$Pb@Pb_8$ basket-Like Cluster based Lead Tellurate-Nitrate Kleinman-forbidden Nonlinear Optical Crystal: $Pb_9Te_2O_{13}(OH)(NO_3)_3$

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Table S1. Atomic coordinates ($Å \times 10^4$) and equivalent isotropic displacements parameters ($Å^2 \times 10^3$) for $Pb_9Te_2O_{13}(OH)(NO_3)_3$

Atom	x	y	z	U(eq)
Pb(5)	-1942.9(5)	4499.5(4)	6420.1(3)	26.26(14)
Pb(4)	1340.5(5)	5024.4(4)	6289.8(3)	25.71(14)
Pb(2)	3031.8(4)	3031.8(4)	5000	22.68(16)
Pb(3)	2843.7(5)	2931.7(4)	7469.4(3)	27.70(14)
Pb(1)	5139.8(4)	4347.7(5)	3817.5(4)	28.81(15)
Te(1)	497.1(7)	2418.7(6)	6293.7(5)	18.76(18)
O(2)	4250(7)	2894(8)	3574(6)	23.1(19)
O(3)	1935(8)	1921(8)	6336(7)	24.1(19)
O(6)	175(8)	1530(8)	5253(6)	22.9(19)
O(7)	-921(7)	2940(8)	6194(6)	19.4(18)
O(4)	857(8)	3318(9)	7294(6)	23(2)
O(1)	5009(8)	3662(8)	5411(6)	23.0(19)
O(5)	945(8)	3487(8)	5433(6)	22.8(19)
O(12)	2187(14)	1677(13)	10743(12)	59(4)
O(8)	2285(19)	4672(16)	8436(14)	102(5)
O(11)	3280(20)	2180(30)	9830(30)	81(12)
O(10)	1407(15)	5582(18)	9449(13)	87(5)
N(2)	2251(18)	5210(20)	9180(15)	99(5)
O(9)	3051(17)	5340(30)	9665(17)	114(6)
N(1)	2249(19)	2249(19)	10000	88(9)

Table S2. Bond lengths (Å) and angles (deg.) for $Pb_9Te_2O_{13}(OH)(NO_3)_3$

Pb(1)-O(2)	2.198(10)	Pb(5)-O(5a)	2.332(9)
Pb(1)-O(1c)	2.345(10)	Pb(5)-O(3b)	2.334(10)
Pb(1)-O(1)	2.477(9)	Pb(5)-O(7)	2.395(9)
Pb(1)-O(9f)	2.64(3)		
Pb(2)-O(2c)	2.592(9)	Te(1)-O(1b)	1.899(9)

Pb(2)-O(2)	2.592(9)	Te(1)-O(4)	1.904(10)
Pb(2)-O(7d)	2.626(9)	Te(1)-O(7)	1.929(9)
Pb(2)-O(7e)	2.626(9)	Te(1)-O(6)	1.930(9)
Pb(2)-O(1)	2.708(10)	Te(1)-O(5)	1.933(9)
Pb(2)-O(1c)	2.708(10)	Te(1)-O(3)	1.937(10)
Pb(3)-O(2c)	2.261(10)		
Pb(3)-O(3)	2.386(9)	H(6)-O(6)	0.9601
Pb(3)-O(7e)	2.560(9)		
Pb(3)-O(4)	2.588(10)	O(8)-N(2)	1.274(16)
Pb(3)-O(8)	2.716(14)	N(2)-O(9)	1.250(17)
Pb(4)-O(2c)	2.218(10)	O(10)-N(2)	1.241(17)
Pb(4)-O(5)	2.372(10)	O(11)-N(1)	1.34(2)
Pb(4)-O(4d)	2.455(9)	O(12)-N(1)	1.30(2)
Pb(4)-O(4)	2.687(10)		
O(2)-Pb(1)-O(1c)	88.0(3)	O(5a)-Pb(5)-O(3b)	96.1(4)
O(2)-Pb(1)-O(1)	79.6(3)	O(5a)-Pb(5)-O(7)	78.5(3)
O(1c)-Pb(1)-O(1)	68.1(4)	O(3b)-Pb(5)-O(7)	70.6(3)
O(1c)-Pb(1)-O(9f)	114.9(6)		
O(1)-Pb(1)-O(9f)	71.2(5)	O(1b)2-Te(1)-O(4)	92.9(4)
O(2c)-Pb(2)-O(7d)	103.9(3)	O(1b)-Te(1)-O(7)	89.4(4)
O(2)-Pb(2)-O(7d)	74.9(3)	O(4)-Te(1)-O(7)	94.3(4)
O(2c)-Pb(2)-O(1)	73.1(3)	O(1b)-Te(1)-O(6)	89.0(4)
O(2)-Pb(2)-O(1)	68.9(3)	O(7)-Te(1)-O(6)	86.8(4)
O(7d)-Pb(2)-O(1)	116.5(3)	O(4)-Te(1)-O(5)	89.9(4)
O(7e)-Pb(2)-O(1)	60.6(3)	O(7)-Te(1)-O(5)	89.2(4)
O(2)-Pb(2)-O(1c)	73.1(3)	O(6)-Te(1)-O(5)	88.2(4)
O(7d)-Pb(2)-O(1c)	60.6(3)	O(1b)-Te(1)-O(3)	93.0(4)
O(7e)-Pb(2)-O(1c)	116.5(3)	O(4)-Te(1)-O(3)	86.8(4)
O(1)-Pb(2)-O(1c)	59.9(4)	O(6)-Te(1)-O(3)	91.9(4)
O(2c)-Pb(3)-O(3)	87.3(3)	O(5)-Te(1)-O(3)	88.4(4)
O(2c)-Pb(3)-O(7e)	82.1(3)		
O(3)-Pb(3)-O(7e)	67.0(3)	O(10)-N(2)-O(9)	118.3(17)
O(2c)-Pb(3)-O(4)	79.7(3)	O(10)-N(2)-O(8)	120.3(18)
O(3)-Pb(3)-O(4)	64.0(3)	O(9)-N(2)-O(8)	121.3(18)
O(2c)-Pb(3)-O(8)	75.4(6)	O(12)-N(1)-O(12h)	128(3)
O(4)-Pb(3)-O(8)	68.9(6)	O(12)-N(1)-O(11h)	113(2)
O(2c)-Pb(4)-O(5)	82.5(4)	O(12)-N(1)-O(11)	100(2)
O(2c)-Pb(4)-O(4d)	96.5(4)	O(11h)-N(1)-O(11)	100(4)
O(5)-Pb(4)-O(4d)	86.0(3)		
O(2c)-Pb(4)-O(4)	78.3(3)		
O(5)-Pb(4)-O(4)	64.5(3)		

Symmetry codes: (a) y-1/2, -x+1/2, z+1/4; (b) x-1/2, -y+1/2, -z+5/4; (c) y, x, -z+1; (d) -y+1/2, x+1/2, z-1/4; (e) x+1/2, -y+1/2, -z+5/4; (f) -x+1, -y+1, z-1/2; (g) -x+1, -y+1,

z+1/2; (h) y, x, -z+2

Table S3. Energy-Dispersive Spectrometry (EDS) for $Pb_9Te_2O_{13}(OH)(NO_3)_3$

Point 1				Point 2			
Element	Weight %	Atomic %	Formula	Element	Weight %	Atomic %	Formula
O K	17.87	72.38		O K	12.87	62.95	
Te L	9.97	5.06	1.0	Te L	10.77	6.55	1.0
Pb M	72.16	22.55	4.45	Pb M	76.81	30.50	4.65
Totals	100			Totals	100		
Point 3							
Element	Weight %	Atomic %	Formula	The average Pb: Te molar ratio: 4.51:1			
O K	13.81	65.79					
Te L	10.48	6.28	1.0				
Pb M	75.70	27.91	4.44				
Totals	100						

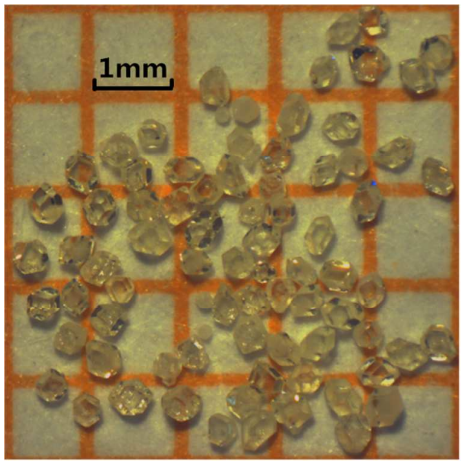


Figure S1. The morphology for $Pb_9Te_2O_{13}(OH)(NO_3)_3$.

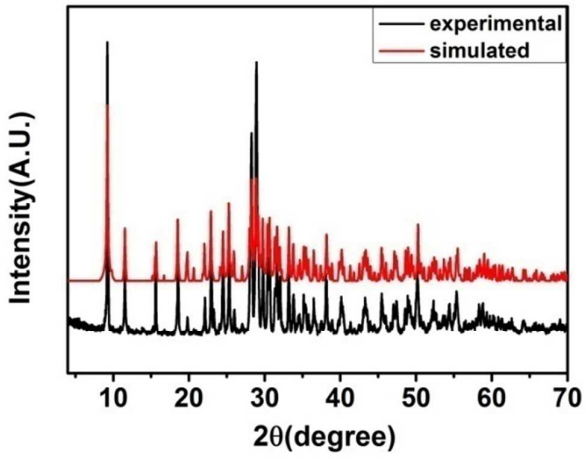


Figure S2. Experimented powder X-ray diffraction patterns (black line) of $Pb_9Te_2O_{13}(OH)(NO_3)_3$ compared to the calculated from the crystal data (red line).

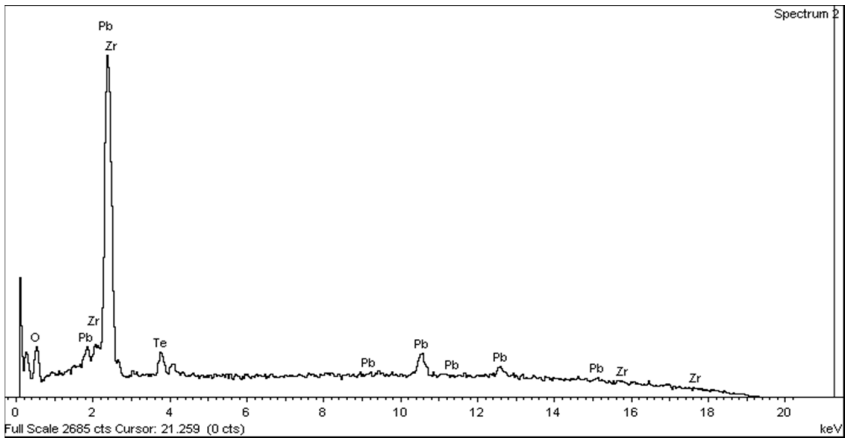


Figure S3. Energy-Dispersive Spectrometry (EDS) for $Pb_9Te_2O_{13}(OH)(NO_3)_3$.

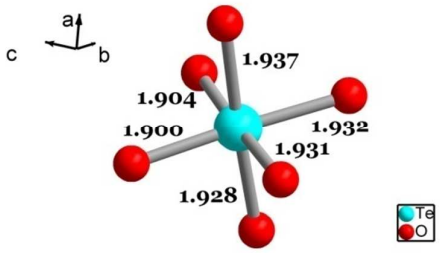
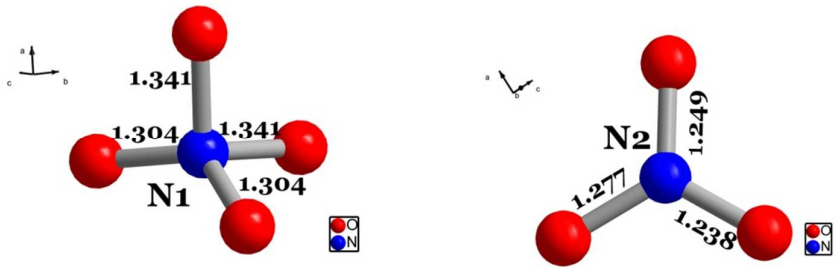


Figure S4.The coordinate environments of the Te^{6+} cations of $Pb_9Te_2O_{13}(OH)(NO_3)_3$.



(a) (b)

Figure S5. The coordinate environments of the N^{5+} cations of $Pb_9Te_2O_{13}(OH)(NO_3)_3$; $N(1)O^{3-}$ (a) and $N(2)O^{3-}$ (b).

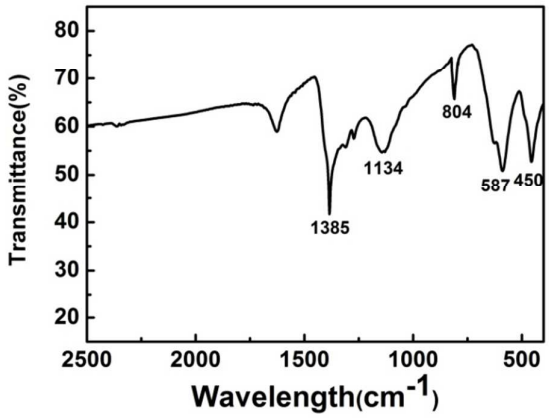


Figure S6. Infrared spectra of $Pb_9Te_2O_{13}(OH)(NO_3)_3$.

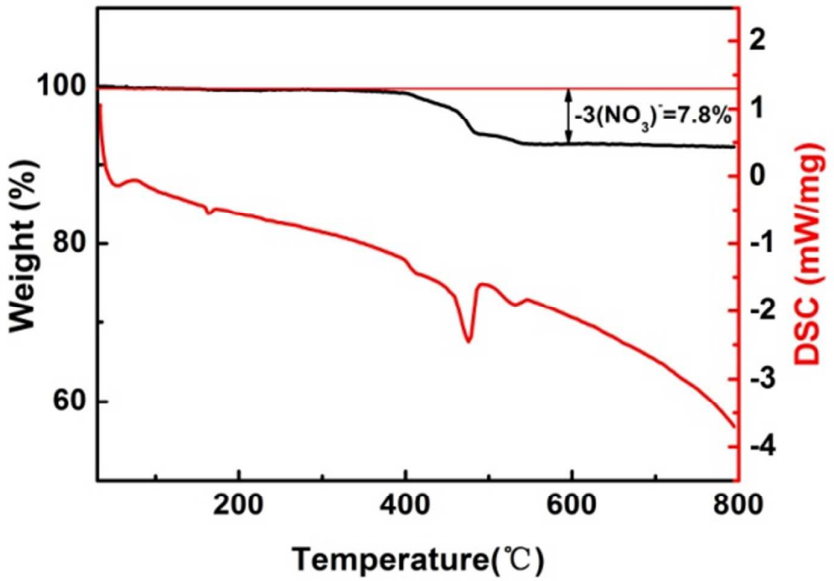


Figure S7. The TGA and DSC curves for $Pb_9Te_2O_{13}(OH)(NO_3)_3$ in 30-800°C range.

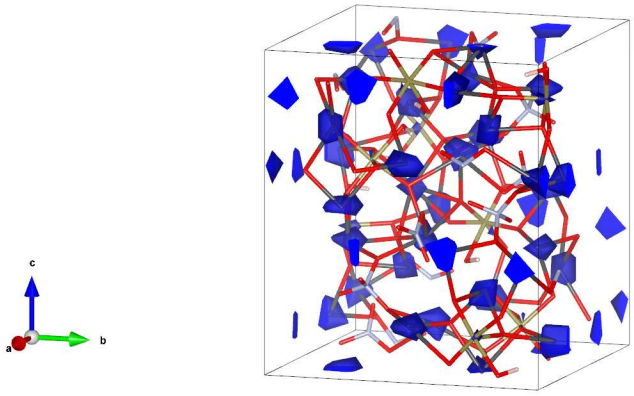


Figure S8. Isosurface of Electron Localization Function (ELF) for$Pb_9Te_2O_{13}(OH)(NO_3)_3$ with the value of 0.55; dark gray represents Pb atoms.