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

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 = 7.8788(1) 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 / 20
Goodness-of-fit on F^2	1.263
Final R indices [I>2sigma(I)]	R1 = 0.0400, wR2 = 0.0841
R indices (all data)	R1 = 0.0401, wR2 = 0.0841
Extinction coefficient	0.0030(4)
Largest diff. peak and hole	3.874 and -3.319 e.A^-3

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

	x	y	z	U(eq)
Sn(1)	7930(1)	6233(1)	5000	9(1)
Sn(2)	5000	5000	2232(1)	8(1)
O(1)	5909(9)	7177(15)	3548(11)	74(4)

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

Sn(1)-O(1)	2.195(8)
Sn(1)-O(1)#1	2.195(8)
Sn(1)-O(1)#2	2.221(8)
Sn(1)-O(1)#3	2.221(8)
Sn(2)-O(1)#2	2.208(8)
Sn(2)-O(1)#4	2.208(8)
Sn(2)-O(1)#5	2.208(8)
Sn(2)-O(1)	2.208(8)
O(1)-Sn(1)-O(1)#1	73.6(5)
O(1)-Sn(1)-O(1)#2	73.1(4)
O(1)#1-Sn(1)-O(1)#2	114.7(7)
O(1)-Sn(1)-O(1)#3	114.7(7)
O(1)#1-Sn(1)-O(1)#3	73.1(4)
O(1)#2-Sn(1)-O(1)#3	72.7(4)
O(1)#2-Sn(2)-O(1)#4	73.1(3)
O(1)#2-Sn(2)-O(1)#5	114.6(7)
O(1)#4-Sn(2)-O(1)#5	73.1(3)
O(1)#2-Sn(2)-O(1)	73.1(3)
O(1)#4-Sn(2)-O(1)	114.6(7)
O(1)#5-Sn(2)-O(1)	73.1(3)
Sn(1)-O(1)-Sn(2)	107.2(4)
Sn(1)-O(1)-Sn(1)#5	106.7(4)
Sn(2)-O(1)-Sn(1)#5	106.3(4)

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_I. 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)	11(1)	11(1)	0	0	-2(1)
Sn(2)	10(1)	10(1)	5(1)	0	0	0
O(1)	25(3)	115(8)	82(6)	-86(6)	-37(4)	44(4)