Table 1. Crystal data and structure refinement for Sn6O4(OH)4_II.

Identification code	HR514_0m
Empirical formula	H4 O8 Sn6
Formula weight	844.17
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Tetragonal, P4/mnc
Unit cell dimensions	a = 7.87880(10) A c = 9.0582(2) A
Volume	562.292(19) A^3
Z, Calculated density	2, 4.986 Mg/m^3
Absorption coefficient	13.133 mm^-1
F(000)	736
Crystal size	0.075 x 0.073 x 0.073 mm
Theta range for data collection	3.657 to 34.963 deg.
Limiting indices	-12<=h<=12, -12<=k<=12, -14<=l<=14
Reflections collected / unique	50033 / 657 [R(int) = 0.0600]
Completeness to theta = 25.242	99.6 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	657 / 0 / 30
Goodness-of-fit on F^2	1.557
Final R indices [I>2sigma(I)]	R1 = 0.0220, wR2 = 0.0605
R indices (all data)	R1 = 0.0221, wR2 = 0.0605
Extinction coefficient	0.0028(3)
Largest diff. peak and hole	1.709 and -1.596 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Sn6O4(OH)4_II.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Sn(1)	7929(1)	6233(1)	5000	9(1)
Sn(2)	5000	5000	2232(1)	8(1)
O(1)	6046(8)	7494(9)	3319(8)	9(1)
O(2)	5770(8)	6845(8)	3785(7)	8(1)

Table 3. Bond lengths [A] and angles [deg] for Sn6O4(OH)4_II.

Sn(1)-O(2)#1	2.083(6)
Sn(1)-O(2)	2.083(6)
Sn(1)-O(2)#2	2.105(6)
Sn(1)-O(2)#3	2.105(6)
Sn(1)-O(1)	2.347(7)
Sn(1)-O(1)#1	2.347(7)
Sn(1)-O(1)#2	2.379(7)
Sn(1)-O(1)#3	2.379(7)
Sn(2)-O(2)	2.112(6)
Sn(2)-O(2)#2	2.112(6)
Sn(2)-O(2)#4	2.112(6)
Sn(2)-O(2)#5	2.112(6)
Sn(2)-O(1)	2.347(7)
Sn(2)-O(1)#2	2.347(7)
Sn(2)-O(1)#4	2.347(7)
Sn(2)-O(1)#5	2.347(7)
O(1)-O(2)	0.697(8)
O(2)#1-Sn(1)-O(2)	63.8(3)
O(2)#1-Sn(1)-O(2)#2	96.8(4)
O(2)-Sn(1)-O(2)#2	64.3(3)
O(2)#1-Sn(1)-O(2)#3	64.3(3)
O(2)-Sn(1)-O(2)#3	96.8(4)
O(2)#2-Sn(1)-O(2)#3	63.1(3)
O(2)#1-Sn(1)-O(1)	74.2(2)
O(2)-Sn(1)-O(1)	16.8(2)
O(2)#2-Sn(1)-O(1)	73.8(2)
O(2)#3-Sn(1)-O(1)	113.6(3)
O(2)#1-Sn(1)-O(1)#1	16.8(2)
O(2)-Sn(1)-O(1)#1	74.2(2)
O(2)#2-Sn(1)-O(1)#1	113.6(3)
O(2)#3-Sn(1)-O(1)#1	73.8(2)
O(1)-Sn(1)-O(1)#1	80.9(3)
O(2)#1-Sn(1)-O(1)#2	113.3(3)
O(2)-Sn(1)-O(1)#2	73.7(2)
O(2)#2-Sn(1)-O(1)#2	16.5(2)
O(2)#3-Sn(1)-O(1)#2	73.2(2)
O(1)-Sn(1)-O(1)#2	79.2(3)
O(1)#1-Sn(1)-O(1)#2	130.1(3)
O(2)#1-Sn(1)-O(1)#3	73.7(2)
O(2)-Sn(1)-O(1)#3	113.3(3)
O(2)#2-Sn(1)-O(1)#3	73.2(2)
O(2)#3-Sn(1)-O(1)#3	16.5(2)
O(1)-Sn(1)-O(1)#3	130.1(3)
O(1)#1-Sn(1)-O(1)#3	79.2(3)
O(1)#2-Sn(1)-O(1)#3	79.6(3)
O(2)-Sn(2)-O(2)#2	63.7(2)
O(2)-Sn(2)-O(2)#4	96.5(4)
O(2)#2-Sn(2)-O(2)#4	63.7(2)
O(2)-Sn(2)-O(2)#5	63.7(2)
O(2)#2-Sn(2)-O(2)#5	96.5(4)
O(2)#4-Sn(2)-O(2)#5	63.7(2)
O(2)-Sn(2)-O(1)	16.9(2)
O(2)#2-Sn(2)-O(1)	73.7(2)
O(2)#4-Sn(2)-O(1)	113.4(3)

O(2)#5-Sn(2)-O(1)	73.8(2)
O(2)-Sn(2)-O(1)#2	73.8(2)
O(2)#2-Sn(2)-O(1)#2	16.9(2)
O(2)#4-Sn(2)-O(1)#2	73.7(2)
O(2)#5-Sn(2)-O(1)#2	113.4(3)
O(1)-Sn(2)-O(1)#2	79.9(1)
O(2)-Sn(2)-O(1)#4	113.4(3)
O(2)#2-Sn(2)-O(1)#4	73.8(2)
O(2)#4-Sn(2)-O(1)#4	16.9(2)
O(2)#5-Sn(2)-O(1)#4	73.7(2)
O(1)-Sn(2)-O(1)#4	130.4(3)
O(1)#2-Sn(2)-O(1)#4	79.9(1)
O(2)-Sn(2)-O(1)#5	73.7(2)
O(2)#2-Sn(2)-O(1)#5	113.4(3)
O(2)#4-Sn(2)-O(1)#5	73.8(2)
O(2)#5-Sn(2)-O(1)#5	16.9(2)
O(1)-Sn(2)-O(1)#5	79.9(1)
O(1)#2-Sn(2)-O(1)#5	130.4(3)
O(1)#4-Sn(2)-O(1)#5	79.9(1)
Sn(1)-O(1)-Sn(2)	98.1(3)
Sn(1)-O(1)-Sn(1)#5	97.1(3)
Sn(2)-O(1)-Sn(1)#5	97.1(2)
O(2)-O(1)-H(1)	171.3
Sn(1)-O(1)-H(1)	116.3
Sn(2)-O(1)-H(1)	112.8
Sn(1)#5-O(1)-H(1)	129.8
O(1)-O(2)-Sn(1)	103.6(8)
O(1)-O(2)-Sn(1)#5	104.6(8)
Sn(1)-O(2)-Sn(1)#5	115.5(3)
O(1)-O(2)-Sn(2)	101.0(8)
Sn(1)-O(2)-Sn(2)	115.3(3)
Sn(1)#5-O(2)-Sn(2)	114.3(3)

Symmetry transformations used to generate equivalent atoms:
#1 x,y,-z+1 #2 y,-x+1,z #3 y,-x+1,-z+1
#4 -x+1,-y+1,z #5 -y+1,x,z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for Sn6O4(OH)4_II. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Sn(1)	6(1)	10(1)	11(1)	0	0	-2(1)
Sn(2)	10(1)	10(1)	5(1)	0	0	0
O(1)	9(2)	8(2)	11(2)	3(2)	3(2)	-2(2)
O(2)	6(2)	9(3)	9(2)	0(2)	2(2)	-1(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Sn6O4(OH)4_II.

	x	y	z	U(eq)
H(1)	6617	8383	2500	10(20)

Table 6. Hydrogen bonds for Sn6O4(OH)4_II [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(2)#6	1.12	1.81	2.875(11)	158.5

Symmetry transformations used to generate equivalent atoms:
#1 x,y,-z+1 #2 y,-x+1,z #3 y,-x+1,-z+1 #4 -x+1,-y+1,z
#5 -y+1,x,z #6 -y+3/2,-x+3/2,-z+1/2