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

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 / 29
Goodness-of-fit on F^2	1.228
Final R indices [I>2sigma(I)]	R1 = 0.0147, wR2 = 0.0324
R indices (all data)	R1 = 0.0164, wR2 = 0.0327
Extinction coefficient	0.00142(7)
Largest diff. peak and hole	1.496 and -1.939 e.A^-3

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

	x	y	z	U(eq)
Pb(1)	8000(1)	6336(1)	5000	8(1)
Pb(2)	5000	5000	2213(1)	7(1)
O(1)	6001(8)	7614(8)	3286(7)	8(1)
O(2)	5766(7)	6975(8)	3742(7)	8(1)

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

Pb(1)-O(2)	2.188(6)
Pb(1)-O(2)#1	2.188(6)
Pb(1)-O(2)#2	2.199(6)
Pb(1)-O(2)#3	2.199(6)
Pb(1)-O(1)#2	2.468(6)
Pb(1)-O(1)#3	2.468(6)
Pb(1)-O(1)#1	2.470(6)
Pb(1)-O(1)	2.470(6)
Pb(2)-O(2)#2	2.205(6)
Pb(2)-O(2)#5	2.205(6)
Pb(2)-O(2)#6	2.205(6)
Pb(2)-O(2)	2.205(6)
Pb(2)-O(1)	2.443(6)
Pb(2)-O(1)#2	2.443(6)
Pb(2)-O(1)#5	2.443(6)
Pb(2)-O(1)#6	2.443(6)
O(1)-O(2)	0.689(7)
O(2)-Pb(1)-O(2)#1	64.4(3)
O(2)-Pb(1)-O(2)#2	65.9(3)
O(2)#1-Pb(1)-O(2)#2	99.1(4)
O(2)-Pb(1)-O(2)#3	99.1(4)
O(2)#1-Pb(1)-O(2)#3	65.9(3)
O(2)#2-Pb(1)-O(2)#3	64.1(3)
O(2)-Pb(1)-O(1)#2	74.4(2)
O(2)#1-Pb(1)-O(1)#2	114.7(3)
O(2)#2-Pb(1)-O(1)#2	15.6(2)
O(2)#3-Pb(1)-O(1)#2	73.8(2)
O(2)-Pb(1)-O(1)#3	114.7(3)
O(2)#1-Pb(1)-O(1)#3	74.4(2)
O(2)#2-Pb(1)-O(1)#3	73.8(2)
O(2)#3-Pb(1)-O(1)#3	15.6(2)
O(1)#2-Pb(1)-O(1)#3	80.2(3)
O(2)-Pb(1)-O(1)#1	73.9(2)
O(2)#1-Pb(1)-O(1)#1	15.5(2)
O(2)#2-Pb(1)-O(1)#1	114.6(3)
O(2)#3-Pb(1)-O(1)#1	74.5(2)
O(1)#2-Pb(1)-O(1)#1	130.2(3)
O(1)#3-Pb(1)-O(1)#1	79.4(3)
O(2)-Pb(1)-O(1)	15.5(2)
O(2)#1-Pb(1)-O(1)	73.9(2)
O(2)#2-Pb(1)-O(1)	74.5(2)
O(2)#3-Pb(1)-O(1)	114.6(3)
O(1)#2-Pb(1)-O(1)	79.4(3)
O(1)#3-Pb(1)-O(1)	130.2(3)
O(1)#1-Pb(1)-O(1)	80.1(3)
O(2)#2-Pb(2)-O(2)#5	65.6(2)
O(2)#2-Pb(2)-O(2)#6	99.9(4)
O(2)#5-Pb(2)-O(2)#6	65.6(2)
O(2)#2-Pb(2)-O(2)	65.6(2)
O(2)#5-Pb(2)-O(2)	99.9(4)
O(2)#6-Pb(2)-O(2)	65.6(2)
O(2)#2-Pb(2)-O(1)	75.0(2)
O(2)#5-Pb(2)-O(1)	115.9(3)
O(2)#6-Pb(2)-O(1)	74.6(2)

O(2)-Pb(2)-O(1)	16.0(2)
O(2)#2-Pb(2)-O(1)#2	16.0(2)
O(2)#5-Pb(2)-O(1)#2	75.0(2)
O(2)#6-Pb(2)-O(1)#2	115.9(3)
O(2)-Pb(2)-O(1)#2	74.6(2)
O(1)-Pb(2)-O(1)#2	80.5(1)
O(2)#2-Pb(2)-O(1)#5	74.6(2)
O(2)#5-Pb(2)-O(1)#5	16.0(2)
O(2)#6-Pb(2)-O(1)#5	75.0(2)
O(2)-Pb(2)-O(1)#5	115.9(3)
O(1)-Pb(2)-O(1)#5	131.9(3)
O(1)#2-Pb(2)-O(1)#5	80.5(1)
O(2)#2-Pb(2)-O(1)#6	115.9(3)
O(2)#5-Pb(2)-O(1)#6	74.6(2)
O(2)#6-Pb(2)-O(1)#6	16.0(2)
O(2)-Pb(2)-O(1)#6	75.0(2)
O(1)-Pb(2)-O(1)#6	80.5(1)
O(1)#2-Pb(2)-O(1)#6	131.9(3)
O(1)#5-Pb(2)-O(1)#6	80.5(1)
Pb(2)-O(1)-Pb(1)#6	97.0(2)
Pb(2)-O(1)-Pb(1)	97.0(2)
Pb(1)#6-O(1)-Pb(1)	97.1(2)
Pb(1)-O(2)-Pb(1)#6	115.0(3)
Pb(1)-O(2)-Pb(2)	113.7(3)
Pb(1)#6-O(2)-Pb(2)	113.3(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+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_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
Pb(1)	5(1)	9(1)	10(1)	0	0	-3(1)
Pb(2)	9(1)	9(1)	4(1)	0	0	0
O(1)	11(3)	7(2)	8(3)	4(2)	4(2)	-1(2)
O(2)	6(2)	10(3)	8(2)	-1(2)	-1(2)	0(2)