Dimensional and Coordination Number Reductions in a Large Family of Lanthanide Tellurite Sulfates

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Supporting Information

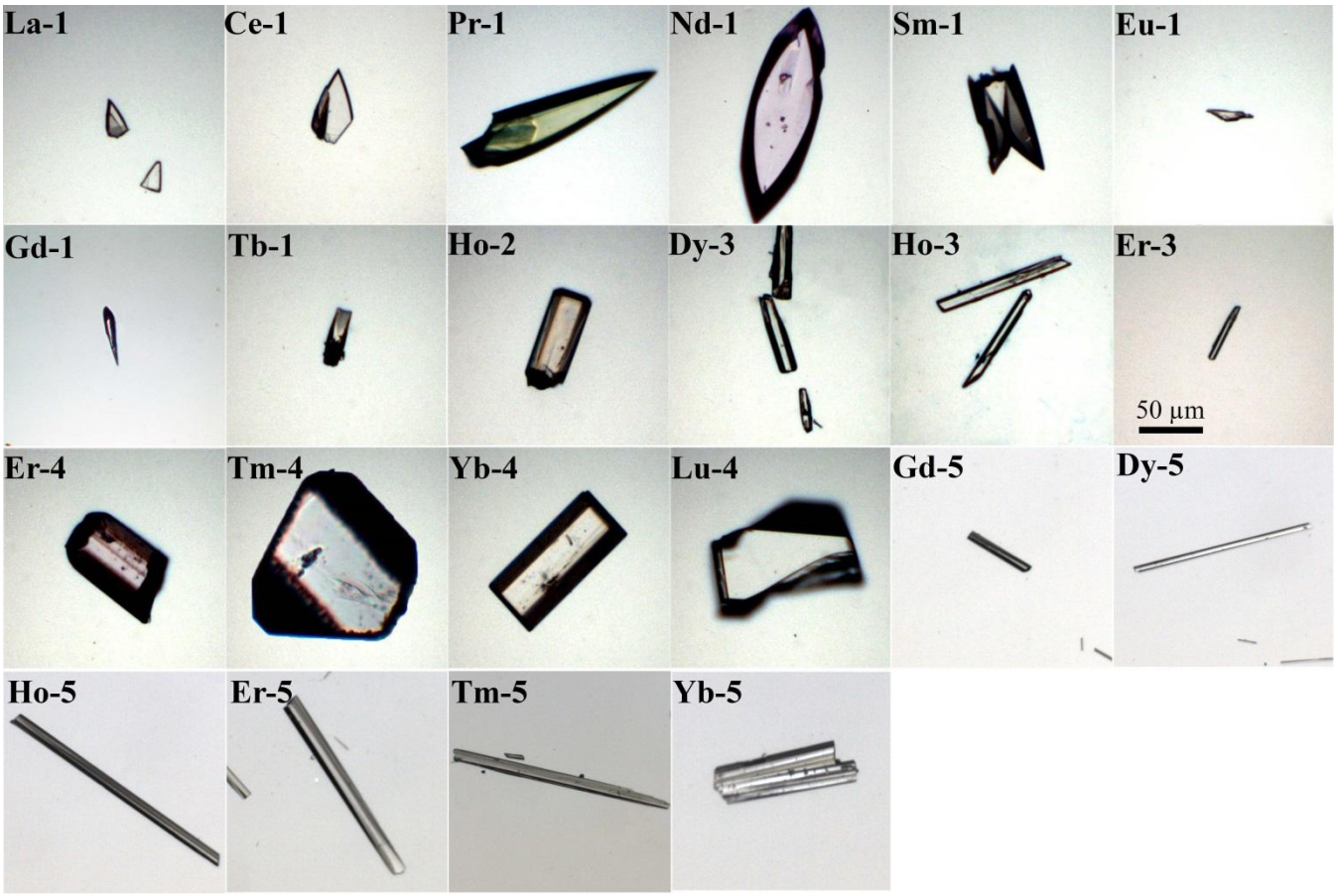

Figure S1. Crystal images of lanthanide tellurite sulfates

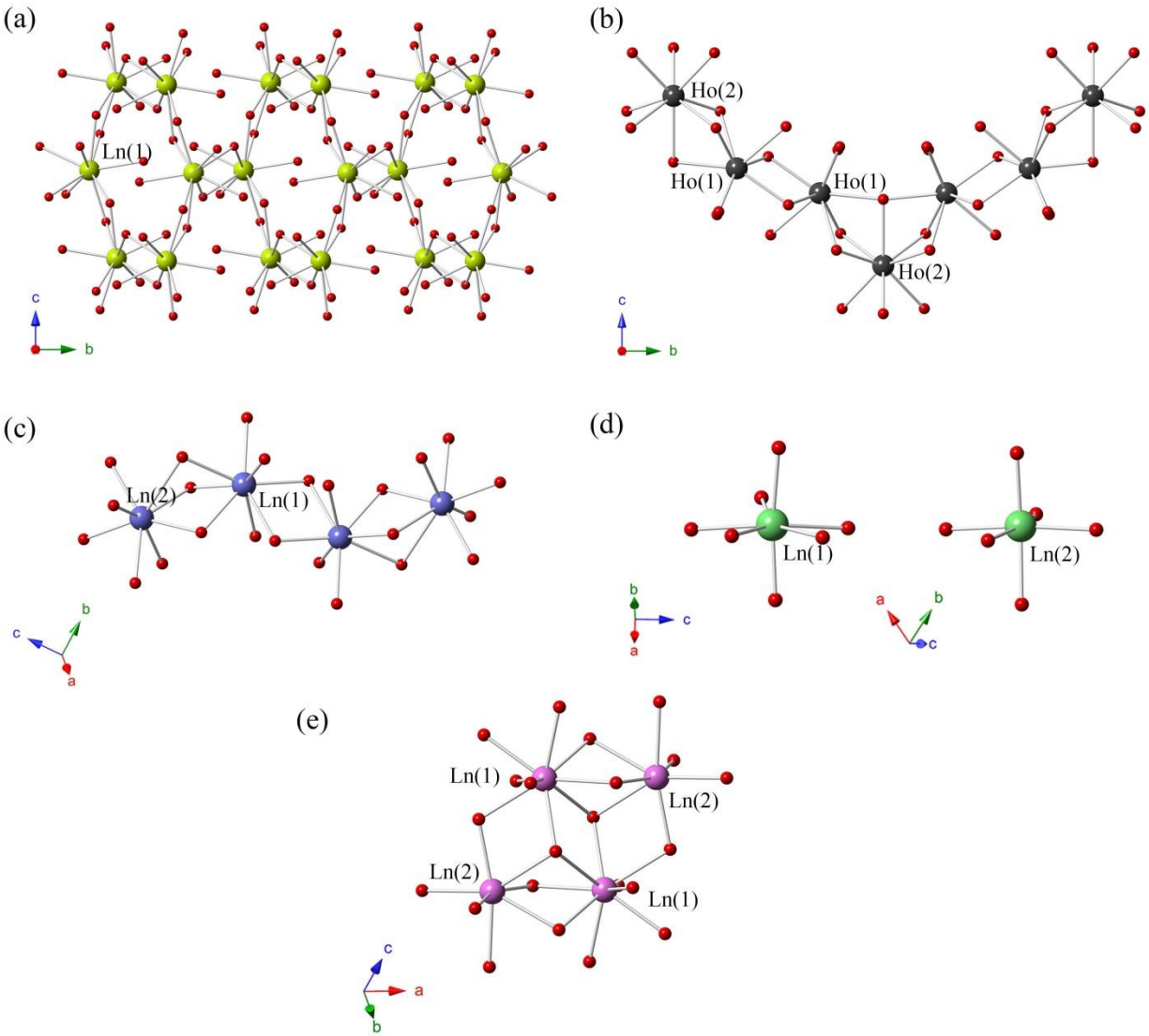

Figure S2. Ball-and-stick representations of Ln polyhedra bonding geometries in **LnTeSO-1**, **LnTeSO-2**, **LnTeSO-3**, **LnTeSO-4**, and **LnTeSO-5**.

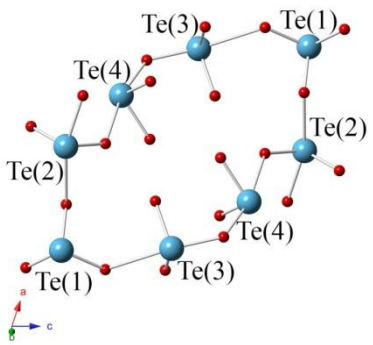

Figure S3. Ball-and-stick image of the $Te_4O_{10}^{4-}$ polymer of **LnTeSO-5**.

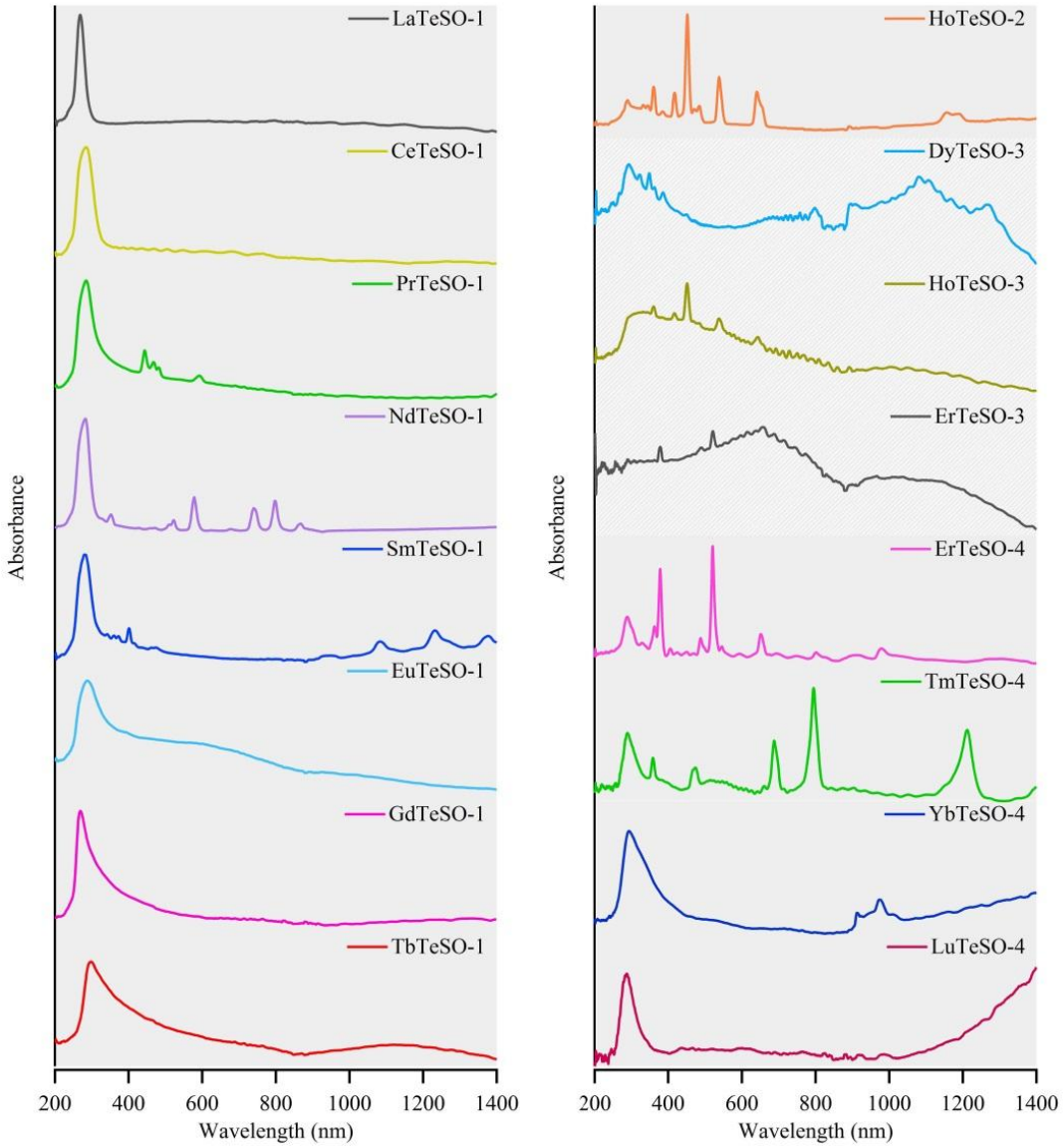

Figure S4. Normalized UV−vis−NIR spectra of **LnTeSO-1**, **LnTeSO-2**, **LnTeSO-3**, and **LnTeSO-4**.

Table S1. Crystallographic Data for **LnTeSO-1**, **LnTeSO-2**, **LnTeSO-3**, **LnTeSO-4**, and **LnTeSO-5**.

Compound	La-1	Ce-1	Pr-1	Nd-1	Sm-1	Eu-1	Gd-1	Tb-1	Ho-2	Dy-3	Ho-3
Formula Mass	805.14	807.56	809.14	815.80	828.02	831.24	841.82	845.16	1073.11	728.72	733.58
Color	Colorless	Colorless	Green	Purple	Colorless	Colorless	Colorless	Colorless	Pink	Colorless	Pink
Habit	Sphenoid	Sphenoid	Sphenoid	Sphenoid	Sphenoid	Sphenoid	Sphenoid	Sphenoid	Tablet	Columnar	Columnar
Space Group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/m$	$P\bar{1}$	$P\bar{1}$
a (Å)	9.6300(19)	9.597(3)	9.575(5)	9.5838(5)	9.5721(7)	9.5815(18)	9.5855(9)	9.6120(5)	5.4548(4)	5.3523(9)	5.3462(7)
b (Å)	6.9840(14)	6.9391(18)	6.934(4)	6.8832(4)	6.8269(5)	6.8132(13)	6.7774(6)	6.7491(4)	15.3443(10)	8.2283(14)	8.2012(11)
c (Å)	8.2879(16)	8.248(2)	8.212(4)	8.1783(5)	8.0964(6)	8.0687(15)	7.9941(8)	7.9564(4)	8.0291(5)	12.341(2)	12.3034(17)
α (deg)	90	90	90	90	90	90	90	90	90	90.774(2)	90.7190(10)
β (deg)	106.317(2)	106.452(3)	106.640(5)	106.758(1)	106.984(1)	107.113(2)	107.688(2)	107.934(1)	99.492(1)	101.525(2)	101.505(2)
γ (deg)	90	90	90	90	90	90	90	90	90	103.895(3)	103.809(2)
V ($Å^3$)	534.96(18)	526.8(2)	522.4(5)	516.59(5)	506.01(6)	503.41(16)	494.78(8)	491.07(5)	662.84(8)	515.87(15)	512.30(12)
Z	2	2	2	2	2	2	2	2	2	2	2
T (K)	100	100	100	100	100	100	100	100	298	298	100
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Maximum 2θ (deg.)	27.510	27.690	27.590	27.490	27.530	27.500	27.520	27.500	28.520	27.540	27.500
ρ_{calcd} (g cm^{-3})	4.998	5.091	5.144	5.245	5.435	5.484	5.651	5.716	5.362	4.666	4.730
μ (Mo Kα) (cm^{-1})	13.686	14.429	15.163	15.953	17.631	18.516	19.567	20.611	22.450	17.619	18.601
R(F) for $F_o^2 > 2\sigma(F_o^2)^a$	0.0391	0.0424	0.0390	0.0376	0.0376	0.0512	0.0351	0.0456	0.0239	0.0267	0.0297
$R_w(F_o^2)^b$	0.0923	0.1237	0.0951	0.0969	0.0892	0.1394	0.0794	0.0951	0.0604	0.0660	0.0707

Compound	Er-3	Er-4	Tm-4	Yb-4	Lu-4	Gd-5	Dy-5	Ho-5	Er-5	Tm-5	Yb-5
Formula Mass	734.26	861.84	865.18	873.40	877.26	1080.96	1091.46	1096.32	1100.98	1104.32	1112.54
Color	Purple	Purple	Colorless	Colorless	Colorless	Colorless	Colorless	Colorless	Pink	Colorless	Pink
Habit	Columnar	Tablet	Tablet	Tablet	Tablet	Acicular	Acicular	Acicular	Acicular	Acicular	Acicular

Space Group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a (Å)	5.332(3)	5.3243(11)	5.2912(4)	5.3243(6)	5.289(3)	6.8584(8)	6.8248(5)	6.8115(3)	6.7819(17)	6.7692(6)	6.7434(5)
b (Å)	8.155(5)	8.2705(17)	8.2255(6)	8.2148(9)	8.193(5)	9.3454(11)	9.3245(6)	9.3149(5)	9.259(2)	9.2956(8)	9.2433(7)
c (Å)	12.264(8)	13.220(3)	13.1589(9)	13.2547(14)	13.144(8)	9.9200(12)	9.8785(7)	9.8627(5)	9.838(3)	9.8114(8)	9.7798(8)
α (deg)	90.522(9)	89.007(2)	89.005(2)	88.4150(10)	89.033(6)	89.744(2)	89.8550(10)	89.8870(10)	89.901(5)	89.932(2)	89.937(2)
β (deg)	101.425(9)	87.485(2)	87.6410(10)	87.2720(10)	87.531(6)	72.406(2)	72.4430(10)	72.4970(10)	72.535(4)	72.498(1)	72.493(2)
γ (deg)	103.814(9)	72.328(2)	72.3330(10)	72.2410(10)	72.455(6)	87.498(2)	87.9530(10)	88.1390(10)	88.596(5)	88.385(2)	88.825(2)
V ($Å^3$)	506.7(5)	554.1(2)	545.23(7)	551.43(10)	542.6(6)	605.47(12)	598.96(7)	596.47(5)	589.1(3)	588.54(9)	581.22(8)
Z	2	2	2	2	2	2	2	2	2	2	2
T (K)	298	100	100	298	100	100	298	100	100	100	100
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Maximum 2θ (deg.)	27.490	27.480	27.530	27.590	27.620	27.570	27.600	27.580	27.660	27.430	27.530
ρ_{calcd} (g cm^{-3})	4.813	5.166	5.270	5.260	5.370	5.929	6.052	6.104	6.207	6.232	6.357
μ (Mo Kα) (cm^{-1})	27.490	20.648	21.865	22.489	23.814	20.555	22.181	23.011	24.114	24.952	26.092
R(F) for $F_o^2 > 2\sigma(F_o^2)$[a]	0.0771	0.0337	0.0200	0.0186	0.0252	0.0239	0.0178	0.0163	0.0194	0.0336	0.0230
R_w (F_o^2)[b]	0.2041	0.1086	0.0470	0.0461	0.0606	0.0525	0.0401	0.0411	0.0485	0.0736	0.0445

Table S2. Selected Bond Distances (Å) for lanthanide tellurite sulfates.

	La-1	Ce-1	Pr-1	Nd-1	Sm-1	Eu-1	Gd-1	Tb-1
Ln(1)-O(2)	2.470(13)	2.441(16)	2.434(14)	2.413(12)	2.388(15)	2.367(9)	2.365(8)	2.342(10)
Ln(1)-O(3)#1	2.482(7)	2.463(8)	2.448(7)	2.435(7)	2.406(7)	2.387(17)	2.374(15)	2.384(10)
Ln(1)-O(5)	2.497(7)	2.465(8)	2.462(7)	2.436(7)	2.406(7)	2.392(9)	2.382(7)	2.387(16)
Ln(1)-O(3)	2.526(7)	2.511(8)	2.495(7)	2.479(6)	2.444(7)	2.431(9)	2.401(8)	2.378(9)
Ln(1)-O(6)	2.531(7)	2.513(7)	2.498(6)	2.485(7)	2.446(7)	2.441(9)	2.426(7)	2.422(9)
Ln(1)-O(4)	2.570(6)	2.535(7)	2.525(6)	2.515(6)	2.474(7)	2.448(8)	2.436(7)	2.413(9)
Ln(1)-O(7)#2	2.577(6)	2.563(7)	2.542(6)	2.535(6)	2.514(7)	2.504(10)	2.485(7)	2.491(9)
Ln(1)-O(4)#1	2.615(6)	2.589(8)	2.585(6)	2.576(6)	2.553(7)	2.542(9)	2.520(7)	2.490(9)
Ln(1)-O(7)	2.702(6)	2.703(8)	2.683(6)	2.672(7)	2.670(7)	2.701(11)	2.658(7)	2.690(10)
Te(1A)-O(3)	1.845(8)	1.832(10)	1.840(8)	1.832(8)	1.861(8)	1.881(12)	1.825(8)	1.821(10)
Te(1A)-O(2)#3	1.931(16)	1.935(18)	1.930(16)	1.96(2)	2.017(17)	1.95(2)	2.12(2)	2.23(2)
Te(1A)-O(1)#1	2.093(17)	2.10(2)	2.104(16)	2.138(17)	2.19(2)	2.15(3)	2.16(2)	2.28(3)
Te(1A)-O(1)	2.290(18)	2.25(2)	2.24(2)	2.22(2)	2.25(2)	2.17(3)	2.19(2)	2.15(2)
Te(1A)-O(2)	2.366(15)	2.352(18)	2.364(16)	2.341(17)	2.342(19)	2.341(19)	2.355(17)	2.327(18)
Te(1B)-O(3)	1.850(8)	1.846(9)	1.850(8)	1.841(8)	2.31(3)	1.883(12)	1.893(8)	2.37(3)
Te(1B)-O(2)	2.130(15)	2.083(17)	2.070(15)	2.024(15)	1.815(9)	1.966(19)	1.950(16)	2.51(3)
Te(1B)-O(1)	2.154(17)	2.19(2)	2.199(18)	2.21(2)	1.932(19)	2.17(3)	2.09(3)	1.908(10)
Te(1B)-O(1)#1	2.314(17)	2.23(2)	2.225(17)	2.226(18)	2.16(3)	2.24(3)	2.22(2)	1.946(17)
Te(1B)-O(2)#3	2.318(16)	2.308(18)	2.317(17)	2.35(2)	2.21(2)	2.28(4)	2.25(2)	1.99(3)
Te(1B)-O(1)#4	2.46(2)	2.48(3)	2.46(3)	2.38(3)	2.433(17)	2.37(2)	2.27(2)	2.24(2)
S(1)-O(5)#5	1.449(7)	1.455(8)	1.455(6)	1.452(7)	1.446(7)	1.452(9)	1.454(7)	1.445(9)
S(1)-O(6)#6	1.466(7)	1.456(8)	1.469(6)	1.460(6)	1.466(7)	1.449(9)	1.455(7)	1.458(9)
S(1)-O(7)	1.483(6)	1.488(8)	1.490(6)	1.483(6)	1.485(6)	1.495(9)	1.494(7)	1.494(9)
S(1)-O(4)#1	1.487(6)	1.497(7)	1.497(6)	1.488(6)	1.490(6)	1.501(11)	1.496(7)	1.497(9)

	Ho-2		Dy-3	Ho-3	Er-3		Er-4	Tm-4	Yb-4	Lu-4
Ho(1)-O(2)#1	2.313(5)	Ln(1)-O(2)#1	2.283(5)	2.282(5)	2.462(16)	Ln(1)-O(3)#1	2.136(8)	2.103(3)	2.098(3)	2.100(5)
Ho(1)-O(6)	2.329(5)	Ln(1)-O(1)#2	2.313(4)	2.308(6)	2.293(17)	Ln(1)-O(6)	2.268(7)	2.240(4)	2.215(3)	2.217(5)
Ho(1)-O(9)	2.3301(11)	Ln(1)-O(6)	2.319(5)	2.306(6)	2.266(18)	Ln(1)-O(7)	2.298(8)	2.274(3)	2.284(3)	2.255(5)
Ho(1)-O(3)	2.349(5)	Ln(1)-O(3)	2.327(5)	2.321(5)	2.326(19)	Ln(1)-O(4)	2.299(8)	2.287(4)	2.285(3)	2.269(5)
Ho(1)-O(7)	2.350(5)	Ln(1)-O(5)	2.334(5)	2.320(6)	2.346(17)	Ln(1)-O(2)	2.309(7)	2.292(4)	2.290(3)	2.277(5)
Ho(1)-O(1)#2	2.417(5)	Ln(1)-O(4)	2.465(5)	2.459(6)	2.42(2)	Ln(1)-O(5)	2.340(7)	2.321(3)	2.322(3)	2.307(5)
Ho(1)-O(2)#2	2.419(5)	Ln(1)-O(9)	2.514(5)	2.499(6)	2.488(18)	Ln(1)-O(1)	2.444(7)	2.436(4)	2.429(3)	2.415(5)
Ho(1)-O(4)	2.439(5)	Ln(1)-O(2)#2	2.530(5)	2.500(5)	2.307(18)					
						Ln(2)-O(9)	2.154(7)	2.140(4)	2.129(3)	2.124(5)
Ho(2)-O(1)#4	2.284(5)	Ln(2)-O(1)	2.264(5)	2.253(5)	2.210(18)	Ln(2)-O(11)#2	2.209(8)	2.187(3)	2.176(3)	2.177(4)
Ho(2)-O(1)	2.284(5)	Ln(2)-O(11)	2.268(5)	2.256(6)	2.26(3)	Ln(2)-O(8)#3	2.223(7)	2.198(3)	2.205(3)	2.184(5)
Ho(2)-O(8)	2.331(7)	Ln(2)-O(12)	2.281(5)	2.265(6)	2.26(2)	Ln(2)-O(10)#4	2.253(7)	2.236(4)	2.226(3)	2.217(5)
Ho(2)-O(3)#5	2.359(5)	Ln(2)-O(10)	2.314(5)	2.304(6)	2.30(2)	Ln(2)-O(13)#2	2.258(7)	2.241(3)	2.228(3)	2.227(5)
Ho(2)-O(3)#6	2.359(5)	Ln(2)-O(3)#4	2.383(4)	2.381(5)	2.366(18)	Ln(2)-O(12)#5	2.304(7)	2.281(4)	2.276(3)	2.274(5)
Ho(2)-O(5)#7	2.409(5)	Ln(2)-O(7)#5	2.412(5)	2.396(6)	2.394(19)					
Ho(2)-O(5)#8	2.409(5)	Ln(2)-O(8)	2.446(5)	2.439(6)	2.431(18)	Te(1)-O(3)	1.791(8)	1.801 (3)	1.796 (3)	1.794 (4)
Ho(2)-O(9)#6	2.467(8)	Ln(2)-O(9)#4	2.741(5)	2.735(6)	2.751(19)	Te(1)-O(2)	1.911(7)	1.914 (3)	1.911 (3)	1.916 (5)
						Te(1)-O(2)#6	2.131(7)	2.133 (4)	2.130 (3)	2.131 (4)
Te(1)-O(3)	1.851(5)	Te(1)-O(3)	1.835(5)	1.825(5)	1.791(18)	Te(1)-O(1)	2.149(7)	2.143 (3)	2.148 (3)	2.145 (4)
Te(1)-O(1)	1.857(5)	Te(1)-O(1)	1.858(5)	1.854(5)	1.838(18)	Te(2)-O(8)	1.827(7)	1.835 (4)	1.836 (3)	1.841 (5)
Te(1)-O(2)	1.866(5)	Te(1)-O(2)	1.870(5)	1.869(6)	1.883(18)	Te(2)-O(9)	1.848(7)	1.854 (3)	1.854 (3)	1.849 (5)
						Te(2)-O(1)	1.931(7)	1.935 (4)	1.935 (3)	1.938 (4)
S(1)-O(6)#1	1.464(5)	S(1)-O(6)#4	1.461(5)	1.462(6)	1.460(19)					
S(1)-O(7)#3	1.464(5)	S(1)-O(7)	1.477(5)	1.473(6)	1.454(19)	S(1)-O(13)	1.465(7)	1.460 (4)	1.456 (3)	1.462 (5)
S(1)-O(5)	1.477(5)	S(1)-O(5)	1.478(5)	1.478(6)	1.478(18)	S(1)-O(4)	1.467(8)	1.462 (4)	1.457 (4)	1.463 (5)
S(1)-O(4)	1.493(5)	S(1)-O(4)#1	1.488(5)	1.488(6)	1.519(19)	S(1)-O (12)	1.474(8)	1.469 (4)	1.458 (3)	1.465 (4)
		S(2)-O(13)	1.430(6)	1.447(6)	1.45 (2)	S(1)-O (10)	1.478(8)	1.480 (4)	1.474 (3)	1.485 (5)
		S(2)-O(12)#6	1.464(6)	1.475(6)	1.46 (2)	S(2)-O(6)#1	1.451(8)	1.462 (4)	1.460 (3)	1.468 (5)
		S(2)-O(11)#7	1.475(5)	1.479(6)	1.46 (2)	S(2)-O(5)	1.479(8)	1.463 (4)	1.463 (4)	1.471 (5)
		S(2)-O(10)	1.488(5)	1.486(6)	1.46 (2)	S(2)-O(7)#7	1.477(8)	1.463 (3)	1.466 (4)	1.474 (5)

S2—O11	1.485(8)	1.477 (4)	1.473 (3)	1.482 (4)

	Gd-5	Dy-5	Ho-5	Er-5	Tm-5	Yb-5
Ln(1)-O(1)	2.380(5)	2.353(3)	2.346(3)	2.332(3)	2.289(9)	2.304(5)
Ln(1)-O(4)	2.492(4)	2.467(3)	2.456(3)	2.431(3)	2.329(9)	2.411(5)
Ln(1)-O(6)#2	2.470(4)	2.430(3)	2.418(3)	2.393(3)	2.331(9)	2.364(4)
Ln(1)-O(7)#1	2.345(4)	2.350(3)	2.345(3)	2.334(3)	2.316(8)	2.325(4)
Ln(1)-O(9)	2.824(4)	2.783(3)	2.764(3)	2.722(3)	2.379(9)	2.698(5)
Ln(1)-O(9)#1	2.384(4)	2.363(3)	2.353(3)	2.345(3)	2.432(9)	2.321(5)
Ln(1)-O(10)	2.427(5)	2.431(3)	2.435(3)	2.435(3)	2.444(10)	2.435(4)
Ln(1)-O(11)#3	2.458(4)	2.446(4)	2.445(3)	2.429(3)	2.437(9)	2.429(5)
Ln(1)-O(13)	2.340(5)	2.311(4)	2.302(3)	2.286(3)	2.765(9)	2.270(5)
Ln((2)-O(2)#2	2.446(4)	2.416(3)	2.409(3)	2.398(3)	2.137(10)	2.372(4)
Ln(2)-O(4)#1	2.477(4)	2.444(3)	2.434(3)	2.410(3)	2.251(9)	2.384(5)
Ln(2)-O(5)#4	2.198(5)	2.158(4)	2.148(3)	2.142(3)	2.275(9)	2.112(5)
Ln(2)-O(6)#2	2.365(4)	2.331(3)	2.321(3)	2.301(3)	2.308(9)	2.271(4)
Ln(2)-O(7)	2.319(4)	2.279(3)	2.269(3)	2.255(3)	2.396(9)	2.218(4)
Ln(2)-O(9)#1	2.484(4)	2.472(3)	2.460(3)	2.435(3)	2.405(9)	2.412(5)
Ln(2)-O(10)#2	2.314(5)	2.292(3)	2.286(3)	2.274(3)	2.428(9)	2.258(4)
Te(1)-O(1)	1.856 (4)	1.851 (3)	1.850 (3)	1.857 (3)	1.845 (9)	1.855 (5)
Te(1)-O(2)	1.859 (5)	1.861 (3)	1.864 (3)	1.868 (3)	1.860 (9)	1.874 (4)
Te(1)-O(3)	1.913 (5)	1.907 (3)	1.909 (3)	1.910 (3)	1.893 (10)	1.899 (5)
Te(2)-O(5)	1.813 (5)	1.823 (4)	1.824 (3)	1.820 (3)	1.816 (10)	1.828 (5)
Te(2)-O(4)	1.885 (4)	1.885 (3)	1.887 (3)	1.887 (3)	1.882 (9)	1.881 (4)
Te(2)-O(3)	2.037 (4)	2.026 (3)	2.026 (3)	2.025 (3)	2.023 (9)	2.031 (4)
Te(2)-O(2)#5	2.320 (4)	2.323 (3)	2.323 (3)	2.299 (3)	2.306 (9)	2.282 (5)
Te(3)-O(7)	1.865 (4)	1.860 (3)	1.861 (3)	1.865 (3)	1.850 (9)	1.868 (4)
Te(3)-O(6)	1.862 (4)	1.863 (3)	1.861 (3)	1.865 (3)	1.856 (8)	1.870 (4)
Te(3)-O(8)	1.925 (4)	1.926 (3)	1.922 (3)	1.931 (3)	1.905 (9)	1.924 (4)

Te(3)-O(1)#2	2.515 (5)	2.509 (4)	2.502 (3)	2.470 (3)	2.490 (9)	2.463 (5)
Te(4)-O(10)	1.863 (5)	1.867 (3)	1.864 (3)	1.864 (3)	1.860 (9)	1.869 (5)
Te(4)-O(9)	1.894 (4)	1.886 (3)	1.890 (3)	1.892 (3)	1.895 (8)	1.892 (5)
Te(4)-O(8)	1.956 (4)	1.940 (3)	1.947 (3)	1.939 (3)	1.957 (9)	1.939 (4)
Te(4)-O(4)	2.467 (4)	2.457 (3)	2.450 (3)	2.445 (3)	2.441 (8)	2.440 (4)
S(1)-O(12)	1.463 (5)	1.456 (4)	1.461 (3)	1.462 (3)	1.447 (11)	1.466 (5)
S(1)-O(13)	1.465 (5)	1.465 (4)	1.464 (3)	1.473 (4)	1.461 (11)	1.471 (5)
S(1)-O(11)	1.481 (5)	1.478 (4)	1.472 (3)	1.479 (3)	1.461 (10)	1.475 (5)
S(1)-O(14)	1.473 (5)	1.469 (4)	1.475 (3)	1.488 (4)	1.467 (10)	1.481 (5)

Table S3. The closest Ln^{3+}–Ln^{3+} distances for the compounds magnetism measurement.

Ln	Ln-Ln (Å)	Ln	Ln-Ln (Å)
Ce-1	4.298(1)	Ho-5	3.7256(3)
Pr-1	4.282(2)	Er-4	5.142(7)
Nd-1	4.263(1)	Er-5	3.6849(7)
Sm-1	4.220(1)	Tm-4	5.112(5)
Tb-1	4.142(1)	Tm-5	3.6915(9)
Gd-5	3.7889(5)	Yb-4	5.160(4)
Dy-5	3.7458(4)		