10.1071/CH21233
Australian Journal of Chemistry

Supplementary Material

Monometallic Ln^{3+} and heterometallic Ln^{3+}–Cd^{2+} complexes based on pentafluorophenylacetic acid: efficient control of dimension and luminescent properties

Y. A. Belousov[A,B,*], *M. A. Kiskin*[C], *A. V. Sidoruk*[A], *E. A. Varaksina*[B], *M. A. Shmelev*[C], *N. V. Gogoleva*[C], *I. V. Taydakov*[B,D] and *I. L. Eremenko*[C]

[A]Chemistry Department, Moscow State University, Leninskie Gory, Moscow 119991, Russia.

[B]P. N. Lebedev Physical Institute of Russian Academy of Sciences, Moscow 119991, Russia.

[C]Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow 119991, Russia.

[D]G. V. Plekhanov Russian University of Economics, Moscow 117997, Russia.

*Correspondence to: Email: belousov@inorg.chem.msu.ru

Monometallic Ln^{3+} and heterometallic Ln^{3+}- Cd^{2+}complexes based on pentafluorophenylacetic acid: efficient control of dimension and luminescent properties

Belousov Y.A.[a,b], Kiskin M.A.[c], Sidoruk A.V.[a], Varaksina E.A.[b], Shmelev M.A.[c], Gogoleva N.V.[c], and Taidakov I.V.[b], Eremenko I.L.[c]

a Chemistry Department, Moscow State University, Leninskie Gory, Moscow 119991, Russia;

b P. N. Lebedev Physical Institute of Russian Academy of Sciences, Moscow 119991, Russia;

c Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow 119991, Russia.

Supplementary data

Supplementary data title	Page
Figure SI1. Calculated for sample **1** (*a*) and experimental diffractograms for samples **1** (*b*) and **2** (*c*)**.**	**2**
Figure SI2. Calculated for sample **3** (*a*) and experimental diffractograms for samples **3** (*b*) and **4** (*c*)**.**	**3**
Table SI1. Continuous Shape Measures (CShM) values for the potential coordination polyhedron of Eu and Cd in **1** and **3**	**4**
Table SI2. D-H…A (D = O, C, A = O, F) interactions in crystals **1** and **3**.	**5**
Table SI3. C-F… π interactions in the crystal **1** (Cg is centroid of 6-memmberd ring (Cg1: C3->C8; Cg2: C11->C16; Cg3: C19->C24); F-Perp is perpendicular distance of F on ring; Gamma is angle F->Cg vector and normal to ring plane).	**6**
Figure SI3. Fragment of luminescence spectra of complexes 3 (a) and 4 (b) at λ_{ex}=280 nm and T=300 K.	**7**

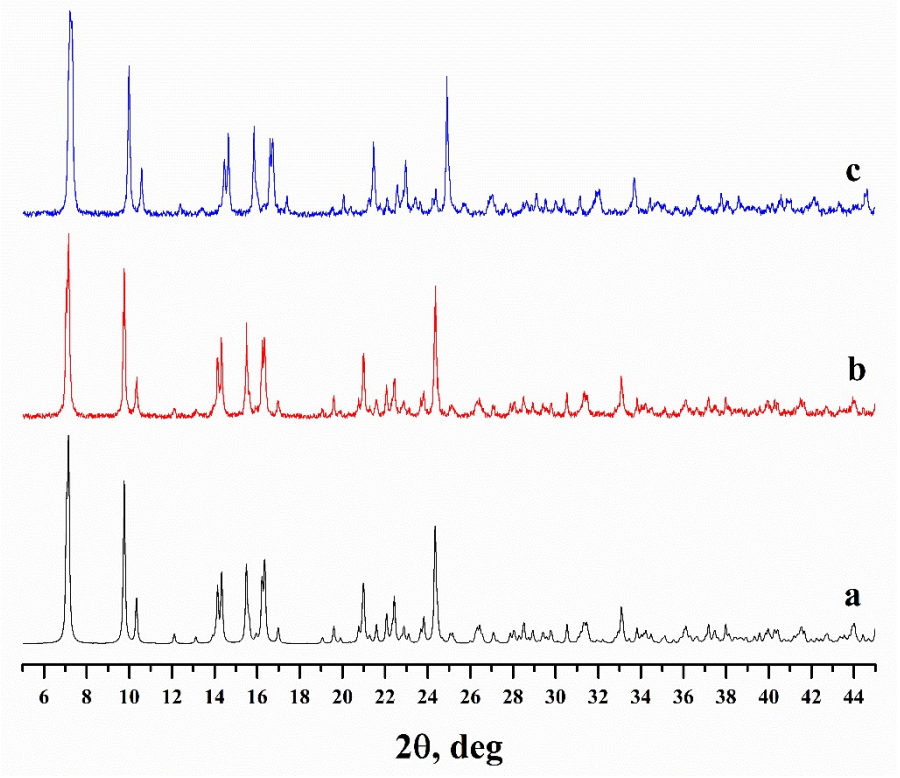

Figure SI1. Calculated for sample **1** (*a*) and experimental diffractograms for samples **1** (*b*) and **2** (*c*)**.**

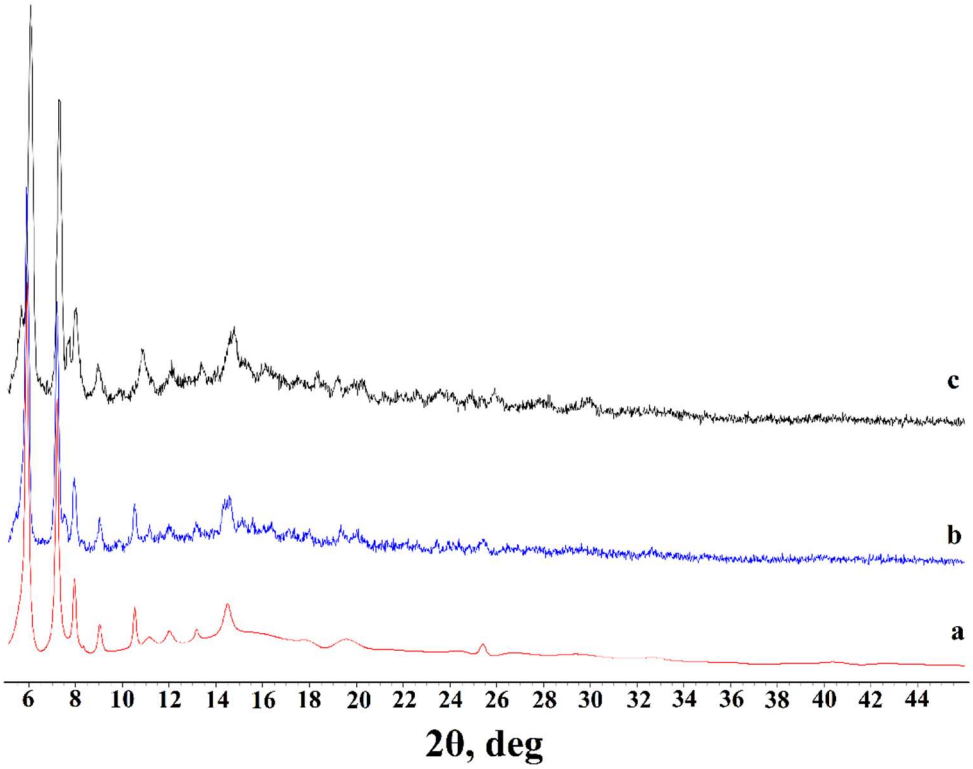

Figure SI2. Calculated for sample **3** (*a*) and experimental diffractograms for samples **3** (*b*) and **4** (*c*)**.**

Table SI1. Continuous Shape Measures (CShM) values for the potential coordination polyhedron of Eu and Cd in **1** and **3**

EuO_{10} in **1**	EuO_9 in **2**	CdN_2O_4 in **1**
Decagon, D_{10h} - 31.728	Enneagon, D_{9h} - 35.638	Hexagon, D_{6h} - 32.974
Enneagonal pyramid, C_{9v} - 24.895	Octagonal pyramid, C_{8v} - 23.184	Pentagonal pyramid, C_{5v} - 23.010
Octagonal bipyramid, D_{8h} - 18.446	Heptagonal bipyramid, D_{7h} - 18.593	Octahedron, O_h - 3.993
Pentagonal prism, D_{5h} - 11.564	Johnson triangular cupola J3, C_{3v} - 15.338	Trigonal prism, D_{3h} - 12.304
Pentagonal antiprism, D_{5d} - 13.202	Capped cube J8, C_{4v} - 10.630	Johnson pentagonal pyramid J2, C_{5v} - 27.334
Bicapped cube J15, D_{4h} - 10.368	Spherical-relaxed capped cube, C_{4v} - 9.076	
Bicapped square antiprism J17, D_{4d} - 2.854	Capped square antiprism J10, C_{4v} - 2.951	
Metabidiminished icosahedron J62, C_{2v} - 9.025	Spherical capped square antiprism, C_{4v} - 2.026	
Augmented tridiminished icosahedron J64, C_{3v} - 18.225	Tricapped trigonal prism J51, D_{3h} - 3.849	
Sphenocorona J87, C_{2v} - 2.740	*Spherical tricapped trigonal prism*, D_{3h} - 2.130	
Staggered Dodecahedron (2:6:2), D_2 - 4.871	Tridiminished icosahedron J63, C_{3v} - 10.206	
Tetradecahedron (2:6:2), C_{2v} - 4.135	Hula-hoop, C_{2v} - 10.156	
Hexadecahedron (2:6:2) or (1:4:4:1), D_{4h} - 9.377	Muffin, C_s - 1.913	

Table SI2. D-H…A (D = O, C, A = O, F) interactions in crystals **1** and **3**.

Interaction	D-H, Å	H…A, Å	D…A, Å	D-H-A, deg.
1				
Intramolecular				
O7-H7A...O4(-*x*,1-*y*,1-*z*)	0.89	2.54	2.864(5)	102
O7-H7B...O1(1-*x*,1-*y*,1-*z*)	0.89	1.85	2.694(5)	159
O8-H8A. ..O6(1-*x*,1-*y*,1-*z*)	0.89	2.44	2.809(5)	105
O8-H8B...O2(-*x*,1-*y*,1-*z*)	0.89	1.81	2.677(5)	167
C2-H2B...F1	0.99	2.42	2.850(8)	105
C10-H10A...F6	0.99	2.45	2.865(7)	105
C10-H10B...O6(1-*x*,1-*y*,1-*z*)	0.99	2.35	3.260(7)	152
C18-H18B...F11	0.99	2.45	2.827(8)	102
C18-H18B...O4(-*x*,1-*y*,1-*z*)	0.99	2.58	3.283(6)	128
Intermolecular				
O8-H8A...F14(-1+*x*,*y*,1+*z*)	0.89	2.44	3.001(6)	144
2				
Intramolecular				
O11-H11...O8(1-*x*,-*y*,1-*z*)	0.82	1.91	2.677(10)	154
C41-H41B...O6	0.97	2.60	3.118(13)	147
C2-H2A...F8	0.97	2.50	2.875(12)	103
C2-H2B...O8	0.97	2.41	3.298(12)	152
C10-H10A...F16	0.97	2.44	2.863(13)	106
C18-H18A...F20	0.97	2.39	2.809(15)	105
C26-H26A...F31	0.97	2.42	2.809(12)	103
C34-H34A...F40	0.97	2.50	2.846(13)	101
Intermolecular				
C45-H45...O1(2-*x*,1-*y*,2-*z*)	0.93	2.44	3.259(13)	114
C18-H18A...F5(-1+x,*y*,*z*)	0.97	2.47	3.249(15)	137

Table SI3. C-F… π interactions in the crystal **1** (Cg is centroid of 6-memmberd ring (Cg1: C3->C8; Cg2: C11->C16; Cg3: C19->C24); F-Perp is perpendicular distance of F on ring; Gamma is angle F->Cg vector and normal to ring plane).

Interaction	F…Cg, Å	F-Perp, Å	Gamma, deg.	C-F…Cg, deg.	C…Cg, Å
C6-F3…Cg1(1-*x*, -*y*, 1-*z*)	3.195(5)	3.192	2.83	89.5(3)	3.447(7)
C13-F7…Cg1(-*x*, -*y*, 1-*z*)	3.456(5)	-3.224	21.09	105.2(3)	4.024(7)
C16-F10…Cg3(1-*x*, 1-*y*, 1-*z*)	3.661(5)	3.485	17.86	93.0(3)	3.965(7)
C20-F11…Cg2(-*x*, 1-*y*, 1-*z*)	3.707(6)	-3.334	25.96	103.9(4)	4.237(7)
C21-F12…Cg2(1-*x*, 1-*y*, 1-*z*)	3.567(6)	3.532	7.94	96.0(4)	3.942(8)

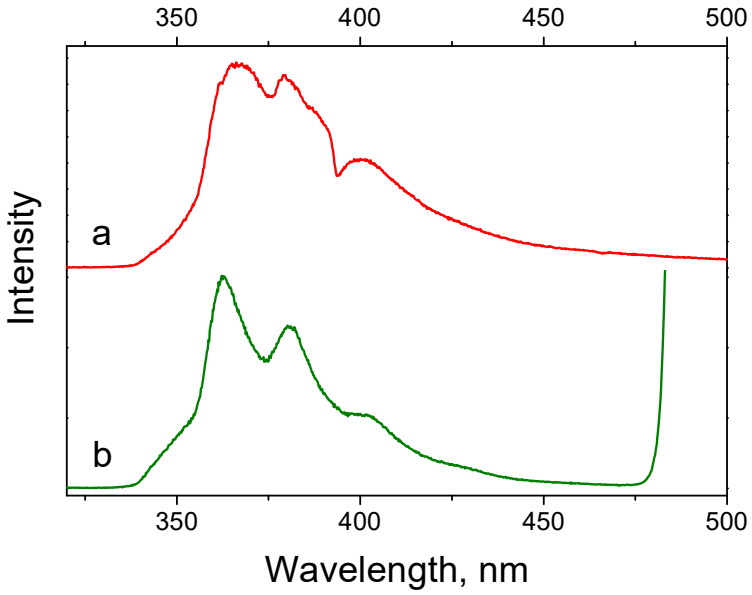

Figure SI3. Fragment of luminescence spectra of complexes 3 (a) and 4 (b) at λ_{ex}=280 nm and T=300 K.