

SUPPLEMENTARY MATERIALS

Table S1. Fractional site coordinates (xyz), site multiplicities (Q), equivalent displacement parameters (U_{eq} , Å²) and site occupancy factor for for compounds [Cd₆Cl₂₄][Ce₁₂(TeO)₁₂] (**1**), [Mn₆Cl₂₄][Nd₁₂(TeO)₁₂] (**2**), [Mn₆Br₂₄][La₁₂(TeO)₁₂] (**3**), [Co₆Cl₂₄][Eu₁₂(TeO)₁₂] (**4**) and [Co₆Cl₂₄][Gd₁₂(TeO)₁₂] (**5**).

Cl		x	y	z	Q	$U_{eq/iso}^*$	s.o.f.
Ln1	1	0.5	0.5	1	2	0.0696(1)	Ce
	2	0	0	0	2	0.0828(1)	Nd
	3	0	0	0	2	0.0055(5)	La
	4	0	0	0	2	0.0073(6)	Eu
	5	0	0	0	2	0.0123(7)	Gd
Ln2	1	0.57	0.57	1	4	0.0101(1)	Ce
	2	-1/4	-1/4	0	4	0.0107(1)	Nd
	3	1/4	1/4	0	4	0.0073(5)	La
	4	1/4	1/4	0	4	0.0110(6)	Eu
	5	1/4	1/4	0	4	0.0168(7)	Gd
Ln3	1	0.7530(1)	0.5	1	8	0.0923(1)	Ce
	2	-0.2529(6)	0	0	8	0.0968(1)	Nd
	3	0.2515(1)	0	0	8	0.0072(5)	La
	4	0.2540(1)	0	0	8	0.0105(5)	Eu
	5	0.2536(2)	0	0	8	0.0160(6)	Gd
Ln4	1	0.6218(1)	0.1218(1)	0.2317(1)	8	0.0141(1)	Ce
	2	-0.3782(1)	-0.1218(1)	0.2403(1)	8	0.0124(1)	Nd
	3	0.3762(1)	0.1238(1)	0.2256(2)	8	0.0166(4)	La
	4	0.3783(1)	0.1217(1)	0.2347(2)	8	0.0150(3)	Eu
	5	0.3785(1)	0.1215(1)	0.2355(2)	8	0.0200(3)	Gd
Ln5	1	1	0.5	1	2	0.0142(2)	Ce
	2	0	-1/2	0	2	0.0136(2)	Nd
	3	1/2	0	0	2	0.0101(1)	La
	4	1/2	0	0	2	0.0224(9)	Eu
	5	1/2	0	0	2	0.0251(9)	Gd
Te1	1	0.6434(1)	0.3782(1)	0.8147(1)	16	0.0871(1)	Te
	2	-0.1428(1)	-0.1220(1)	0.1904(4)	16	0.0115(1)	Te
	3	0.1436(1)	0.1223(1)	0.1795(1)	16	0.0162(3)	Te
	4	0.1411(1)	0.1222(1)	0.1920(2)	16	0.0132(3)	Te
	5	0.1410(2)	0.1220(1)	0.1929(2)	16	0.0190(3)	Te
Te2	1	0.8853(1)	0.6147(1)	0.8399(3)	8	0.0103(1)	Te
	2	-0.3849(2)	0.1151(1)	0.1652(1)	8	0.0128(1)	Te
	3	0.6138(1)	0.1138(1)	0.1592(1)	8	0.0168(3)	Te
	4	0.6156(1)	0.1156(1)	0.1679(3)	8	0.0147(4)	Te
	5	0.6157(1)	0.1157(1)	0.1682(3)	8	0.0189(5)	Te

M1	1	0	0	$\frac{1}{2}$	2	0.248(3)	Cd
	2	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	2	0.0433(1)	Mn _{0.72}
	3	0	0	$\frac{1}{2}$	2	0.098(5)	Mn _{0.8}
	4	0	0	$\frac{1}{2}$	2	0.110(8)*	Co _{0.88}
	5	0	0	$\frac{1}{2}$	2	0.089(8)	Co _{0.76}
M2	1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{2}$	4	0.0387(2)	Cd
	2	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{2}$	4	0.0479(1)	Mn _{0.53}
	3	0.75	$\frac{1}{4}$	$\frac{1}{2}$	4	0.0454(1)	Mn
	4	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{2}$	4	0.085(5)*	Co
	5	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{2}$	4	0.063(4)	Co _{0.83}
M3	1	0.2458(1)	0	$\frac{1}{2}$	8	0.0589(1)	Cd _{0.70}
	2	-0.2528(2)	$-\frac{1}{2}$	$-\frac{1}{2}$	8	0.0313(1)	Mn _{0.12}
	3	0.2543(4)	0	$\frac{1}{2}$	8	0.045(3)	Mn _{0.6}
	4	0.2428(6)	0	$\frac{1}{2}$	8	0.069(4)*	Co _{0.78}
	5	0.2441(7)	0	$\frac{1}{2}$	8	0.095(6)	Co _{0.89}
O1	1	0.7517(1)	0.3774(1)	0.8677(3)	16	0.0119(8)	O
	2	-0.2533(2)	-0.1241(2)	0.1367(4)	16	0.0146(1)	O
	3	0.2526(5)	0.1233(5)	0.1294(1)	16	0.0114(1)	O
	4	0.2531(6)	0.1255(7)	0.136(1)	16	0.013(3)	O
	5	0.2538(7)	0.1254(8)	0.137(1)	16	0.022(4)	O
O2	1	0.8585(1)	0.6415(1)	0.9659(4)	8	0.0162(1)	O
	2	-0.3616(3)	0.1384(3)	0.0248(1)	8	0.0188(1)	O
	3	0.6366(1)	0.1366(1)	0.0255(1)	8	0.024(3)	O
	4	0.6420(8)	0.1420(8)	0.022(1)	8	0.020(4)	O
	5	0.642(1)	0.142(1)	0.027(2)	8	0.036(6)	O
O3	1	0.7116(1)	0.6192(1)	0.9001(2)	16	0.0128(1)	O
	2	-0.1207(2)	-0.214(2)	0.126(3)	16	0.0133(1)	O
	3	0.1221(1)	0.2114(1)	0.0977(1)	16	0.021(1)	O
	4	0.1205(7)	0.2146(7)	0.1010(9)	16	0.012(2)*	O
	5	0.1206(7)	0.2169(8)	0.104(1)	16	0.022(4)	O
O4	1	0.8771(1)	0.5026(1)	0.8754(3)	16	0.0138(1)	O
	2	-0.3777(2)	0.0002(2)	0.1260(3)	16	0.0112(1)	O
	3	0.6223(1)	0.0009(1)	0.1216(1)	16	0.019(2)	O
	4	0.6239(8)	0.0011(6)	0.126(1)	16	0.017(4)	O
	5	0.6227(9)	0.0005(7)	0.121(1)	16	0.020(4)	O
O5	1	0.6223(1)	0.4677(1)	0.9006(3)	16	0.0133(1)	O
	2	-0.1236(2)	-0.0328(2)	0.0994(3)	16	0.0137(1)	O
	3	0.1225(6)	0.0351(1)	0.0975(1)	16	0.022(2)	O
	4	0.1242(7)	0.0297(7)	0.102(1)	16	0.016(4)	O

	5	0.1223(7)	0.0319(7)	0.1000(8)	16	0.011(2)*	O
<i>X1</i>	1	0.1302(1)	0.1302(1)	$\frac{1}{2}$	8	0.0508(9)	Cl
	2	-0.3771(1)	-0.3771(1)	$-\frac{1}{2}$	8	0.0537(1)	Cl
	3	0.8709(1)	0.1292(1)	$\frac{1}{2}$	8	0.0530(1)	Br
	4	0.1285(6)	0.1285(6)	$\frac{1}{2}$	8	0.072(4)	Cl
	5	0.1277(6)	0.1277(6)	$\frac{1}{2}$	8	0.073(4)*	Cl
<i>X2</i>	1	0.2556(1)	0.0353(1)	0.3180(1)	16	0.0362(5)	Cl
	2	0.2436	-0.4	-0.3	16	0.0448	Cl
	3	0.2553(1)	0.9951(1)	0.3101(2)	16	0.0227(5)	Br
	4	0.2568(4)	0.9989(3)	0.3246(8)	16	0.034(3)	Cl
	5	0.2582(4)	0.9980(3)	0.3258(8)	16	0.040(3)	Cl
<i>X3</i>	1	0.3663(1)	0.1339(1)	0.5210(3)	8	0.0524(1)	Cl
	2	-0.1318(1)	-0.3683(1)	-0.4779(4)	8	0.0701(1)	Cl
	3	0.6336(1)	0.1336(1)	0.5191(1)	8	0.0300(5)	Br
	4	0.3692(5)	0.1308(5)	0.4804(8)	8	0.061(3)	Cl
	5	0.3681(5)	0.1319(5)	0.4826(9)	8	0.058(3)*	Cl
<i>X4</i>	1	$\frac{1}{2}$	0	0.3311(1)	4	0.0486(1)	Cl
	2	$-\frac{1}{2}$	0	0.3254(4)	4	0.0305(1)	Cl
	3	$\frac{1}{2}$	0	0.3233(3)	4	0.0194(1)	Br
	4	$\frac{1}{2}$	0	0.328(1)	4	0.040(3)	Cl
	5	$\frac{1}{2}$	0	0.326(1)	4	0.043(4)	Cl
<i>X5</i>	1	0	0	0.3229(1)	4	0.9352(1)	Cl
	2	$-\frac{1}{2}$	$-\frac{1}{2}$	-0.3158(4)	4	0.0297(1)	Cl
	3	0	0	0.3216(3)	4	0.0171(1)	Br
	4	0	0	0.3263(9)	4	0.029(3)	Cl
	5	0	0	0.3258(8)	4	0.032(3)	Cl
<i>X6</i>	1	0.2524(1)	0.2477(1)	0.3099(1)	8	0.0229(1)	Cl
	2	0.2472(1)	-0.2529(1)	-0.3221(1)	8	0.0417(1)	Cl
	3	0.7454(1)	0.2454(1)	0.3101(2)	8	0.0188(1)	Br
	4	0.2484(3)	0.2516(3)	0.322(1)	8	0.041(3)	Cl
	5	0.2491(3)	0.2509(3)	0.3221(8)	8	0.035(3)*	Cl

Table S2. Selected interatomic distances (Å) for compounds **1 - 5**.

Bond		Length [Å]				
		1	2	3	4	5
<i>Ln1</i>	O5	2.42(2) × 8	2.411(1) × 8	2.473(4) × 8	2.394(12) × 8	2.358(11) × 8
<i>mean</i>		2.42	2.411	2.473	2.394	2.358
<i>Ln2</i>	O2	2.529(2) × 2	2.555(3) × 2	2.661(3) × 2	2.443(13) × 2	2.441(16) × 2
	O3	2.591(3) × 4	2.509(2) × 4	2.564(3) × 4	2.477(11) × 4	2.478(13) × 4
	O1	2.709(3) × 4	2.665(2) × 4	2.719(3) × 4	2.607(11) × 4	2.612(13) × 4
<i>mean</i>		2.626	2.401	2.645	2.522	2.524
<i>Ln3</i>	O3	2.433(3) × 2	2.407(5) × 2	2.489(2) × 2	2.376(11) × 2	2.378(13) × 2
	O5	2.599(1) × 2	2.487(1) × 2	2.562(4) × 2	2.468(12) × 2	2.477(11) × 2
	O4	2.556(2) × 2	2.563(2) × 2	2.647(3) × 2	2.497(13) × 2	2.470(14) × 2
	O1	2.654(4) × 2	2.642(1) × 2	2.675(3) × 2	2.619(12) × 2	2.621(14) × 2
	O2	2.898(4) × 2	2.399(1) × 2	2.923(2) × 2	2.811(13) × 2	2.810(16) × 2
<i>mean</i>		2.628	2.450	2.659	2.554	2.551
<i>Ln4</i>	O1	2.443(1) × 2	2.399(2) × 2	2.412(1) × 2	2.339(12) × 2	2.325(12) × 2
	O4	2.458(2) × 2	2.438(1) × 2	2.485(1) × 2	2.375(13) × 2	2.405(12) × 2
	X2	3.066(1) × 2	2.987(1) × 2	3.150(3) × 2	2.965(7) × 2	2.953(7) × 2
	X4	3.089(2)	2.971(1)	3.167(4)	2.971(5)	2.944(5)
	X3	3.232(3)	3.022(5)	3.456(6)	3.069(10)	3.091(12)
	X6	3.177(3)	3.155(3)	3.248(5)	3.118(6)	3.092(6)
	O2	3.362(1)	3.381(4)	3.404(4)		
<i>mean</i>		2.879	2.818	2.937	2.724	2.721
<i>Ln5</i>	O4	2.604(1) × 8	2.533(1) × 8	2.593(2) × 8	2.519(11) × 8	2.458(12) × 8
	O2	3.277(2) × 4	3.161(1) × 4	3.192(2) × 4	3.204(13) × 4	3.197(16) × 4
<i>mean</i>		2.828	2.742	2.793	2.747	2.704
<i>Te1</i>	O5	1.878(1)	1.866(1)	1.846(3)	1.869(12)	1.861(11)
	O3	1.877(3)	1.896(1)	1.868(2)	1.884(11)	1.898(13)
	O4	1.878(3)	1.903(2)	1.917(3)	1.912(10)	1.917(12)
<i>mean</i>		1.878	1.888	1.877	1.888	1.892
<i>Te2</i>	O4	1.883(1) × 2	1.915(3) × 2	1.932(2) × 2	1.897(13) × 2	1.920(14) × 2
	O2	1.876(2)	1.859(3)	1.881(3)	1.910(16)	1.860(20)
<i>mean</i>		1.881	1.896	1.915	1.901	1.900
<i>M1a</i>	X5	2.308(5) × 2	2.336(2) × 2	2.409(5) × 2	2.165(11) × 2	2.173(10) × 2
	X1	3.013(3) × 4	2.793(2) × 4	3.002(4) × 4	2.888(10) × 4	2.859(10) × 4
<i>mean</i>		2.778	2.641	2.804	2.647	2.630
<i>M1b</i>	X1		1.975(4) × 2	2.144(3) × 2		
	X5		3.039(3) × 2	3.022(4) × 2		
	X2		3.147(1) × 2	3.462(4) × 2		

<i>mean</i>			2.720	2.876		
<i>M2a</i>	X6	$2.492(2) \times 2$	$2.256(3) \times 2$	$2.568(1) \times 2$	$2.215(13) \times 2$	$2.219(10) \times 2$
	X3	$2.691(3) \times 2$	$2.701(4) \times 2$	$2.717(2) \times 2$	$2.690(8) \times 2$	$2.653(8) \times 2$
	X1	$2.759(1) \times 2$	$2.888(4) \times 2$	$2.810(1) \times 2$	$2.731(10) \times 2$	$2.738(10) \times 2$
<i>mean</i>		2.647	2.615	2.698	2.545	2.536
<i>M2b</i>	X3		1.916(1)			
	X1		2.108(4)			
	X2		2.780(1)			
	X6		2.918(2)			
	X2		3.146(2)			
	X6		3.269(3)			
<i>mean</i>			2.689			
<i>M3a</i>	X2	$2.39(3) \times 2$	$2.278(3) \times 2$	$2.567(3) \times 2$	$2.197(10) \times 2$	$2.184(10) \times 2$
	X1	$2.847(3) \times 2$	$2.808(5) \times 2$	$2.957(4) \times 2$	$2.733(11) \times 2$	$2.736(12) \times 2$
	X3	$2.948(1) \times 2$	$2.889(4) \times 2$	$2.879(4) \times 2$	$2.901(10) \times 2$	$2.874(11) \times 2$
<i>mean</i>		2.728	2.658	2.801	2.610	2.598
<i>M3b</i>	X3	$2.206(3) \times 2$	$2.136(3) \times 2$			
	X2	$3.01(2) \times 2$	$2.909(3) \times 2$			
	X4	$3.087(1) \times 2$	$3.051(1) \times 2$			
<i>mean</i>		2.767	2.670			