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A New Congruent-Melting Oxyborate, $Pb_4O(BO_3)_2$ with Optimally Aligned BO_3 Triangles Adopted Layered-type Arrangement

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Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Pb_4O(BO_3)_2$. U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atom	Wyckoff	x	y	z	U_{eq}	BVS
Pb(1)	8b	3822(1)	10492(1)	2267(1)	16(1)	1.966
Pb(2)	8b	3772(1)	6962(1)	2204(1)	14(1)	2.182
Pb(3)	8b	1995(1)	8734(1)	3899(1)	14(1)	1.957
Pb(4)	8b	4179(1)	8757(1)	5299(1)	16(1)	2.175
B(1)	8b	2547(12)	6207(11)	4920(20)	12(4)	2.886
B(2)	8b	5065(12)	6103(13)	4858(19)	16(4)	2.978
O(1)	8b	2583(8)	6207(6)	3460(12)	17(2)	1.744
O(2)	8b	3425(7)	8729(7)	3342(12)	16(2)	2.108
O(3)	8b	4453(8)	8811(8)	1028(13)	20(3)	1.781
O(4)	8b	2376(7)	7321(9)	5540(12)	22(2)	1.955
O(5)	8b	2362(7)	10136(9)	5571(11)	19(2)	2.008
O(6)	4a	5000	10000	4091(16)	29(4)	2.108
O(7)	8b	4694(8)	7087(9)	4269(12)	33(3)	2.176
O(8)	4a	5000	5000	4119(18)	24(4)	1.830

Figure S1. The coordination geometry around each Pb^{2+} ion and the direction of the lone pair.

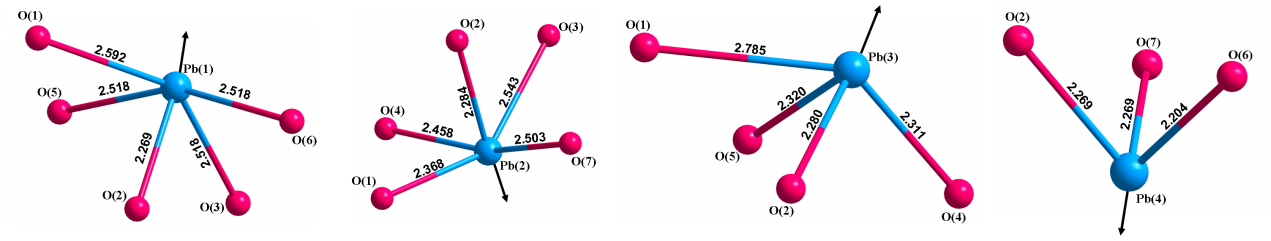

Figure S2. The IR spectrum of $Pb_4O(BO_3)_2$.