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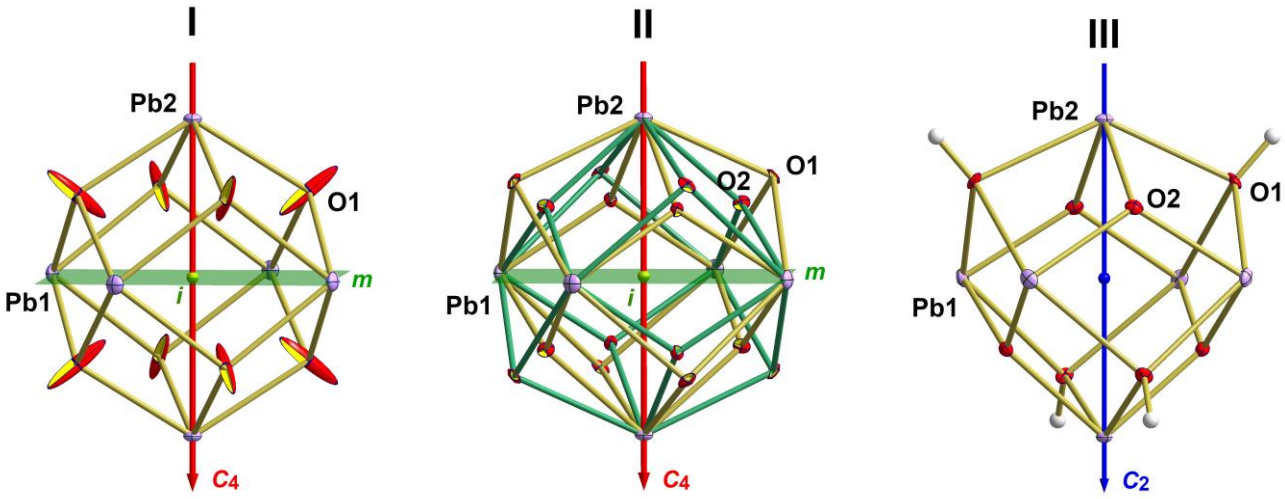

Figure S1. Ball-and-stick models of $Pb_6O_4(OH)_4$. as result of the different structure models in the two different space groups *P*4/*mnc* (**I**, **II**) and $P\bar{4}2_1c$ (**III**); structure model I and II, point group C_{4h} with mirror planes *m* (green), center of symmetry *i* (dark green) and proper rotation axis C_4 (as part of a S_4 rotoinversion axis, red); structure model III, point group S_4 with S_4-rotoinversion axis (blue, blue sphere = center of symmetry of the rotoinversion axis).

Table S1. Summary of the effect of the different space groups and structure models on some dataset, refinement and validation parameters for $Sn_6O_4(OH)_4$ and $Pb_6O_4(OH)_4$.

	$Sn_6O_4(OH)_4$			$Pb_6O_4(OH)_4$		
structure model	**I**	**II**	**III**	**I**	**II**[4]	**III**
space group		*P*4/*mnc*	$P\bar{4}2_1c$		*P*4/*mnc*	$P\bar{4}2_1c$
Z'		1/8	1/4		1/8	1/4
Collected reflections		78097			125245	
Rejected reflections		28064	24737		16461	9169
Measured reflexions		50033	53360		108784	116076
Unique refelxions		647	1242		689	1304
R_{int}		0.0600	0.0600		0.0993	0.0999
R_σ		0.0097	0.0122		0.0122	0.0167
centre of symmetry		yes	no		yes	no
point group		C_{4h}	S_4		C_{4h}	S_4
symmetry elements		C4, σ_h, i	$\bar{4}$, C2		C4, σ_h, i	$\bar{4}$, C2
weighting parameter *p*/*q*	0/24.9653	0/7.6551	0/0.8625	26.9664	0.0091/6.1892	0.0080/5.5214
Goof	1.263	1.557	1.332	1.090	1.228	1.106
R1[1]	0.0400	0.0220	0.0127	0.0280	0.0147	0.0157
wR2[1]	0.0841	0.0605	0.0277	0.0482	0.0324	0.0285
±Δ [e/Å^3], near to	3.87/-3.32, O1	1.71/-1.60, Sn2	0.553/-0.552	4.44/-4.07, O1	1.50/-1.94, Pb2	1.135/-1.880
A-Alerts[3]	5	0	0	5	0	0
B-Alerts[3]	4	1	0	3	0	0
C-Alerts[3]	16	3	0	11	4	4
violations[2]		789	32		46	4

[1]) I > 2σ(I), [2]) systematic absence violations before merging according to SHELXL, [3]) checkCIF, [4]) without H

Table S2. Full list of bond lengths [Å] and angles [°] for $Sn_6O_4(OH)_4$.

Sn(1)-O(2)#1	2.091(2)
Sn(1)-O(2)	2.091(2)
Sn(1)-O(1)	2.334(2)
Sn(1)-O(1)#2	2.392(2)
Sn(2)-O(2)	2.115(2)
Sn(2)-O(2)#3	2.115(2)
Sn(2)-O(1)	2.346(3)
Sn(2)-O(1)#3	2.346(3)
O(1)-H(1)	0.9600
O(2)#1-Sn(1)-O(2)	96.6(1)
O(2)#1-Sn(1)-O(1)	74.2(1)
O(2)-Sn(1)-O(1)	74.3(1)
O(2)#1-Sn(1)-O(1)#2	73.2(1)
O(2)-Sn(1)-O(1)#2	73.0(1)
O(1)-Sn(1)-O(1)#2	130.0(1)
O(2)-Sn(2)-O(2)#3	96.2(1)
O(2)-Sn(2)-O(1)	73.6(1)
O(2)#3-Sn(2)-O(1)	73.8(1)
O(2)-Sn(2)-O(1)#3	73.8(1)
O(2)#3-Sn(2)-O(1)#3	73.6(1)
O(1)-Sn(2)-O(1)#3	130.4(1)
Sn(1)-O(1)-Sn(2)	97.9(1)
Sn(1)-O(1)-Sn(1)#1	97.1(1)
Sn(2)-O(1)-Sn(1)#1	97.4(1)
Sn(1)-O(1)-H(1)	116.0
Sn(2)-O(1)-H(1)	112.6
Sn(1)#1-O(1)-H(1)	130.1
Sn(1)#2-O(2)-Sn(1)	115.7(1)
Sn(1)#2-O(2)-Sn(2)	115.6(1)
Sn(1)-O(2)-Sn(2)	114.1(1)

Symmetry transformations used to generate equivalent atoms: #1 y,-x,-z #2 -y,x,-z #3 -x,-y,z

Table S3. Full list of bond lengths [Å] and angles [°] for $Pb_6O_4(OH)_4$.

Pb(1)-O(2)#1	2.184(5)
Pb(1)-O(2)	2.192(5)
Pb(1)-O(1)	2.456(2)
Pb(1)-O(1)#1	2.475(2)
Pb(2)-O(2)#2	2.204(5)
Pb(2)-O(2)#1	2.204(5)
Pb(2)-O(1)	2.436(6)
Pb(2)-O(1)#3	2.436(6)
O(1)-H(1)	0.9600
O(2)#1-Pb(1)-O(2)	98.3(3)
O(2)#1-Pb(1)-O(1)	74.6(2)
O(2)-Pb(1)-O(1)	73.7(2)
O(2)#1-Pb(1)-O(1)#1	73.4(2)
O(2)-Pb(1)-O(1)#1	73.9(2)
O(1)-Pb(1)-O(1)#1	129.8(2)
O(2)#2-Pb(2)-O(2)#1	99.1(3)
O(2)#2-Pb(2)-O(1)#3	74.6(2)
O(2)#1-Pb(2)-O(1)#3	74.5(2)
O(2)#2-Pb(2)-O(1)	74.5(2)
O(2)#1-Pb(2)-O(1)	74.6(2)
O(1)#3-Pb(2)-O(1)	131.6(3)
Pb(1)-O(1)-Pb(2)	97.2(2)
Pb(1)-O(1)-Pb(1)#2	97.3(2)
Pb(2)-O(1)-Pb(1)#2	97.3(2)
Pb(1)-O(1)-H(1)	121.5
Pb(2)-O(1)-H(1)	106.6
Pb(1)#2-O(1)-H(1)	130.1
Pb(1)#2-O(2)-Pb(1)	115.5(2)
Pb(1)#2-O(2)-Pb(2)#2	113.5(2)
Pb(1)-O(2)-Pb(2)#2	114.0(2)

Symmetry transformations used to generate equivalent atoms: #1 -y+1,x,-z+1 #2 y,-x+1,-z+1 #3 -x+1,-y+1,z

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic/anisotropic displacement parameters ($Å^2$ x 10^3) for $Sn_6O_4(OH)_4$. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$h^2a^{*2}U_{11}$ + ... + 2hka*b*U_{12}]. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	Wyckoff	x	y	z	U_{eq}	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pb(1)	*e*	1234(1)	2929(1)	22(1)	9(1)	11(1)	6(1)	11(1)	-1(1)	3(1)	-2(1)
Pb(2)	*c*	0	0	2768(1)	8(1)	12(1)	9(1)	5(1)	0	0	2(1)
O(1)	*e*	2492(3)	1044(3)	1681(3)	10(1)	10(1)	11(1)	10(1)	-2(1)	-2(1)	-2(1)
O(2)	*e*	-768(3)	1844(3)	1209(2)	8(1)	7(1)	8(1)	8(1)	-1(1)	0(2)	0(1)

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic/anisotropic displacement parameters ($Å^2$ x 10^3) for $Pb_6O_4(OH)_4$. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$h^2a^{*2}U_{11}$ + ... + 2hka*b*U_{12}]. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Bond lengths	**M = Sn**	**M = Pb**	**Bond angles**	**M = Sn**	**M = Pb**
M(1)-O(2)^1	2.091(2)	2.184(5)	O(2)^1-M(1)-O(2)	96.6(1)°	98.3(3)°
M(1)-O(2)	2.091(2)	2.192(5)	O(2)^1-M(1)-O(1)	74.2(1)°	73.4(2)°
M(1)-O(1)	2.334(2)	2.474(5)	O(2)^1-M(1)-O(1)^2	73.2(1)°	74.6(2)°
M(1)-O(1)^2	2.392(2)	2.456(6)	O(2)-M(1)-O(1)	74.3(1)°	73.9(2)°
			O(2)-M(1)-O(1)^2	73.0(1)°	73.6(2)°
			O(1)-M(1)-O(1)^2	130.0(1)°	129.8(2)°
M(2)-O(2)	2.115(2)	2.204(5)	O(2)-M(2)-O(1)	73.6(1)°	74.5(2)°
M(2)-O(2)^3	2.115(2)	2.204(5)	O(2)-M(2)-O(2)^3	96.2(1)°	99.0(3)°
M(2)-O(1)	2.346(3)	2.436(6)	O(2)-M(2)-O(1)^3	73.8(1)°	74.6(2)°
M(2)-O(1)^3	2.346(3)	2.436(6)	O(2)^3-M(2)-O(1)	73.8(1)°	74.6(2)°
			O(2)^3-M(2)-O(1)^3	73.6(1)°	74.5(2)°
			O(1)-M(2)-O(1)^3	130.4(1)°	131.6(3)°

Table S6. Selected bond lengths [Å] and angles for $M_6O_4(OH)_4$ with M = Sn, Pb. Symmetry transformations used to generate equivalent atoms: $^{1)}$ y, -x, -z; $^{2)}$ -y, x, -z; $^{3)}$-x, -y, z for M = Sn; $^{1)}$-y+1, x, -z+1; $^{2)}$y, -x+1, -z+1; $^{3)}$-x+1, -y+1, z for M = Pb.

	Wyckoff	x	y	z	U_{eq}	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pb(1)	*e*	2001(1)	6337(1)	5014(1)	8(1)	5(1)	9(1)	10(1)	2(1)	1(1)	3(1)
Pb(2)	*c*	5000	5000	2213(1)	7(1)	10(1)	8(1)	4(1)	0	0	1(1)
O(1)	*e*	2397(7)	4001(7)	3290(6)	7(1)	6(2)	9(2)	7(2)	-4(2)	-2(2)	-1(2)
O(2)	*e*	4243(7)	6963(7)	3756(6)	7(1)	8(2)	7(2)	6(2)	1(2)	0(2)	2(2)

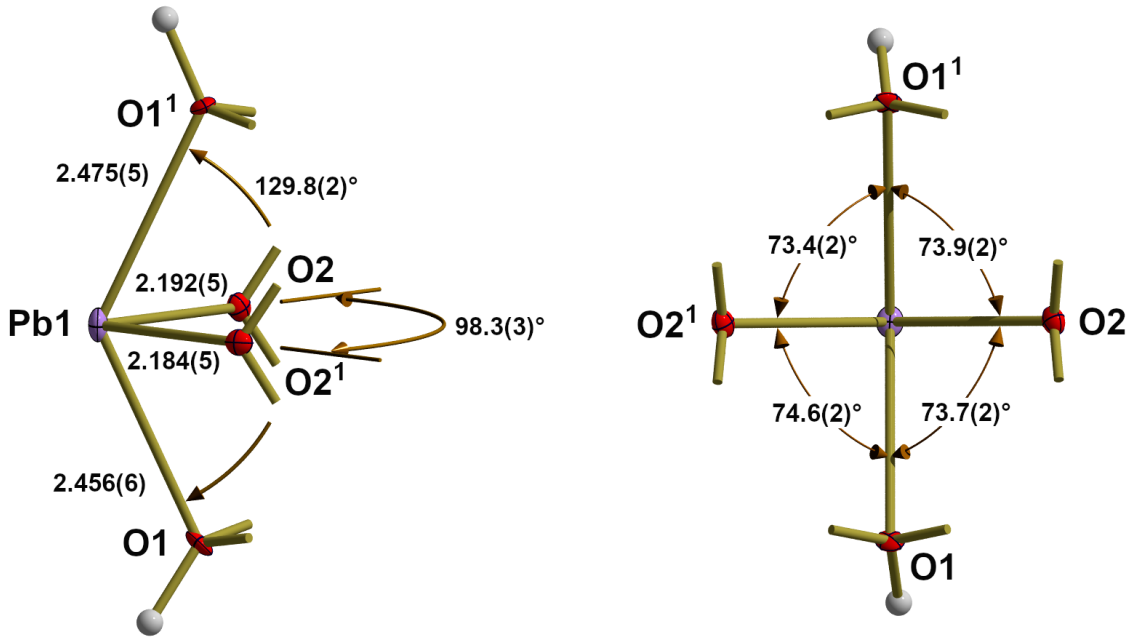

Figure S2. Different views [left side = side view, right side = from bottom up] on the ball-and-stick model of the bended seesaw {PbO_4} coordination of Pb1 with bond lengths [Å] and angles [°]; additional bonds of the oxygen atoms are indicated as shortened sticks; symmetry operations used to generate equivalent atoms: [1]) 1-y,x,1-z.

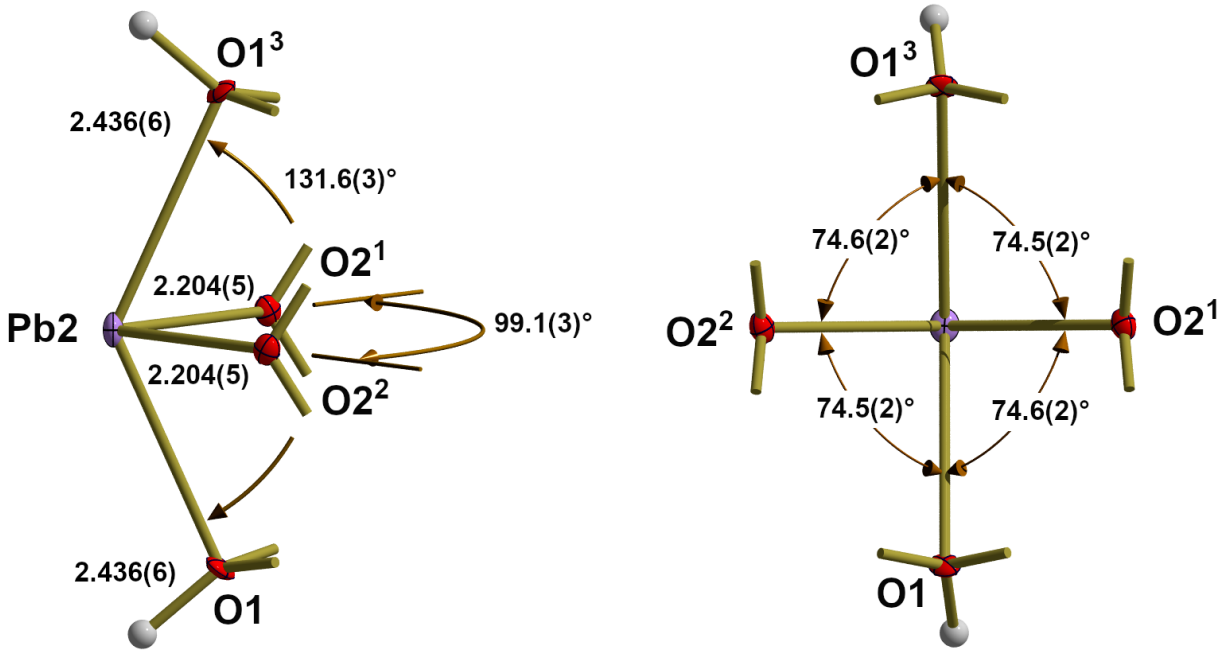

Figure S3. Different views [left side = side view, right side = from bottom up] on the ball-and-stick model of the bended seesaw {PbO_4} coordination of Pb2 with bond lengths [Å] and angles [°]; additional bonds of the oxygen atoms are indicated as shortened sticks; symmetry operations used to generate equivalent atoms: [1])1-y,x,1-z; [2])y,1-x,1-z; [3])1-x,1-y,z.

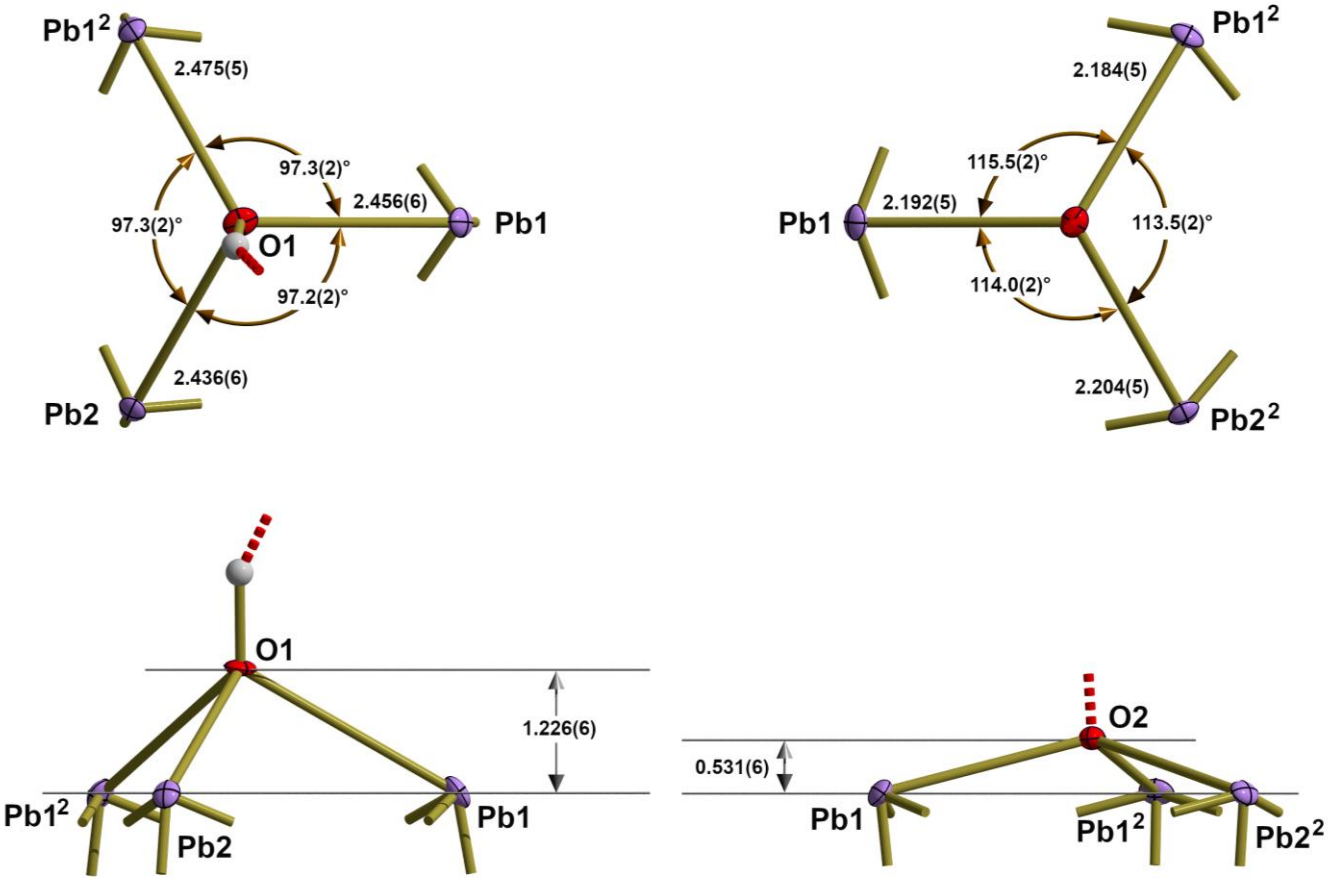

Figure S4. Different views [above = from top, below = side view] on the ball-and-stick models of the trigonal-pyramidal coordination of O1 (left) and O2 (right) with bond lengths [Å] and angles [°] for $Pb_6O_4(OH)_4$; additional bonds of the oxygen atoms are indicated as shortened sticks; symmetry operations used to generate equivalent atoms: $^{2)}$y,1-x,1-z.