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Electronic Supporting Information

Ultraviolet Emission and Electron Spin Characteristics of Th $(C_2O_4)_2.xH_2O:Gd^{3+}$

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Table S1. Position coordinates of various atoms in triclinic (P1) structure of TOHG

Atom	Wyc.	x	y	z	U(eq) Å^2
Th1	1a	-0.0060(8)	-0.0026(8)	-0.0023(6)	0.0414
C1	1a	0.0411(13)	0.5053(3)	0.09856(16)	0.0414
O1	1a	1.088(5)	0.3343(7)	0.1812(8)	0.0414
O2	1a	0.061(2)	0.6573(9)	0.8182(4)	0.0414
C2	1a	1.0007(6)	0.4968(2)	0.90687(14)	0.0414
O3	1a	0.020(7)	0.7356(11)	0.1937(7)	0.0414
O4	1a	1.027(4)	0.2630(7)	0.8093(5)	0.0414
C3	1a	0.4992(5)	1.0038(15)	0.9022(2)	0.0414
O5	1a	0.6563(10)	0.079(3)	0.8177(5)	0.0414
O6	1a	0.3463(9)	0.950(6)	0.1802(7)	0.0414
C4	1a	0.5145(4)	-0.0127(16)	0.09440(17)	0.0414
O7	1a	0.2657(8)	0.974(6)	0.8127(5)	0.0414
O8	1a	0.7376(9)	0.067(3)	0.1885(5)	0.0414
O11W*	1a	0.2830	0.7170	0.5000	0.0414
O12W*	1a	0.7170	0.2830	0.5000	0.0414
O13W*	1a	0.7160	0.7160	0.4810	0.0414
O14W*	1a	0.2840	0.2840	0.5190	0.0414
O15W*	1a	0.5000	0.5000	0.0000	0.0414
O16W*	1a	0.0000	0.0000	0.5000	0.0414

*W: Water molecule and no hydrogen atom is considered. Kept fixed as the equivalent positions in monoclinic lattice in the refinement

Triclinic (P1)

a = 6.4696 Å, b = 6.4617 Å, c = 7.8796 Å, α = 90.43°, β = 91.96°, γ = 89.89°

Rp: 18.9 % Rwp: 24.1 %; R_B: 16.2 %

Table S2. Typical bond lengths (Å) and angles (°) in TOHG. The water molecules are not considered.

Bonds lengths		**Angles**				**Torsion angles**	
Th1-O1	2.664(10)	O4-Th1-O5	65.8(7)	Th1-O1-C1	111.9(8)	O4-Th1-O1-C1	22.1(16)
Th1-O2	2.648(8)	O1-Th1-O4	73.4(3)	Th1-O2-C2	108.2(3)	O5-Th1-O1-C1	-35.1(18)
Th1-O3	2.301(9)	O4-Th1-O8	111.3(7)	Th1-O3-C1	111.2(3)	O8-Th1-O1-C1	-98.9(18)
Th1-O4	2.293(7)	O2-Th1-O4	104.8(3)	Th1-O4-C2	111.2(4)	O2-Th1-O1-C1	110.8(17)
Th1-O5	2.619(9)	O4-Th1-O7	63.2(10)	Th1-O5-C3	106.9(5)	O7-Th1-O1-C1	78.7(19)
Th1-O6	2.671(9)	O3-Th1-O4	170.4(13)	Th1-O6-C4	113.8(6)	O3-Th1-O1-C1	-167.2(19)
Th1-O7	2.326(7)	O4-Th1-O6	109.9(9)	Th1-O7-C3	115.1(4)	O6-Th1-O1-C1	142.3(19)
Th1-O8	2.318(8)	O1-Th1-O5	107.4(7)	Th1-O8-C4	106.2(4)	O4-Th1-O6-C4	-35(2)
		O5-Th1-O8	73.2(2)	O3-C1-C2	117.2(4)	O1-Th1-O6-C4	-97(2)
C1-C2	1.525(2)	O2-Th1-O5	91.6(4)	O1-C1-O3	123.2(5)	O8-Th1-O6-C4	-156(2)
C3-C4	1.519(2)	O5-Th1-O7	107.9(3)	O1-C1-C2	119.6(3)	O2-Th1-O6-C4	72(2)
		O3-Th1-O5	123.7(11)	O2-C2-O4	115.0(5)	O7-Th1-O6-C4	16(2)
C1-O1	1.316(9)	O5-Th1-O6	174.9(9)	O4-C2-C1	117.2(3)	O3-Th1-O6-C4	143(3)
C1-O3	1.669(8)	O1-Th1-O8	69.5(7)	O2-C2-C1	117.2(3)	Th1-O3-C1-C2	-11(3)
C2-O2	1.322(7)	O1-Th1-O2	157.4(8)	O5-C3-O7	122.1(6)	Th1-O3-C1-O1	169.8(19)
C2-O4	1.701(6)	O1-Th1-O7	103.0(10)	O7-C3-C4	116.3(3)	Th1-O4-C2-O2	166.0(9)
C3-O5	1.329(10)	O1-Th1-O3	103.2(4)	O5-C3-C4	120.2(4)	Th1-O4-C2-C1	22.2(15)
C3-O7	1.656(7)	O1-Th1-O6	68.2(10)	O8-C4-C3	116.2(4)	Th1-O7-C3-O5	-151.5(14)
C4-O6	1.324(9)	O2-Th1-O8	129.5(5)	O6-C4-O8	122.7(5)	Th1-O7-C3-C4	15(2)
C4-O8	1.680(9)	O7-Th1-O8	172.2(10)	O6-C4-C3	119.8(3)	Th1-O8-C4-C3	-31.8(12)
		O3-Th1-O8	75.0(10)			Th1-O8-C4-O6	161(2)
		O6-Th1-O8	106.8(3)			O3-C1-C2-O4	179(2)
		O2-Th1-O7	58.4(9)			O7-C3-C4-O8	-167.3(17)
		O2-Th1-O3	74.8(3)				
		O2-Th1-O6	92.2(8)				
		O3-Th1-O7	109.7(12)				
		O6-Th1-O7	71.4(2)				
		O3-Th1-O6	60.7(12)				

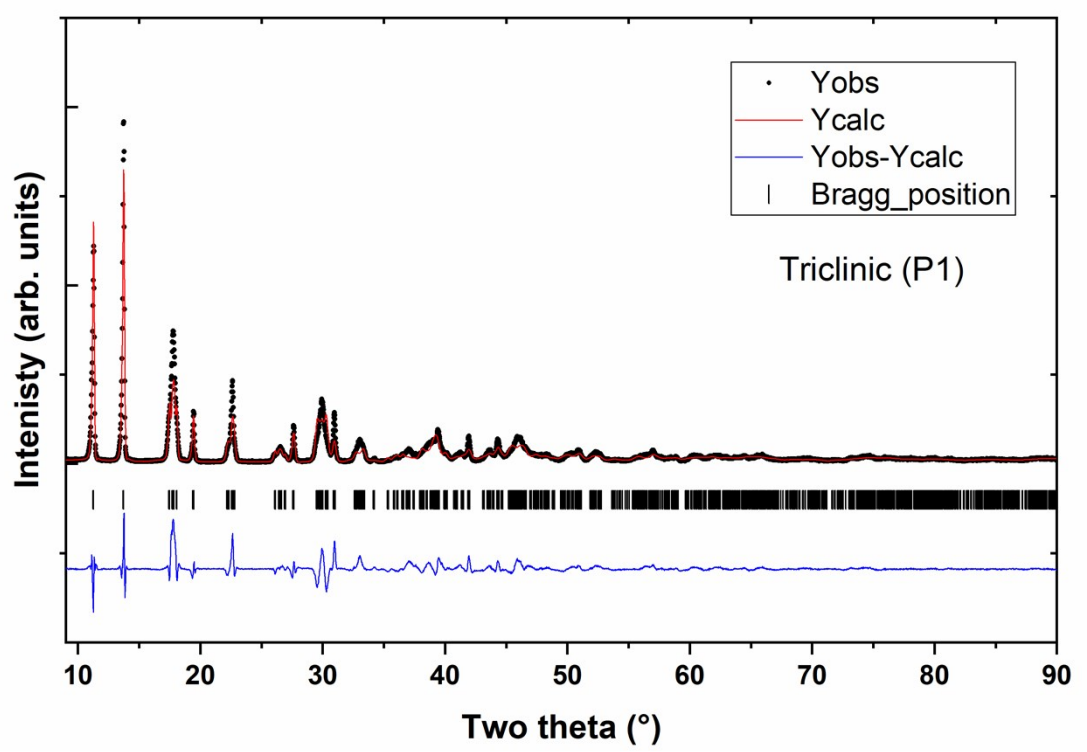

Figure S1. Rietveld refinement plot of TOHG in triclinic (P1) model structure

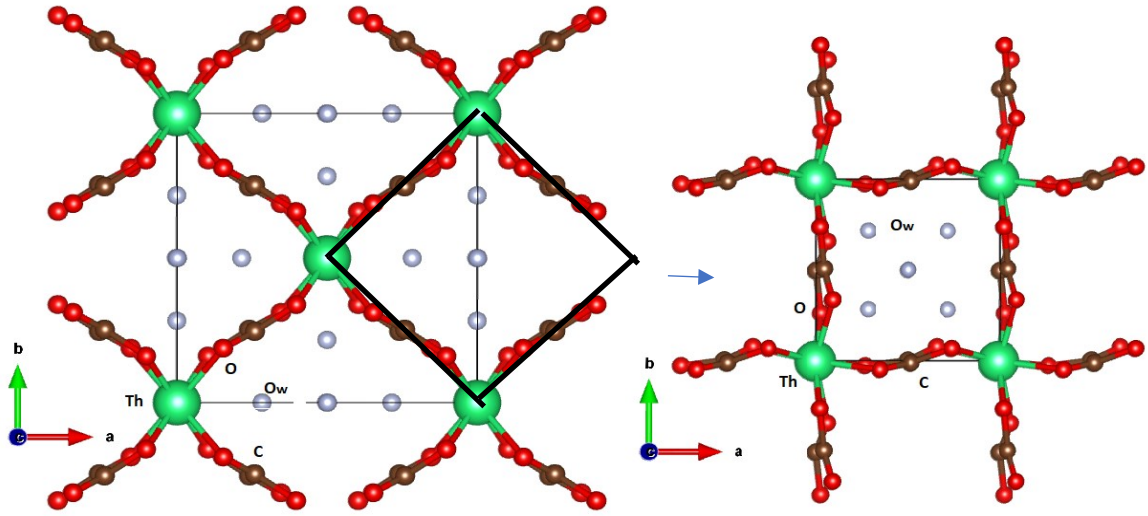

Figure S2. Relation between monoclinic, C2/m (left) and triclinic, P1 (right) structure of TOHG.