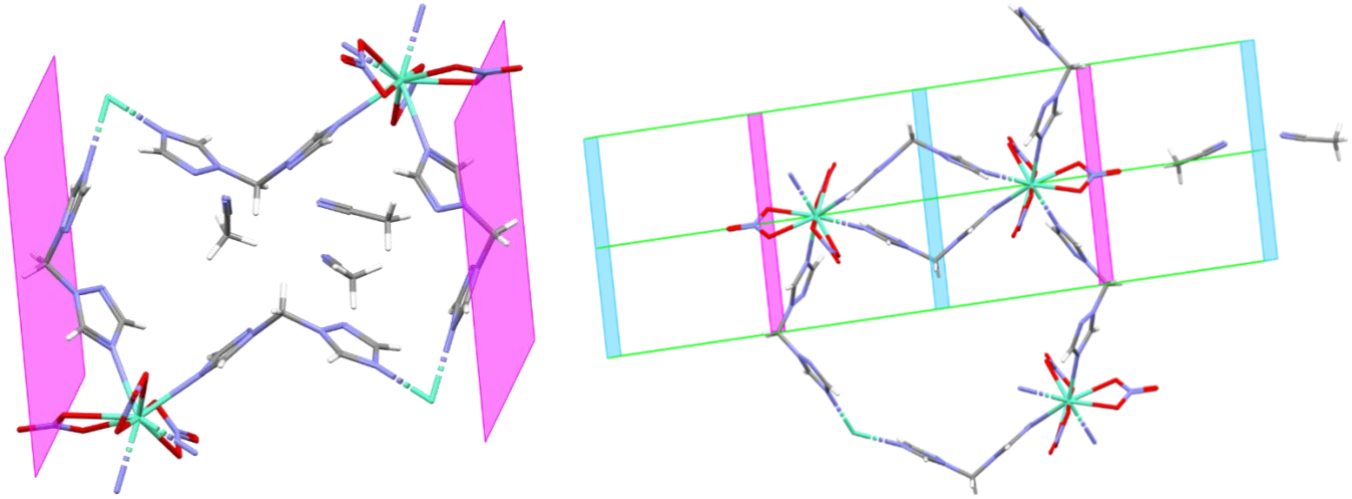
Supplementary Materials

Photoluminescent lanthanide(III) coordination polymers with bis(1,2,4-triazol-1-yl)methane linker

Elizaveta A. Ivanova [1], Ksenia S. Smirnova [1], Ivan P. Pozdnyakov [2], Andrei S. Potapov [1,*] and Elizaveta V. Lider [1,*]

[1] Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk 630090, Russia; ivanovaea@niic.nsc.ru (E.A.I.), smirnova@niic.nsc.ru (K.S.S.); potapov@niic.nsc.ru (A.S.P.); lider@niic.nsc.ru (E.V.L.)
[2] Voevodsky Institute of Chemical Kinetics and Combustion, SB RAS, Novosibirsk 630090, Russia; pozdnyak@kinetics.nsc.ru (I.P.P.)
* Correspondence: potapov@niic.nsc.ru (A.S.P.), lider@niic.nsc.ru (E.V.L.)



(**a**) (**b**)

Figure S1. Selected symmetry elements in the crystal substructures of compound **1**: (a) *P*2$_1$/*n* space group; (b) *C*2/*m* space group. Color code: purple – glide planes, blue – mirror planes, green – 2-fold axes.

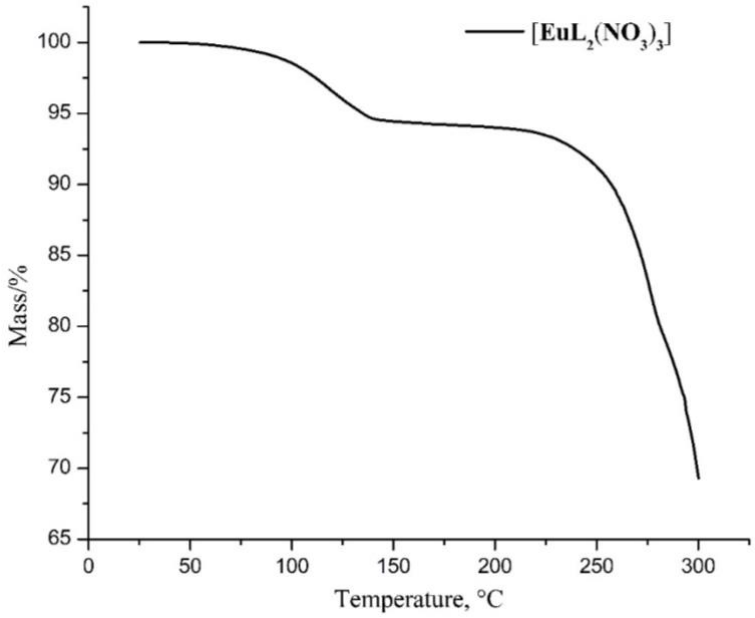


Figure S2. The thermogravimetric curve for compound **1**.

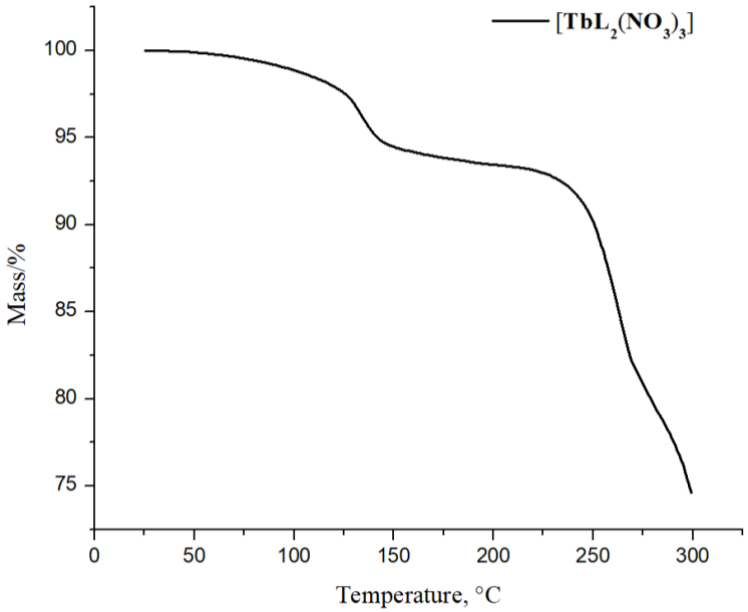


Figure S3. The thermogravimetric curve for compound **2**.

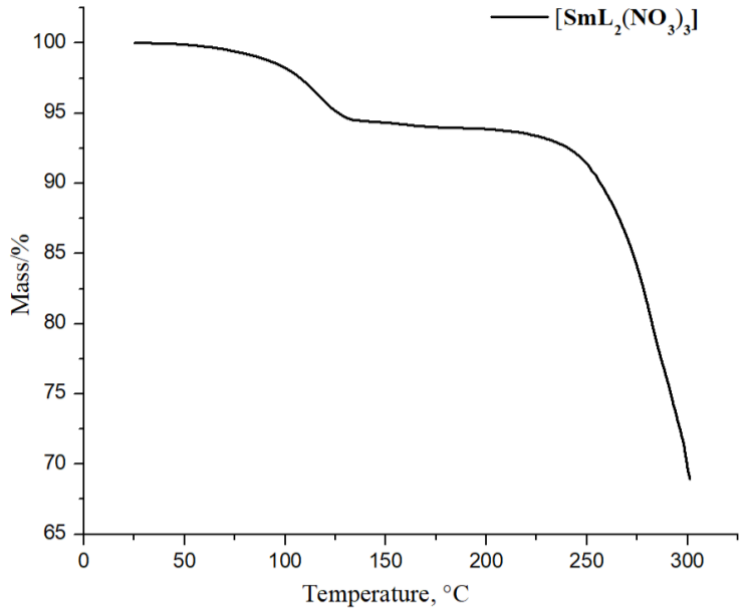


Figure S4. The thermogravimetric curve for compound **3**.

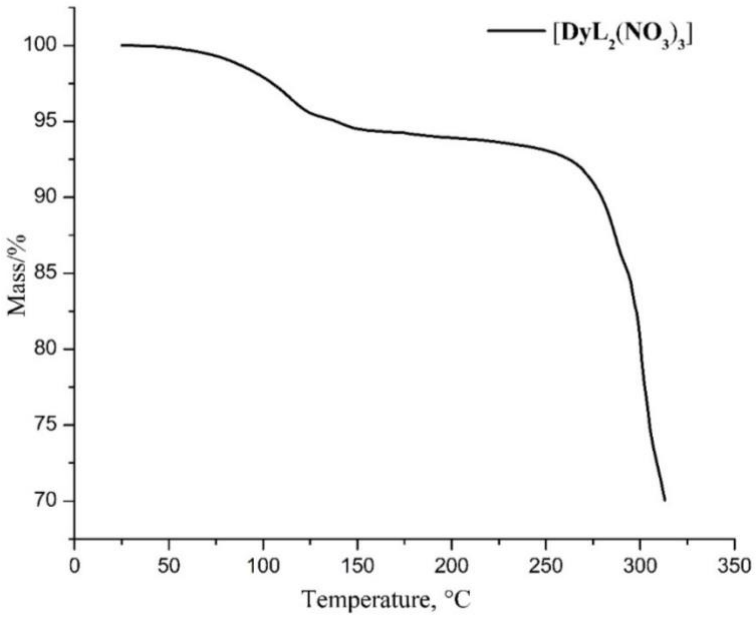


Figure S5. The thermogravimetric curve for compound **4**.

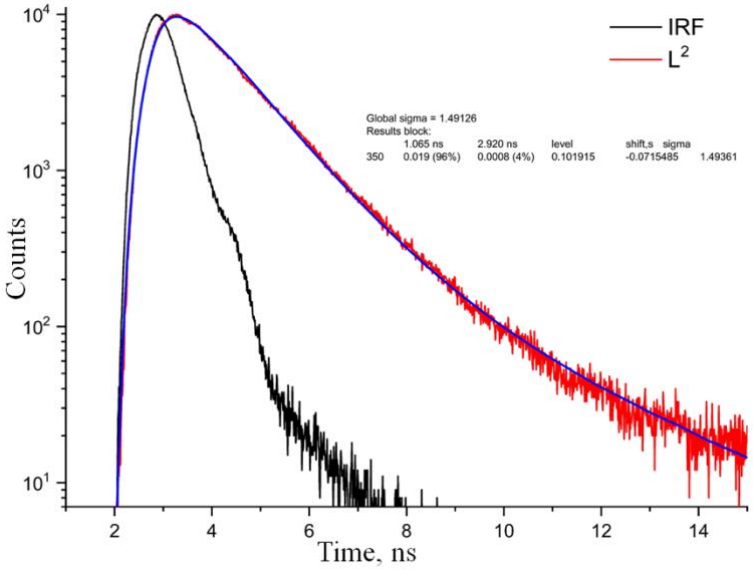


Figure S6. Luminescence decay plot for bis(1,2,4-triazol-1-yl)methane (btrm).

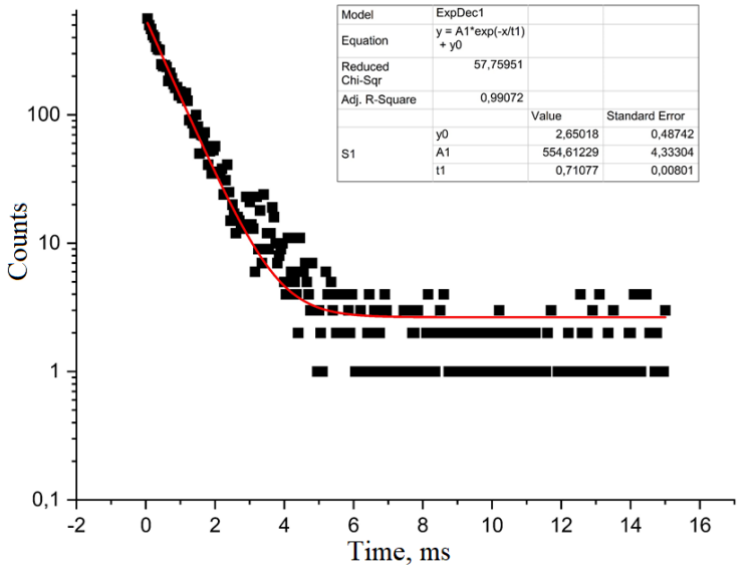


Figure S7. Luminescence decay plot for compound **1**.

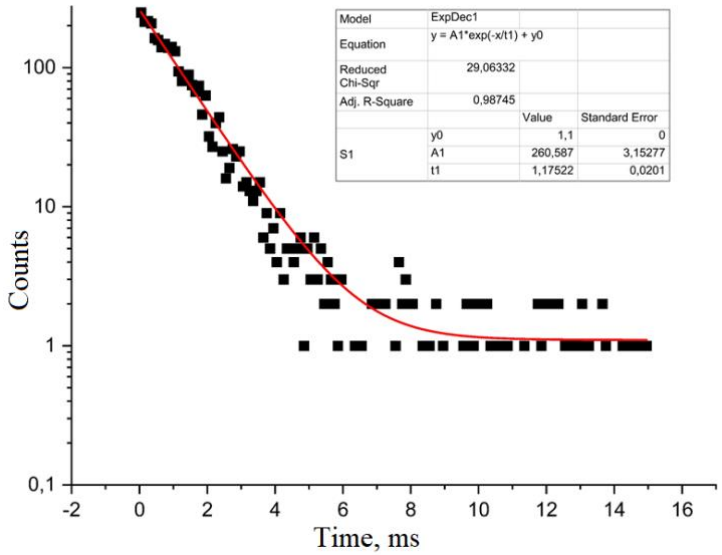


Figure S8. Luminescence decay plot for compound **2**.

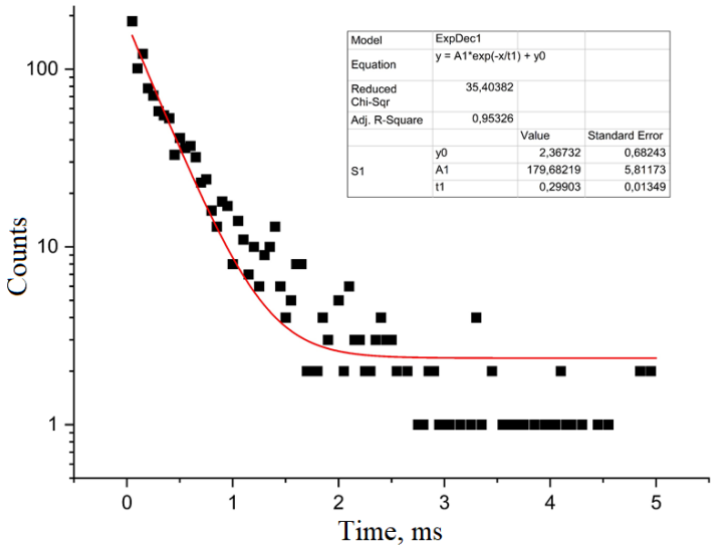


Figure S9. Luminescence decay plot for compound **3**.

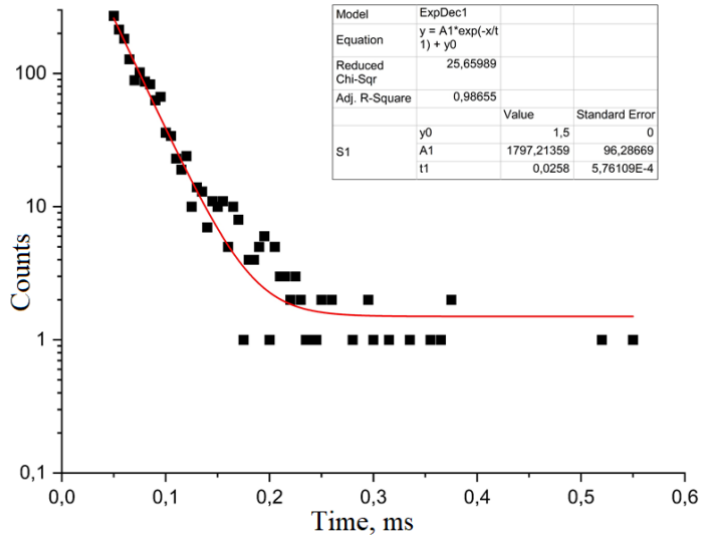


Figure S10. Luminescence decay plot for compound **4**.

Table S1. Assignment of the IR bands (cm^{-1}) of bis(1,2,4-triazol-1-yl)methane (btrm) and coordination polymers **1**-**5**

Compound	ν(O–H)	ν(C–H)	δ(C–H)	ν_{ring}	$\nu(NO_3^-)$
btrm	–	3112, 3098, 3015, 2929, 2851	1463, 1421, 1379, 1204, 1132, 1076, 1019	1553, 1506, 1345, 1275	–
$[EuL_2(NO_3)_3]_n \cdot 4H_2O$ (**1**)	3366	3125, 3055, 2925, 2855	1456, 1435, 1200, 1174, 1021	1560, 1557, 1275	1490, 1308
$[TbL_2(NO_3)_3]_n \cdot 3H_2O$ (**2**)	3359	3124, 3056, 2923, 2857	1462, 1434, 1202, 1121, 1077, 1025	1538, 1518, 1275	1493, 1306
$[SmL_2(NO_3)_3]_n \cdot H_2O$ (**3**)	3362	3126, 3053	1450, 1412, 1201, 1124, 1074 1023,	1536, 1511, 1275	1491, 1312
$[DyL_2(NO_3)_3]_n \cdot 2H_2O$ (**4**)	3365	3127, 3053, 2929, 2851	1458, 1434, 1203, 1122, 1075, 1023	1538, 1518, 1275	1495, 1312
$[GdL_2(NO_3)_3] \cdot H_2O$ (**5**)	3363	3124, 3053, 2926, 2853	1456, 1435, 1202, 1121, 1075, 1025	1537, 1518, 1275	1493, 1308

Table S2. Crystallographic data and structure refinement details for the coordination polymers

Compound	1a	1b	2a	3a	4a	4b
Molecular formula	$C_{16}H_{21}N_{18}O_9Eu$	$C_{16}H_{21}N_{18}O_9Eu$	$C_{10}H_{12}N_{15}O_9Tb$	$C_{16}H_{21}N_{18}O_9Sm$	$C_{16}H_{21}N_{18}O_9Dy$	$C_{16}H_{21}N_{18}O_9Dy$
Formula weight	761.47	761.47	645.27	759.86	772.01	772.01
Crystal system, space group	Monoclinic, $P2_1/n$	Monoclinic, $C2/m$	Monoclinic, $C2/m$	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/n$	Monoclinic, $C2/m$
Temperature (K)	150	150	150	150	150	150
a/Å	8.8102(7)	11.6706(17)	11.4936(5)	8.8102(3)	8.7580(5)	11.6627(6)
b/Å	31.082(3)	31.082(3)	30.9476(11)	31.0793(11)	31.0161(14)	31.0181(13)
c/Å	10.7758(9)	8.8095(15)	8.6690(4)	10.7882(4)	10.7149(5)	8.7576(4)
β/°	107.634(3)	118.366(9)	117.4440(10)	107.7090(10)	107.197(2)	118.628(2)
Volume/Å^3	2812.2 (4)	2811.9(7)	2736.5(2)	2813.99(17)	2780.5(2)	2780.8(2)
Z	4	4	4	4	4	4
ϱ_{calc} g/cm^3	1.799	1.799	1.566	1.794	1.844	1.844
μ/mm^{-1}	2.310	2.311	2.647	2.167	2.768	2.768
Crystal size/mm	0.26×0.22×0.03	0.26×0.22×0.03	0.13×0.04×0.01	0.24× 0.11 × 0.02	0.13 × 0.05 × 0.02	0.13 × 0.05 × 0.02
2Θ range for data collection/°	4.18 to 55.85	4.18 to 55.83	4.20 to 52.75	4.17 to 61.11	4.19 to 55.10	4.19 to 54.19
Index ranges	-11 ≤ h ≤ 11 -40 ≤ k ≤ 38 -14 ≤ l ≤ 14	-15 ≤ h ≤ 15 -40 ≤ k ≤ 38 -11 ≤ l ≤ 11	-14 ≤ h ≤ 14 -38 ≤ k ≤ 38 -9 ≤ l ≤ 10	-12 ≤ h ≤ 12 -44 ≤ k ≤ 44 -15 ≤ l ≤ 15	-9 ≤ h ≤ 11 -40 ≤ k ≤ 40 -13 ≤ l ≤ 13	-14 ≤ h ≤ 14 -39 ≤ k ≤ 39 -11 ≤ l ≤ 9
Reflections collected	39563	20108	16904	54617	28917	14272
Independent reflections	6715 [R_{int} = 0.0523, R_{sigma} = 0.0381]	3431 [R_{int} = 0.0438, R_{sigma} = 0.0321]	2861 [R_{int} = 0.0637, R_{sigma} = 0.0416]	8621 [R_{int} = 0.0690, R_{sigma} = 0.0524]	6382 [R_{int} = 0.0592, R_{sigma} = 0.0526]	3133 [R_{int} = 0.0443, R_{sigma} = 0.0391]
Restraints/parameters	0 / 400	9 / 192	0 / 139	0 / 400	8 / 385	9 / 194
Goodness-of-fit on F^2	1.125	1.107	1.083	1.055	1.056	1.045
Final R indexes [I>=2σ (I)]	R_1 = 0.0405, wR_2 = 0.0903	R_1 = 0.0374, wR_2 = 0.0991	R_1 = 0.0452, wR_2 = 0.1228	R_1 = 0.0440, wR_2 = 0.1008	R_1 = 0.0500, wR_2 = 0.1228	R_1 = 0.0493, wR_2 = 0.1300
Final R indexes [all data]	R_1 = 0.0498, wR_2 = 0.0936	R_1 = 0.0445, wR_2 = 0.1032	R_1 = 0.0522, wR_2 = 0.1279	R_1 = 0.0713, wR_2 = 0.1102	R_1 = 0.0686, wR_2 = 0.1323	R_1 = 0.0648, wR_2 = 0.1422
Largest diff. peak/hole / e/Å^{-3}	1.47/-2.46	1.54/-2.19	1.31/-1.06	1.61/-1.35	3.35/-1.34	1.56/-3.42
CCDC	2270135	2270131	2270136	2270133	2270134	2270132