The complete series of lanthanoid-chloranilato lattices with dimethylsulfoxide: Role of the lanthanoid size on the coordination number and crystal structure

Samia Benmansour [1,*], Antonio Hernández-Paredes [1] and Carlos J. Gómez-García [1,*]

[1] Departamento de Química Inorgánica. Universidad de Valencia. C/ Dr. Moliner 50, 46100 Burjasot (Valencia) Spain.

Correspondence: sam.ben@uv.es (S.B.); carlos.gomez@uv.es (C.J.G.-G)

Table S1. Crystal size and colour, exact amounts and precursors used for the synthesis of compounds **1-13**.

#	Formula	Salt	mass (mg)	Aspect
1	$[La_2(C_6O_4Br_2)_3(dmso)_6]$	$La(NO_3)_3{\cdot}6H_2O$	8.8	Violet block
2	$[Ce_2(C_6O_4Br_2)_3(dmso)_6]$	$Ce(NO_3)_3{\cdot}6H_2O$	8.7	Red block
3	$[Pr_2(C_6O_4Br_2)_3(dmso)_6]$	$Pr(NO_3)_3{\cdot}6H_2O$	8.7	Red prism
4	$[Nd_2(C_6O_4Br_2)_3(dmso)_6]$	$Nd(NO_3)_3{\cdot}6H_2O$	8.8	Violet block
5	$[Sm_2(C_6O_4Br_2)_3(dmso)_6]$	$Sm(NO_3)_3{\cdot}6H_2O$	8.9	Pink prism
6	$[Eu_2(C_6O_4Br_2)_3(dmso)_6]$	$Eu(NO_3)_3{\cdot}6H_2O$	8.9	Red block
7	$[Gd_2(C_6O_4Br_2)_3(dmso)_6]$	$Gd(NO_3)_3{\cdot}6H_2O$	9.0	Violet prism
8	$[Tb_2(C_6O_4Br_2)_3(dmso)_6]$	$Tb(NO_3)_3{\cdot}5H_2O$	8.7	Pink block
9	$[Dy_2(C_6O_4Br_2)_3(dmso)_4]{\cdot}2dmso{\cdot}2H_2O$	$Dy(NO_3)_3{\cdot}5H_2O$	8.8	Pink prism
10	$[Ho_2(C_6O_4Br_2)_3(dmso)_4]{\cdot}2dmso{\cdot}2H_2O$	$Ho(NO_3)_3{\cdot}5H_2O$	8.8	Pink block
11	$[Er_2(C_6O_4Br_2)_3(dmso)_4]{\cdot}2dmso{\cdot}2H_2O$	$Er(NO_3)_3{\cdot}5H_2O$	8.9	Violet block
12	$[Tm_2(C_6O_4Br_2)_3(dmso)_4]{\cdot}2dmso{\cdot}2H_2O$	$Tm(NO_3)_3{\cdot}5H_2O$	8.9	Pink prism
13	$[Yb_2(C_6O_4Br_2)_3(dmso)_4]{\cdot}2dmso{\cdot}2H_2O$	$Yb(NO_3)_3{\cdot}5H_2O$	9.0	Violet prism

Table S2. Crystal data and structure refinement parameters for compounds $[Ln_2(C_6O_4Cl_2)_3(dmso)_6]$ with Ln = La(**1**), Ce(**2**) and Pr(**3**).

Compound	$[La_2(C_6O_4Cl_2)_3(dmso)_6]$	$[Ce_2(C_6O_4Cl_2)_3(dmso)_6]$	$[Pr_2(C_6O_4Cl_2)_3(dmso)_6]$
Ref	**1**	**2**	**3**
CCDC	2142143	2142144	2142145
Empirical formula	$C_{15}H_6Cl_3LaO_9S_3$	$C_{15}H_6CeCl_3O_9S_3$	$C_{15}H_6Cl_3O_9PrS_3$
Formula weight	671.64	672.85	673.64
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$
a (Å)	9.5575(2)	9.5998(2)	9.6249(2)
b (Å)	16.0812(3)	16.0722(2)	16.0534(4)
c (Å)	15.4324(3)	15.4088(3)	15.3742(3)
α (°)	90	**9**0	90
β (°)	90.576(2)	91.128(2)	91.502(2)
γ (°)	90	90	90
Volume ($Å^3$)	2371.78(8)	2376.96(7)	2374.69(9)
Z	4	4	4
Density (calculated) (g/cm^3)	1.881	1.880	1.884
Absorption coefficient (mm^{-1})	2.445	2.558	2.695
F(000)	1296.0	1300.0	1304.0
Crystal size (mm^3)	0.07 × 0.05 × 0.025	0.080 x 0.060 x 0.020	0.07 × 0.035 × 0.02
2θ range for data (°)	5.598 to 50.07	6.612 to 50.076	5.55 to 50.098
Reflections collected	9756	18414	9387
Data	4163	4197	4190
Restraints	78	14	36
Parameters	322	307	312
Goodness-of-fit on F^2	1.039	1.041	1.046
R_1 [I > 2s(I)]	0.0412	0.0394	0.0409
wR_2 (all data)	0.1001	0.0989	0.0996
Largest diff. peak/hole / e $Å^{-3}$	1.93/-0.78	1.572/-0.806	1.24/-1.08

Table S3. Crystal data and structure refinement parameters for compounds $[Ln_2(C_6O_4Cl_2)_3(dmso)_6]$ with Ln = Nd(**4**), Sm(**5**) and Eu(**6**).

Compound	$[Nd_2(C_6O_4Cl_2)_3(dmso)_6]$	$[Sm_2(C_6O_4Cl_2)_3(dmso)_6]$	$[Eu_2(C_6O_4Cl_2)_3(dmso)_6]$
Ref	**4**	**5**	**6**
CCDC	2142146	2142147	2142148
Empirical formula	$C_{15}H_{14}Cl_3NdO_9S_3$	$C_{15}H_{11}Cl_3O_9S_3Sm$	$C_{15}H_{13}Cl_3EuO_9S_3$
Formula weight	685.03	688.12	691.74
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$
a (Å)	9.63840(10)	9.6354(4)	9.6543(2)
b (Å)	16.0436(3)	15.9723(9)	15.9914(4)
c (Å)	15.3468(2)	15.2510(5)	15.2331(3)
α (°)	90	90	90
β (°)	91.915(2)	92.357(4)	92.613(2)
γ (°)	90	90	90
Volume (Å^3)	2371.82(6)	2345.14(18)	2349.33(9)
Z	4	4	4
Density (calculated) (g/cm^3)	1.918	1.949	1.956
Absorption coefficient (mm^{-1})	2.834	3.156	3.321
F(000)	1340.0	1336.0	1348.0
Crystal size (mm^3)	0.1 × 0.06 × 0.05	0.06 × 0.03 × 0.015	0.1 × 0.08 × 0.05
2θ range for data (°)	6.61 to 50.07	5.7 to 50.122	5.704 to 50.07
Reflections collected	8946	8755	8704
Data	4182	4103	4142
Restraints	42	51	95
Parameters	305	309	310
Goodness-of-fit on F^2	1.057	1.039	1.031
R_1 [I > 2s(I)]	0.0386	0.0537	0.0369
wR_2 (all data)	0.0911	0.1188	0.0847
Largest diff. peak/hole / e Å^{-3}	1.72/-0.65	1.52/-0.95	1.72/-0.85

Table S4. Crystal data and structure refinement parameters for compounds $[Ln_2(C_6O_4Cl_2)_3(dmso)_6]$ with Ln = Gd(**7**) and Tb(**8**).

Compound	$[Gd_2(C_6O_4Cl_2)_3(dmso)_6]$	$[Tb_2(C_6O_4Cl_2)_3(dmso)_6]$
Ref	**7**	**8**
CCDC	2142149	2142150
Empirical formula	$C_{15}Cl_3GdO_9S_3$	$C_{15}H_9Cl_3TbO_9S_3$
Formula weight	683.93	694.67
Crystal system	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$
a (Å)	9.6382(3)	9.65790(10)
b (Å)	15.9788(6)	15.9514(2)
c (Å)	15.1628(5)	15.1556(2)
α (°)	90	90
β (°)	92.846(3)	92.8650
γ (°)	90	90
Volume (Å^3)	2332.30(14)	2331.91(5)
Z	4	4
Density (calculated) (g/cm^3)	1.948	1.979
Absorption coefficient (mm^{-1})	3.498	3.688
F(000)	1300.0	1340.0
Crystal size (mm^3)	0.060 × 0.035 × 0.020	0.050 x 0.040 x 0.020
2θ range for data (°)	5.726 to 50.142	6.628 to 50.064
Reflections collected	9385	18382
Data	4111	4105
Restraints	54	12
Parameters	300	299
Goodness-of-fit on F^2	1.052	1.051
R_1 [I > 2s(I)]	0.0460	0.0309
wR_2 (all data)	0.1167	0.0746
Largest diff. peak/hole / e Å^{-3}	1.46/-0.87	1.539/-0.679

Table S5. Crystal data and structure refinement parameters for compounds $[Ln_2(C_6O_4Cl_2)_3(dmso)_4]\cdot 2dmso\cdot 2H_2O$ with Ln = Dy(**9**), Ho (**10**) and Er(**11**).

Compound	$[Dy_2(C_6O_4Cl_2)_3(dmso)_4]$ ·2 dmso·$2H_2O$	$[Ho_2(C_6O_4Cl_2)_3(dmso)_4]$ ·2 dmso·$2H_2O$	$[Er_2(C_6O_4Cl_2)_3(dmso)_4]$ ·2 dmso·$2H_2O$
Ref	**9***	**10**	**11***
CCDC	2054148	2142151	1586537
Empirical formula	$C_{15}H_{14}Cl_3DyO_{10}S_3$	$C_{15}H_{12}Cl_3HoO_{10}S_3$	$C_{15}H_{12}Cl_3ErO_{10}S_3$
Formula weight	719.29	719.71	722.04
Crystal system	triclinic	triclinic	triclinic
Space group	*P*-1	*P*-1	*P*-1
a (Å)	9.7197(6)	9.7331(4)	9.7277(5)
b (Å)	10.6161(7)	10.5508(5)	10.5298(5)
c (Å)	12.7564(7)	12.7644(4)	12.7286(6)
α (°)	78.913(5)	78.898(3)	78.483(4)
β (°)	73.305(5)	73.243(3)	73.193(4)
γ (°)	73.305(5)	84.240(4)	83.957(4)
Volume ($Å^3$)	1235.46(14)	1230.25(9)	1221.41(11)
Z	2	2	2
Density (calculated) (g/cm^3)	1.934	1.943	1.963
Absorption coefficient (mm^{-1})	3.648	3.842	4.067
F(000)	698.0	696.0	698.0
Crystal size (mm^3)	0.140 x 0.120 x 0.020	0.06 × 0.05 × 0.02	0.130 x 0.110 x 0.020
2θ range for data (°)	6.652 to 50.066	6.648 to 50.082	6.796 to 50.062
Reflections collected	8103	15449	8041
Data	4372	4362	4321
Restraints	6	120	30
Parameters	301	316	303
Goodness-of-fit on F^2	1.116	1.064	1.048
R_1 [I > 2s(I)]	0.0520	0.0405	0.0402
wR_2 (all data)	0.1248	0.1027	0.0940
Largest diff. peak/hole / e $Å^{-3}$	1.652/-1.549	1.39/-1.83	1.684/ -1.230

* Data published, see references [1, 2].

Table S6. Crystal data and structure refinement parameters for compounds $[Ln_2(C_6O_4Cl_2)_3(dmso)_4]\cdot 2dmso\cdot 2H_2O$ with Ln = Tm(**12**) and Yb(**13**).

Compound	$[Tm_2(C_6O_4Cl_2)_3(dmso)_4]$ ·2 dmso·$2H_2O$	$[Yb_2(C_6O_4Cl_2)_3(dmso)_4]$ ·2 dmso·$2H_2O$
Ref	**12**	**13**
CCDC	2142152	2142153
Empirical formula	$C_{15}H_{18}Cl_3O_{10}S_3Tm$	$C_{15}H_{18}Cl_3O_{10}S_3Yb$
Formula weight	729.75	732.85
Crystal system	triclinic	triclinic
Space group	*P*-1	*P*-1
a (Å)	9.7002(8)	9.7123(4)
b (Å)	10.5192(10)	10.4665(5)
c (Å)	12.6581(12)	12.7036(7)
α (°)	78.450(8)	78.599(4)
β (°)	73.099(8)	73.267(4)
γ (°)	83.863(7)	84.330(4)
Volume ($Å^3$)	1209.2(2)	1211.08(11)
Z	2	2
Density (calculated) (g/cm^3)	2.004	2.010
Absorption coefficient (mm^{-1})	4.307	4.498
F(000)	712.0	712.0
Crystal size (mm^3)	0.09 × 0.06 × 0.02	0.130 x 0.060 x 0.030
2θ range for data (°)	6.708 to 50.088	6.690 to 50.092
Reflections collected	8462	7722
Data	4264	4278
Restraints	50	0
Parameters	289	293
Goodness-of-fit on F^2	1.046	1.187
R_1 [I > 2s(I)]	0.0696	0.0383
wR_2 (all data)	0.2012	0.0845
Largest diff. peak/hole / e $Å^{-3}$	4.37/-2.40	2.391/-1.616

Table S7. Continuous SHAPE measurement (CShM) values of the 13 possible coordination geometries for the Ln(III) ion with coordination number nine in compounds **1-8**. The minimum values are indicated in bold.

Geometry	Symmetry	1	2	3	4	5	6	7	8
EP-9	D9h	36.422	36.538	36.556	36.737	36.812	36.830	36.712	36.849
OPY-9	C8v	23.269	23.091	23.109	22.834	22.798	22.713	22.815	22.674
HBPY-9	D7h	18.832	18.845	18.851	18.783	19.004	18.973	19.116	19.152
JTC-9	C3v	16.088	16.104	16.088	16.035	16.143	16.201	16.208	16.240
JCCU-9	C4v	10.777	10.817	10.919	10.929	10.828	10.846	10.762	10.713
CCU-9	C4v	9.563	9.632	9.738	9.744	9.858	9.878	9.805	9.776
JCSAPR-9	C4v	1.724	1.575	1.496	1.405	1.287	1.272	1.223	1.186
CSAPR-9	**C4v**	**0.776**	**0.664**	**0.602**	**0.531**	**0.434**	**0.426**	**0.383**	**0.369**
JTCTPR-9	D3h	2.916	2.877	2.853	2.835	2.720	2.706	2.625	2.613
TCTPR-9	D3h	1.361	1.426	1.424	1.394	1.275	1.288	1.218	1.210
JTDIC-9	C3v	11.980	12.282	12.422	12.491	12.508	12.603	12.617	12.612
HH-9	C2v	10.726	10.832	10.879	11.000	11.299	11.250	11.512	11.459
MFF-9	Cs	0.852	0.799	0.772	0.749	0.732	0.706	0.726	0.705

EP-9 = Enneagon; OPY-9 = Octagonal pyramid; HBPY-9 = Heptagonal bipyramid; JTC-9 = Triangular cupola (J3) = trivacant cuboctahedron; JCCU-9 = Capped cube (Elongated square pyramid, J8); CCU-9 = Capped cube; JCSAPR-9 = Capped square antiprism (Gyroelongated square pyramid J10); **CSAPR-9 = Capped square antiprism**; JTCTPR-9 = Tricapped trigonal prism (J51); TCTPR-9 = Tricapped trigonal prism; JTDIC-9 = Tridiminished icosahedron (J63); HH-9 = Hula-hoop; MFF-9 = Muffin.

Table S8. Continuous SHAPE measurement (CShM) values of the 13 possible coordination geometries for the Ln(III) ion with coordination number eight in compounds **9-13**. The minimum values are indicated in bold.

Geometry	Symmetry	9	10	11	12	13
OP-8	D8h	30.366	30.377	30.399	30.229	30.471
HPY-8	C7v	23.156	23.291	23.426	23.348	23.431
HBPY-8	D6h	15.039	15.112	15.034	15.025	15.027
CU-8	Oh	11.281	11.356	11.281	11.224	11.253
SAPR-8	D4d	1.603	1.586	1.602	1.556	1.559
TDD-8	**D2d**	**1.208**	**1.149**	**1.126**	**1.142**	**1.062**
JGBF-8	D2d	13.161	13.081	12.920	12.995	12.947
JETBPY-8	D3h	28.647	28.825	28.806	28.831	28.914
JBTPR-8	C2v	2.267	2.271	2.246	2.324	2.242
BTPR-8	C2v	1.806	1.817	1.814	1.865	1.790
JSD-8	D2d	3.079	2.996	2.929	3.012	2.898
TT-8	Td	12.011	12.092	12.031	11.926	12.002
ETBPY-8	D3h	23.622	23.753	24.080	24.073	24.345

OP-8 = Octagon; HPY-8 = Heptagonal pyramid; HBPY-8 = Hexagonal bipyramid; CU-8 = Cube; SAPR-8 = Square antiprism; **TDD-8 = Triangular dodecahedron**; JGBF-8 = Johnson-Gyrobifastigium (J26); JETBPY-8 = Johnson-Elongated triangular bipyramid (J14); JBTP-8 = Johnson-Biaugmentedtrigonal prism (J50); BTPR-8 = Biaugmentedtrigonal prism; JSD-8 = Snub disphenoid (J84); TT-8 = Triakis tetrahedron.

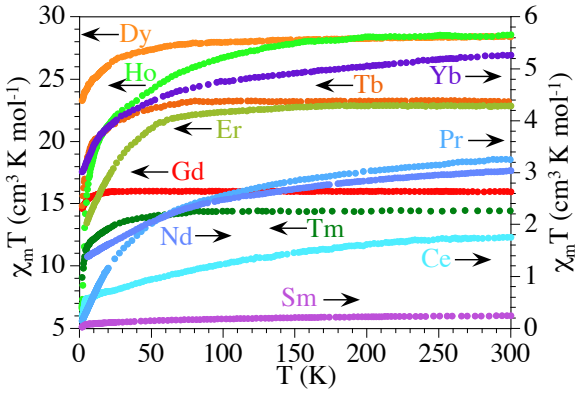

Figure S1. Thermal variation of the $\chi_m T$ product per formula unit (two Ln(III) ions) for compounds **1-13**.

Table S9. Experimental and calculated room temperature $\chi_m T$ values for compounds **1-13**.

#	Ln^{3+}	Ground State	$\chi_m T_{calc.}$ (cm^3 K mol^{-1})	$\chi_m T_{exp}$ (cm^3 K mol^{-1})
1	La^{3+}	$^1F_0$	0	-
2	Ce^{3+}	$^5F_{5/2}$	1.60	1.8
3	Pr^{3+}	$^3H_4$	3.20	3.2
4	Nd^{3+}	$^4I_{9/2}$	3.28	3.1
5	Sm^{3+}	$^6H_{5/2}$	0.18	0.2
6	Eu^{3+}	$^7F_0$	0	-
7	Gd^{3+}	$^8S_{7/2}$	15.76	15.9
8	Tb^{3+}	$^7F_6$	23.64	23.3
9	Dy^{3+}	$^6H_{15/2}$	28.40	28.0
10	Ho^{3+}	$^5I_8$	28.10	28.0
11	Er^{3+}	$^4I_{15/2}$	22.96	22.8
12	Tm^{3+}	$^3H_6$	14.30	14.4
13	Yb^{3+}	$^2F_{7/2}$	5.14	5.3

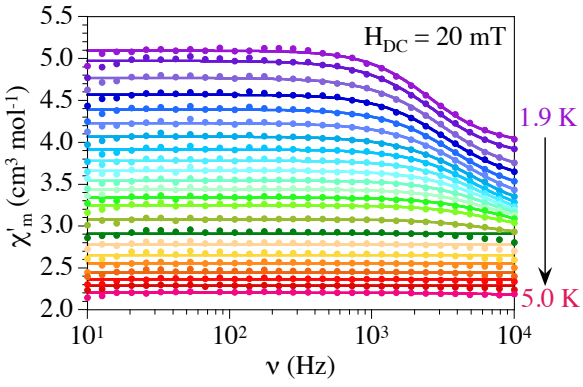

Figure S2. Frequency dependence of χ'_m for compound **11** with H_{dc} = 20 mT in the temperature range 1.9-5.0 K. Solid lines are the best fit to the Debye model.

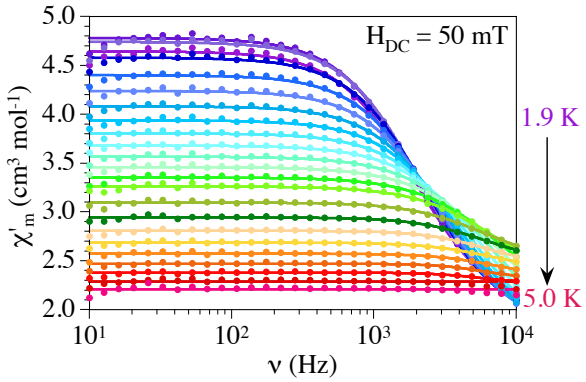

Figure S3. Frequency dependence of χ'_m for compound **11** with H_{dc} = 50 mT in the temperature range 1.9-5.0 K. Solid lines are the best fit to the Debye model.

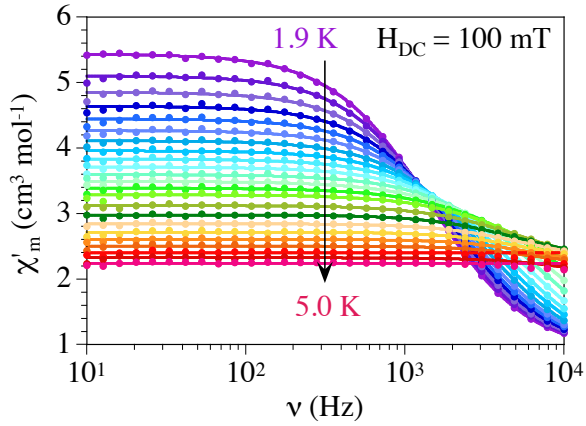

Figure S4. Frequency dependence of χ'_m for compound **11** with H_{dc} = 100 mT in the temperature range 1.9-5.0 K. Solid lines are the best fit to the Debye model.

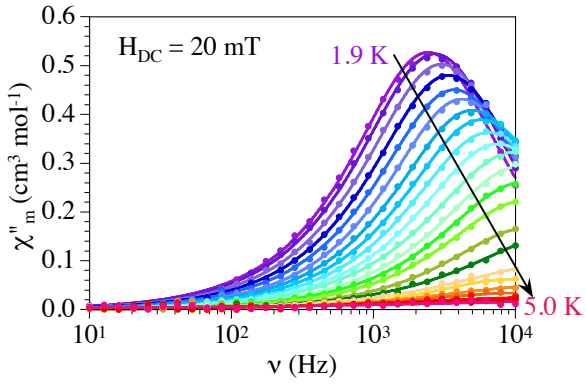

Figure S5. Frequency dependence of χ''_m for compound **11** with H_{dc} = 20 mT in the temperature range 1.9-5.0 K. Solid lines are the best fit to the Debye model.

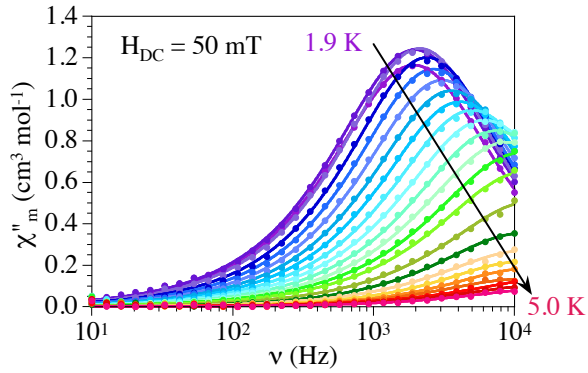

Figure S6. Frequency dependence of χ''_m for compound **11** with H_{dc} = 50 mT in the temperature range 1.9-5.0 K. Solid lines are the best fit to the Debye model.

Table S10. Ln-O bond distances (in Å) in compounds **1**-**8**.

Distance	1 (La)	2 (Ce)	3 (Pr)	4 (Nd)	5 (Sm)	6 (Eu)	7 (Gd)	8 (Tb)
Ln-O2	2.569(3)	2.543(4)	2.546(4)	2.523(4)	2.515(5)	2.515(4	2.456(4)	2.451(3)
Ln-O3	2.587(4)	2.558(4)	2.533(4)	2.524(4)	2.487(5)	2.476(4)	2.497(5)	2.459(3)
Ln-O5	2.602(3)	2.567(4)	2.550(4)	2.544(4)	2.498(5)	2.489(4)	2.458(4)	2.501(3)
Ln-O6	2.579(4)	2.569(4)	2.545(4)	2.520(3)	2.497(5)	2.478(4)	2.475(4)	2.446(3)
Ln-O12	2.539(4)	2.523(4)	2.511(4)	2.492(3)	2.478(6)	2.461(4)	2.451(4)	2.435(3)
Ln-O16	2.557(4)	2.539(4)	2.523(4)	2.506(4)	2.477(6)	2.473(4)	2.454(6)	2.452(3)
Ln-O1D	2.487(4)	2.467(4)	2.412(4)	2.441(4)	2.364(6)	2.388(4)	2.362(5)	2.380(3)
Ln-O11D	2.479(4)	2.460(4)	2.449(4)	2.429(4)	2.397(7)	2.363(4)	2.359(5)	2.358(4)
Ln-O21D	2.453(4)	2.426(4)	2.446(4)	2.394(4)	2.407(6)	2.405(4)	2.386(5)	2.345(3)
Ln-$O_{anilato}$[1]	2.572	2.550	2.535	2.518	2.489	2.482	2.465	2.457
Ln-O_{dmso}[2]	2.473	2.451	2.436	2.421	2.389	2.385	2.369	2.361

[1] Average Ln-O bond distance of the anilato oxygen atoms: O2, O3, O12, O13, O22 and O23 (O13, O22 and O23 correspond to O16, O6 and O5, respectively, in **2**, **4** and **8**).
[2] Average Ln-O bond distance of the dmso oxygen atoms (O1D, O11D and O21D).

Table S11. Ln-O bond distances (in Å) in compounds **9**-**13**.

Compound	9 (Dy)	10 (Ho)	11 (Er)	12 (Tm)	13 (Yb)
Ln-O2	2.374(5)	2.357(5)	2.364(4)	2.351(8)	2.333(4)
Ln-O3*	2.382(6)	2.375(5)	2.349(4)	2.366(8)	2.357(4)
Ln-O12	2.380(6)	2.366(4)	2.355(4)	2.343(9)	2.324(4)
Ln-O13*	2.398(6)	2.389(4)	2.377(4)	2.348(9)	2.348(4)
Ln-O22	2.375(5)	2.354(5)	2.342(4)	2.342(8)	2.329(4)
Ln-O23*	2.393(6)	2.376(5)	2.371(4)	2.348(9)	2.348(4)
Ln-O1D	2.319(6)	2.305(4)	2.298(5)	2.278(7)	2.248(4)
Ln-O11D	2.293(6)	2.275(5)	2.260(5)	2.280(8)	2.283(4)
Ln-$O_{anilato}$[1]	2.384	2.370	2.360	2.350	2.340
Ln-O_{dmso}[2]	2.306	2.290	2.279	2.279	2.266

[1] Average Ln-O bond distance of the anilato oxygen atoms: O2, O3, O12, O13, O22 and O23 (O3, O13 and O23 correspond to O6, O16 and O26, respectively, in **11**).
[2] Average Ln-O bond distance of the dmso oxygen atoms (O1D and O11D).

Table S12. Ln-Ln distances (Å) along the three diagonals and Ln-Ln-Ln angles (º) in the hexagonal rings in **1**-**13**.

#	Ln (III)	Phase	d_1 (Å)	d_2 (Å)	d_3 (Å)	α_1 (º)	α_2 (º)	α_3 (º)	$\Sigma\lvert d_1 - d_{av}\rvert$ (Å)	$\Sigma\lvert 120 - \alpha_i\rvert$ (º)
1	**La**	**I**	20.84	19.51	10.80	90.72	100.16	165.91	12.50	95.03
2	**Ce**	**I**	20.74	19.43	10.73	90.69	100.08	166.15	12.47	95.38
3	**Pr**	**I**	20.65	19.36	10.71	90.81	100.07	166.04	12.39	95.15
4	**Nd**	**I**	20.57	19.29	10.66	90.80	100.02	166.18	12.36	95.35
5	**Sm**	**I**	20.38	19.15	10.63	91.13	99.99	165.79	12.18	94.67
6	**Eu**	**I**	20.33	19.13	10.61	91.20	99.88	165.88	12.16	94.80
7	**Gd**	**I**	20.20	19.05	10.62	91.52	99.86	165.48	12.01	94.10
8	**Tb**	**I**	20.18	19.05	10.58	91.51	99.74	165.68	12.05	94.43
9	**Dy**	**II**	20.25	16.61	14.12	94.87	122.36	141.78	6.51	49.26
10	**Ho**	**II**	20.12	16.60	14.09	95.37	121.94	141.66	6.37	48.23
11	**Er**	**II**	20.08	16.49	14.14	95.35	122.61	141.00	6.35	48.26
12	**Tm**	**II**	20.05	16.37	14.12	95.09	123.17	140.78	6.41	48.86
13	**Yb**	**II**	19.95	16.47	14.07	95.66	122.23	141.15	6.24	47.72

References

1. Benmansour, S.; Pérez-Herráez, I.; Cerezo-Navarrete, C.; López-Martínez, G.; Martínez Hernandez, C.; Gómez-García, C. J. Solvent-Modulation of the Structure and Dimensionality in Lanthanoid-Anilato Coordination Polymers. *Dalton Trans.* **2018**, *47*, 6729-6741.
2. Benmansour, S.; Hernández-Paredes, A.; Bayona-Andrés, M.; Gómez-García, C. J. Slow Relaxation of the Magnetization in Anilato-Based Dy(III) 2D Lattices. *Molecules* **2021**, *26*.