

Supporting Information

An unusual seven-connected lead borate constructed by different cluster building units of {B₆} and {Pb₆}

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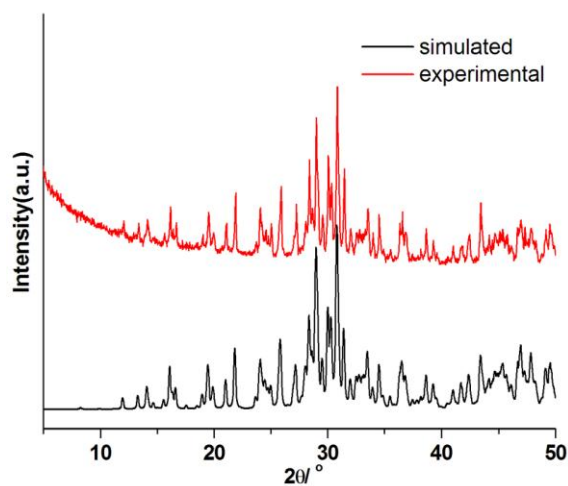


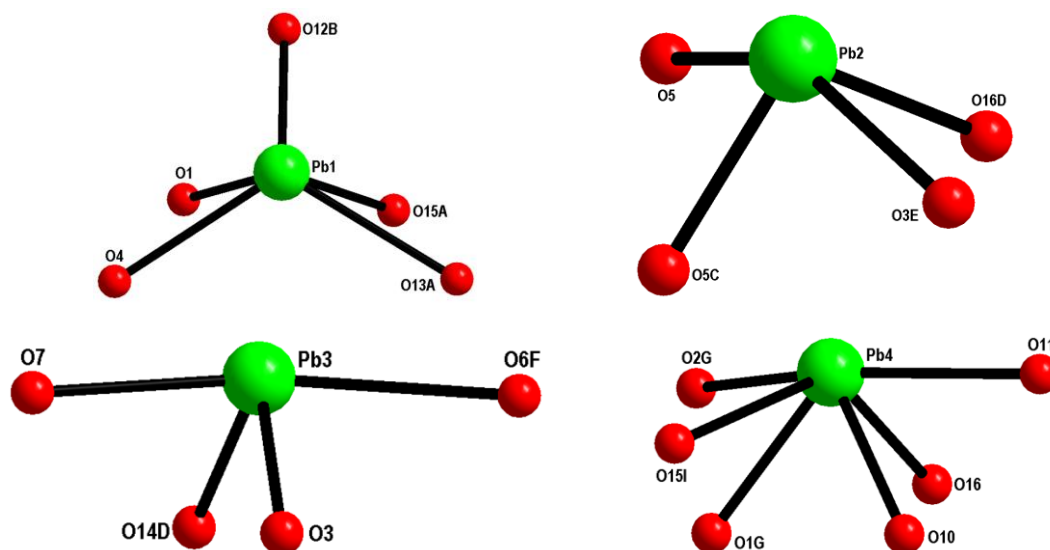
Figure S1. Simulated and experimental PXRD patterns of compound **1**.

Table S1. Selected Bond Lengths (Å) for Compound **1**.

Pb(1)-O(1)	2.292(12)	Pb(4)-O(15I)	2.833(15)	B(2)-O(6)	1.41(3)
Pb(1)-O(15A)	2.343(14)	Pb(5)-O(1B)	2.211(14)	B(3)-O(4)	1.45(3)
Pb(1)-O(12B)	2.347(13)	Pb(5)-O(10H)	2.406(12)	B(3)-O(7)	1.45(2)
Pb(1)-O(4)	2.733(12)	Pb(5)-O(12)	2.413(13)	B(3)-O(8)	1.50(3)
Pb(1)-O(13A)	2.822(16)	Pb(5)-O(16H)	2.695(14)	B(3)-O(6)	1.51(3)
Pb(2)-O(5C)	2.200(16)	Pb(5)-OW	2.72(3)	B(4)-O(11)	1.42(3)
Pb(2)-O(16D)	2.277(13)	Pb(5)-O(3B)	2.898(15)	B(4)-O(7)	1.49(2)

Pb(2)-O(3E)	2.407(13)	Pb(6)-O(12)	2.283(13)	B(4)-O(10)	1.49(2)
Pb(2)-O(5)	2.617(14)	Pb(6)-O(10H)	2.315(12)	B(4)-O(9)	1.51(2)
Pb(3)-O(3)	2.197(13)	Pb(6)-O(14)	2.404(16)	B(5)-O(8)	1.44(2)
Pb(3)-O(14D)	2.408(14)	Pb(6)-O(15F)	2.654(15)	B(5)-O(13)	1.46(3)
Pb(3)-O(7)	2.442(15)	Pb(6)-O(6H)	2.877(14)	B(5)-O(12)	1.50(2)
Pb(3)-O(6F)	2.751(15)	B(1)-O(4)	1.43(2)	B(5)-O(11)	1.51(2)
Pb(4)-O(10)	2.299(13)	B(1)-O(1)	1.48(2)	B(6)-O(14)	1.36(2)
Pb(4)-O(1G)	2.349(13)	B(1)-O(3)	1.49(3)	B(6)-O(13)	1.37(2)
Pb(4)-O(16)	2.396(14)	B(1)-O(2)	1.49(2)	B(6)-O(15)	1.39(2)
Pb(4)-O(11)	2.550(12)	B(2)-O(5)	1.35(3)		
Pb(4)-O(2G)	2.806(13)	B(2)-O(2)	1.37(2)		

^aSymmetry codes: (A) $-x + 4, -y + 1, -z + 1$; (B) $-x + 3, -y + 1, -z + 1$; (C) $-x + 4, -y, -z + 1$; (D) $-x + 7/2, y - 1/2, -z + 3/2$; (E) $-x + 3, -y, -z + 1$; (F) $x - 1, y, z$; (G) $x + 1/2, -y + 1/2, z + 1/2$; (H) $-x + 7/2, y + 1/2, -z + 3/2$; (I) $-x + 9/2, y - 1/2, -z + 3/2$.



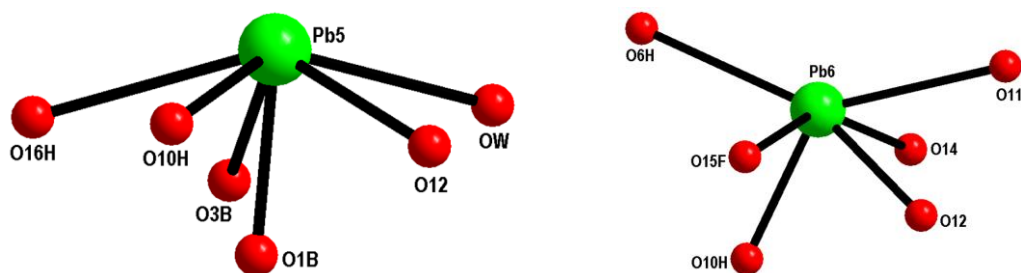


Figure S2. The coordination environments of Pb atoms in compounds **1**, showing the stereoactivity of the lone pair.

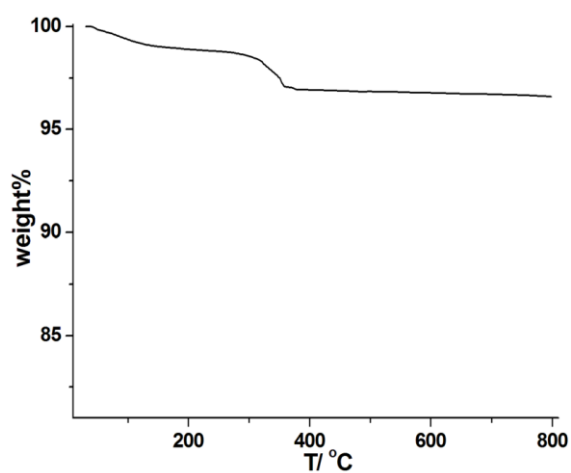


Figure S3. TG curve of **1**.

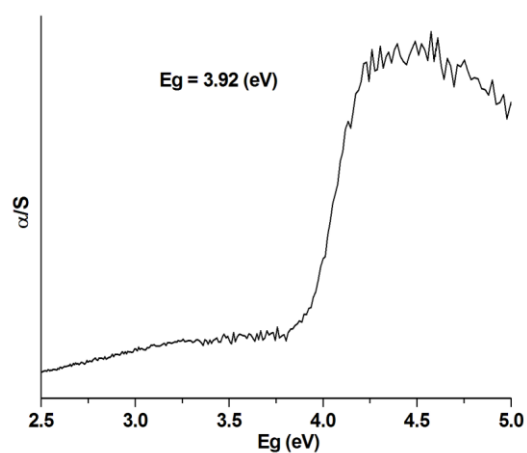


Figure S4. Optical diffuse reflectance spectra of **1**.

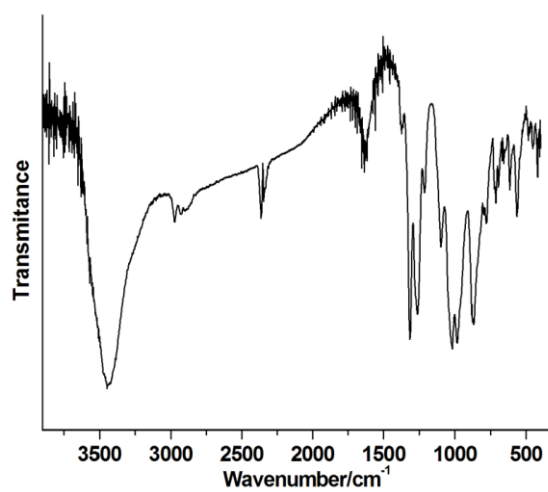


Figure S5. The IR spectra of **1**.