

2D and 3D coordination polymers based on Ln(III) and 2,5-diiodoterephthalates: structures and luminescent behavior

Alexander S. Zaguzin, Mikhail A. Bondarenko, Pavel A. Abramov, Marianna I. Rakhmanova, Maxim N. Sokolov, Vladimir P. Fedin and Sergey A. Adonin

Table S1. XRD Experimental details

For all structures: triclinic, $P\bar{1}$, $Z = 1$.

	1	2
Chemical formula	$C_{42}H_{48}I_6La_2N_6O_{18}$	$C_{36}H_{34}I_6La_2N_4O_{16}$
M_r	1964.08	1817.89
Temperature (K)	100	150
a, b, c (Å)	11.5427(8), 11.7888(5), 13.1459(10)	10.0810 (3), 11.1622 (2), 12.3422 (3)
α, β, γ (°)	110.115(5), 115.234 (8), 97.442(5)	78.164 (1), 70.692 (1), 88.909 (1)
V (Å ³)	1436.89 (19)	1281.05 (6)
Radiation type	Cu Ka	Mo Ka
μ (mm ⁻¹)	37.24	5.33
Crystal size (mm)	0.10 × 0.03 × 0.01	0.12 × 0.05 × 0.05
Diffractometer	SuperNova, Single source at offset/far, HyPix3000	Bruker D8 Venture diffractometer
Absorption correction	Multi-scan <i>CrysAlis PRO</i> 1.171.41.122a (Rigaku Oxford Diffraction, 2021) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	Multi-scan <i>SADABS</i> 2016/2: Krause, L., Herbst- Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.403, 1.000	0.589, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12125, 5313, 4434	17957, 6007, 5294
R_{int}	0.067	0.028
θ values (°)	$\theta_{max} = 70.0$, $\theta_{min} = 4.2$	$\theta_{max} = 27.9$, $\theta_{min} = 1.8$
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.610	0.658
Range of h, k, l	$-12 \leq h \leq 13$, $-14 \leq k \leq 14$, $-15 \leq l \leq 15$	$-13 \leq h \leq 13$, $-14 \leq k \leq 14$, $-16 \leq l \leq 15$
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.078, 0.223, 1.11	0.037, 0.084, 1.09
No. of reflections,	5313, 329, 48	6007, 309, 6

parameters, restraints		
H-atom treatment	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.1277P)^2 + 19.6071P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0215P)^2 + 10.7312P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å ⁻³)	2.34, -3.46	1.49, -2.28

Computer programs: *CrysAlis PRO* 1.171.41.122a (Rigaku OD, 2021), *APEX3* (Bruker-AXS, 2016), *SAINT* (Bruker-AXS, 2016), *SHELXT* 2018/2 (Sheldrick, 2018), *SHELXT* 2014/5 (Sheldrick, 2014), *SHELXL2017/1* (Sheldrick, 2017).

Table S2. Selected geometric parameters (Å)

1			
O1—La1	2.510 (9)	O6—La1 ⁱ	2.715 (9)
O2—La1	2.552 (10)	O7—La1 ⁱ	2.629 (10)
O3—La1	2.475 (9)	O8—La1 ⁱⁱ	2.569 (8)
O4—La1 ⁱ	2.514 (8)	O9—La1 ⁱⁱ	2.579 (10)
O6—La1	2.451 (9)		
2			
O1—La1	2.515 (4)	O5—La1 ⁱ	2.650 (4)
O2—La1	2.555 (4)	O6—La1 ⁱ	2.613 (4)
O3—La1	2.574 (4)	O7—La1 ⁱ	2.503 (4)
O4—La1	2.492 (4)	O8—La1	2.514 (4)
O5—La1	2.539 (4)		

Symmetry code(s): (i) -x+1, -y+1, -z+1; (ii) -x+1, -y+2, -z+1.

Steady-state, room temperature luminescence measurements were conducted using a Jobin Yvon FluoroLog 3 with a 450 W xenon source and pulsed xenon lamps as light sources, cooled detector and double grating excitation and emission monochromators. All excitation and emission spectra were corrected for the sensitivity of the detector and wavelength dependence of the output power of the source. The photoluminescence quantum yields (φ_f) were measured using a Fluorolog 3 Quanta- φ device at 300 K.

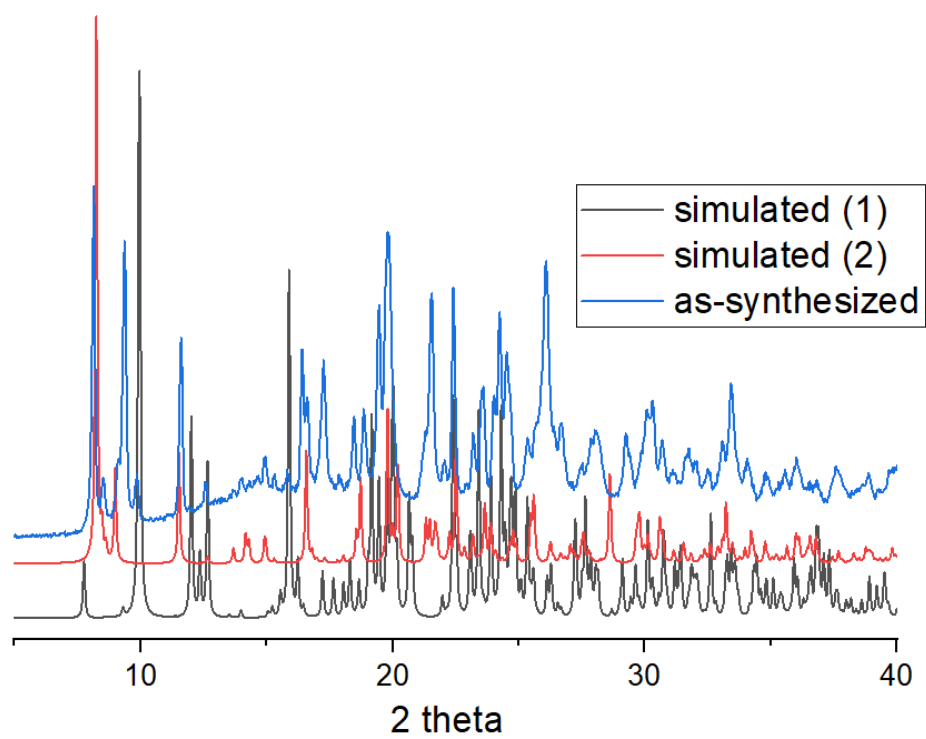


Figure S1. PXRD data for the solid containing **1** and **2**.

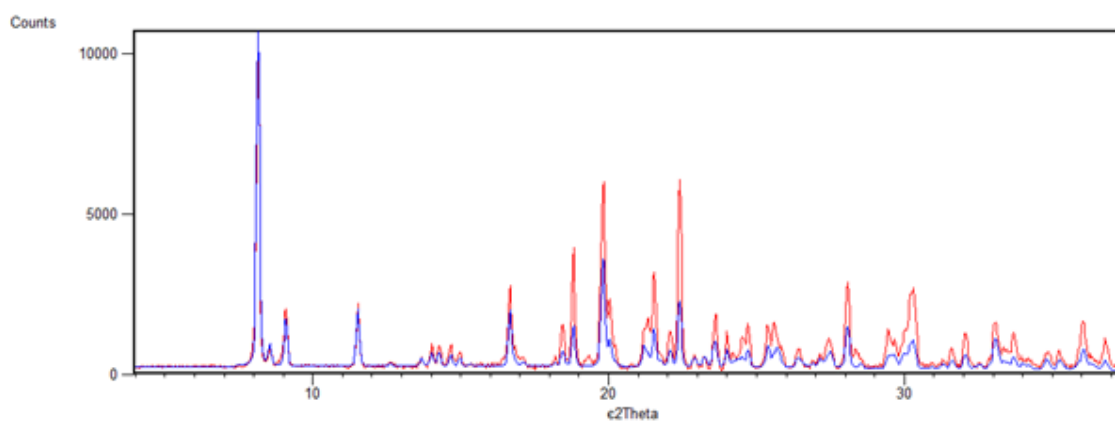


Figure S2. PXRD data for **3** (calculated and experimental).

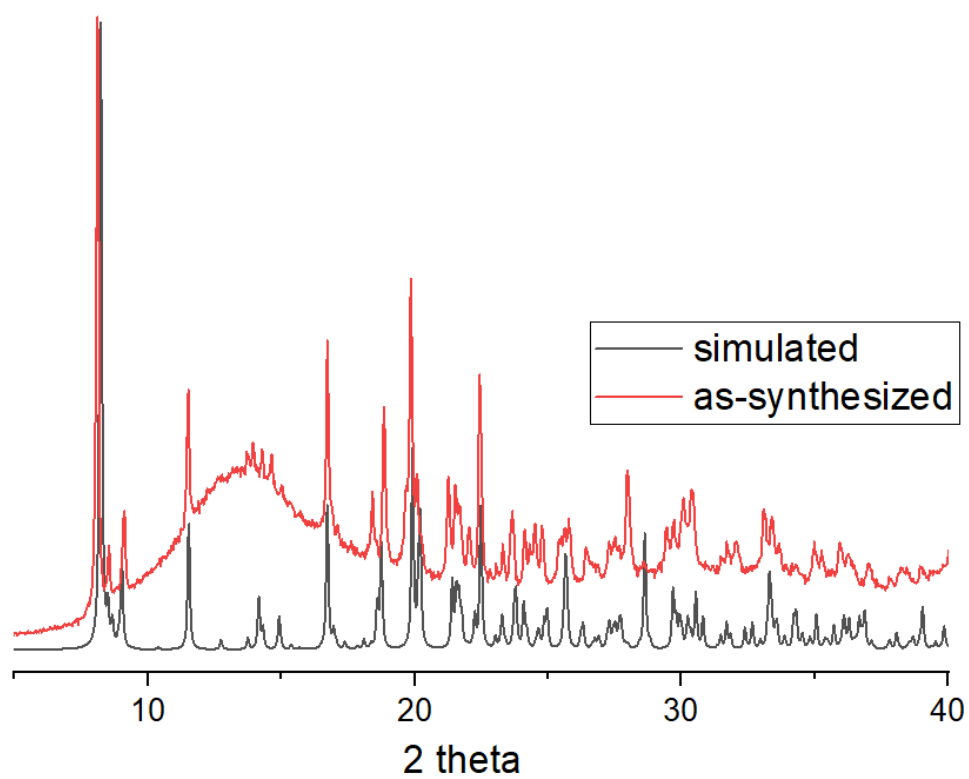


Figure S3. PXRD data for **4** (calculated and experimental).

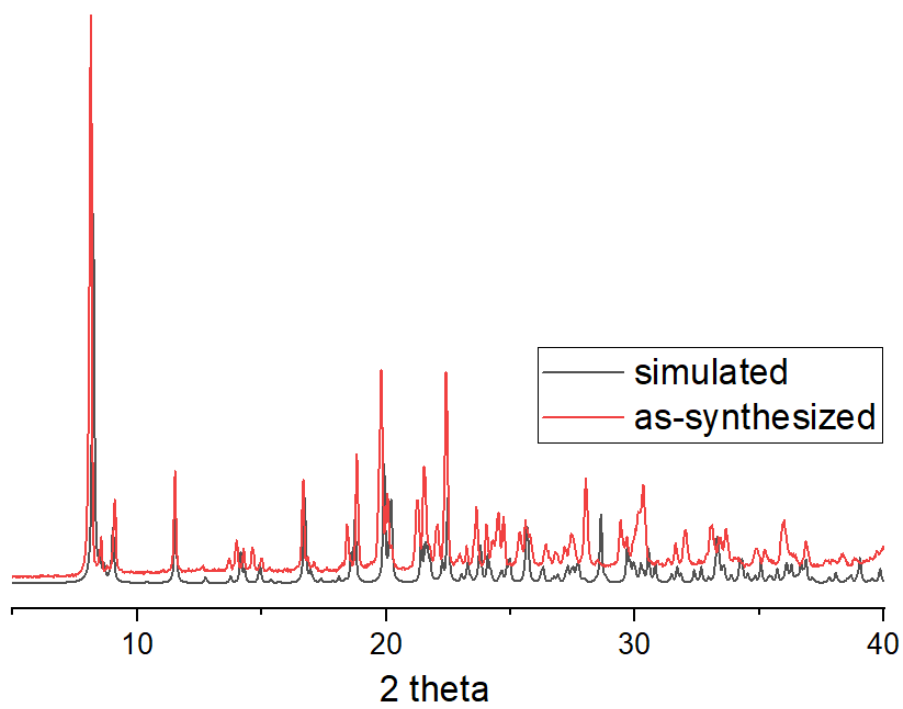


Figure S4. PXRD data for **5** (calculated and experimental).

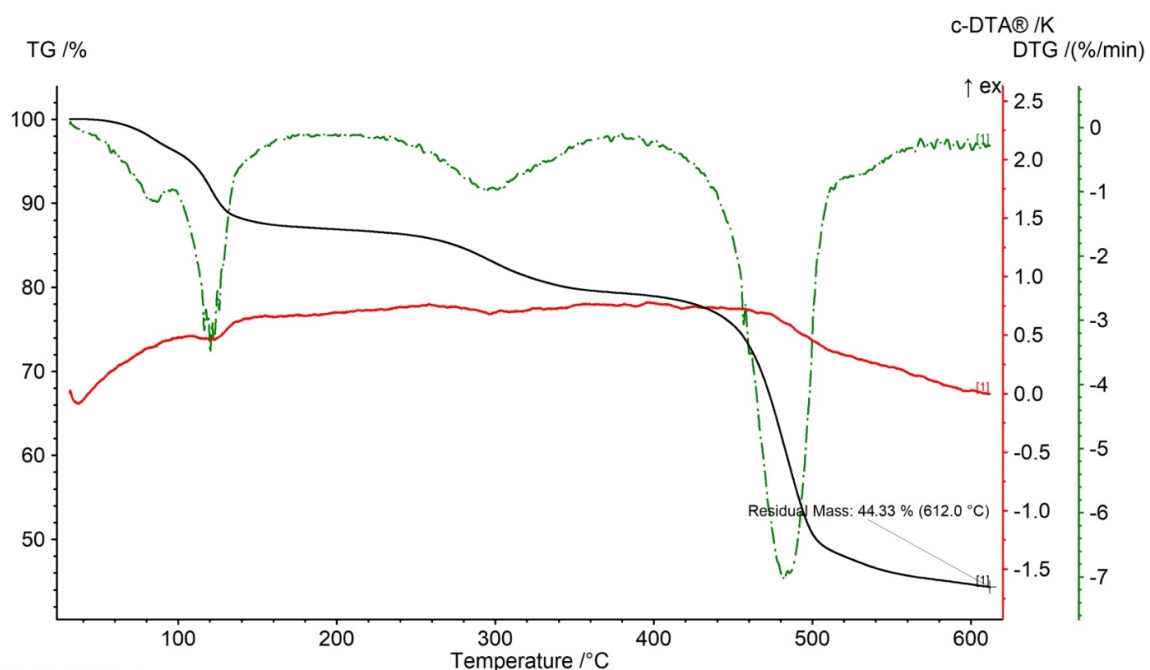


Figure S5. TG, DTA and DSC data for **4**.

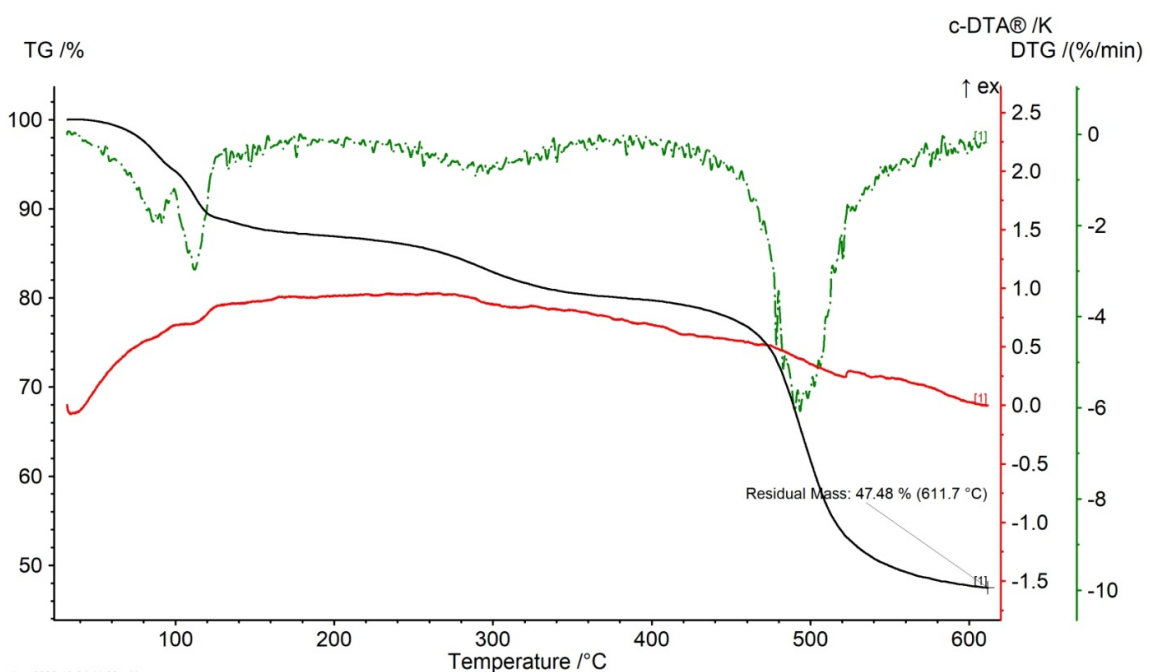
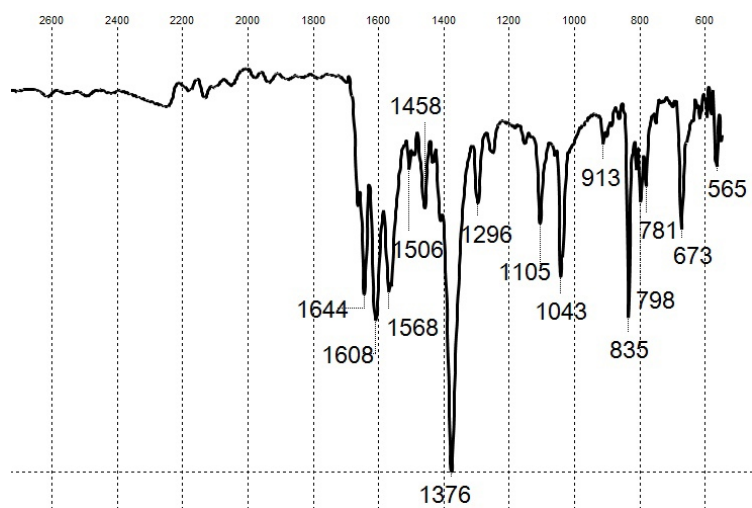


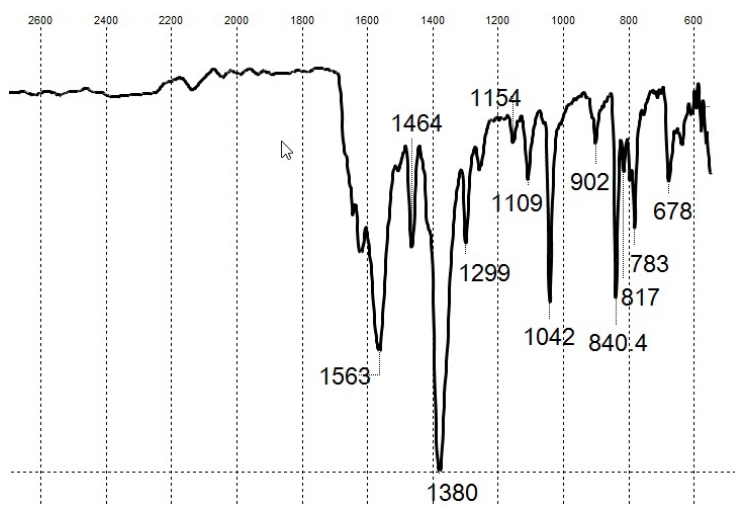
Figure S6. TG, DTA and DSC data for **5**

FTIR data

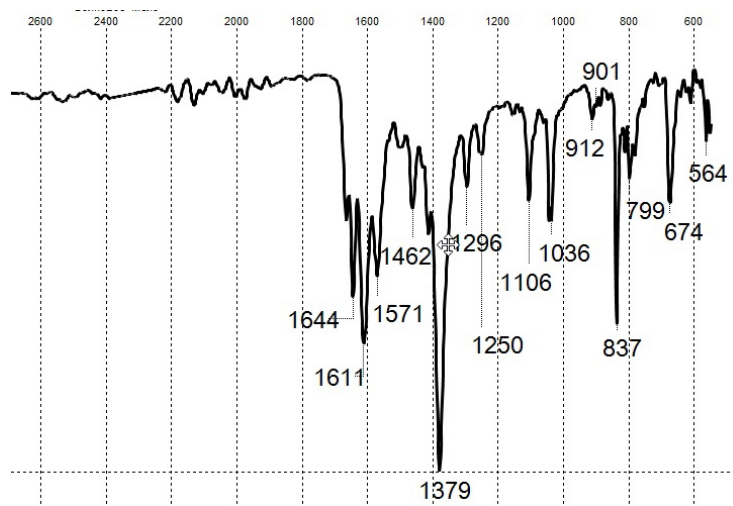
1/2: 1644 m, 1608 m, 1568 m, 1506 m, 1458 m, 1376s, 1296 m, 1105 m, 1043 m, 913 m, 835 s, 798 w, 781 w, 673 m, 565 m.



3: 1647 m, 1610 m, 1563 s, 1464 m, 1380s, 1299 m, 1109 m, 1041 a, 902 w, 817 s, 783 w, 781 w, 678 m.



4: 1644 m, 1611 s, 1571 m, 1462 m, 1379 s, 1296 m, 1106 m, 1036 m, 912 w, 817 s, 799 w, 674 m, 564 w



Element analysis data

	C, H, N (calcd)	C, H, N (found)
3	23.69; 1.88; 3.07	23.78; 1.95; 3.18
4	23.43; 1.86; 3.04	23.53; 1.97; 3.14
5	23.40; 1.86; 3.04	23.54; 1.98; 3.17