Table 1. Crystal data and structure refinement for Pb6O4(OH)4_I.

Identification code	KP2002_0m_d
Empirical formula	H4 O8 Pb6
Formula weight	1375.17
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Tetragonal, P4/mnc
Unit cell dimensions	a = 7.9693(3) A c = 9.2741(3) A
Volume	589.00(5) A^3
Z, Calculated density	2, 7.754 Mg/m^3
Absorption coefficient	85.455 mm^-1
F(000)	1120
Crystal size	0.020 x 0.010 x 0.010 mm
Theta range for data collection	3.371 to 34.939 deg.
Limiting indices	-12<=h<=12, -12<=k<=12, -14<=l<=14
Reflections collected / unique	108784 / 689 [R(int) = 0.0993]
Completeness to theta = 25.242	100.0 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	689 / 0 / 20
Goodness-of-fit on F^2	1.090
Final R indices [I>2sigma(I)]	R1 = 0.0217, wR2 = 0.0421
R indices (all data)	R1 = 0.0237, wR2 = 0.0427
Extinction coefficient	0.00128(7)
Largest diff. peak and hole	4.435 and -4.070 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for Pb6O4(OH)4_I.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pb(1)	7999(1)	6336(1)	5000	8(1)
Pb(2)	5000	5000	2213(1)	7(1)
O(1)	5887(8)	7310(13)	3503(10)	72(4)

Table 3. Bond lengths [A] and angles [deg] for Pb6O4(OH)4_I.

Pb(1)-O(1)#1	2.315(8)
Pb(1)-O(1)	2.315(8)
Pb(1)-O(1)#2	2.317(7)
Pb(1)-O(1)#3	2.317(7)
Pb(2)-O(1)#2	2.307(7)
Pb(2)-O(1)#5	2.307(7)
Pb(2)-O(1)#6	2.307(7)
Pb(2)-O(1)	2.307(7)
O(1)#1-Pb(1)-O(1)	73.7(4)
O(1)#1-Pb(1)-O(1)#2	116.3(6)
O(1)-Pb(1)-O(1)#2	74.0(4)
O(1)#1-Pb(1)-O(1)#3	74.0(4)
O(1)-Pb(1)-O(1)#3	116.3(6)
O(1)#2-Pb(1)-O(1)#3	73.6(4)
O(1)#2-Pb(2)-O(1)#5	74.4(3)
O(1)#2-Pb(2)-O(1)#6	117.5(6)
O(1)#5-Pb(2)-O(1)#6	74.4(3)
O(1)#2-Pb(2)-O(1)	74.4(3)
O(1)#5-Pb(2)-O(1)	117.5(6)
O(1)#6-Pb(2)-O(1)	74.4(3)
Pb(2)-O(1)-Pb(1)	105.5(4)
Pb(2)-O(1)-Pb(1)#6	105.4(4)
Pb(1)-O(1)-Pb(1)#6	106.0(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+1 #5 -x+1,-y+1,z
#6 -y+1,x,z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for Pb6O4(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
Pb(1)	5(1)	9(1)	10(1)	0	0	-2(1)
Pb(2)	9(1)	9(1)	3(1)	0	0	0
O(1)	20(3)	113(7)	83(6)	-89(6)	-32(3)	39(4)