

## Supporting Information

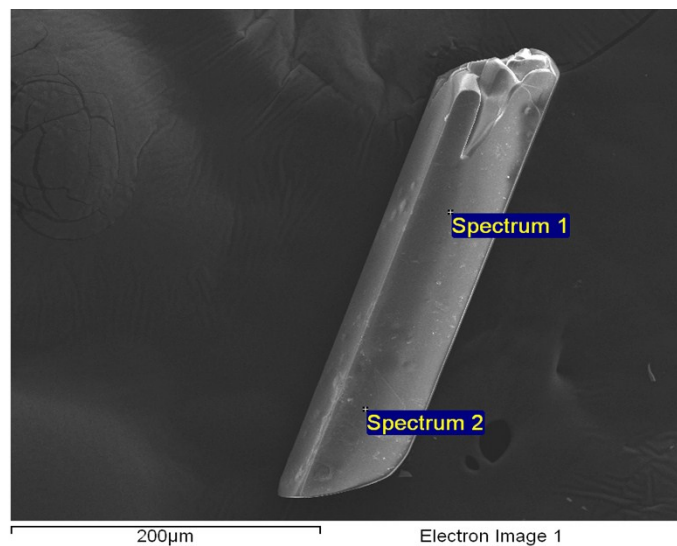
**High-Temperature, High-Pressure Hydrothermal Synthesis, Crystal Structure,  
Infrared and NMR Spectroscopy of a Barium Lead Borate with 2D Layer  
Structure: [Ba<sub>3</sub>Pb(H<sub>2</sub>O)][B<sub>11</sub>O<sub>19</sub>(OH)<sub>3</sub>]**

Yu-Chen Kuo<sup>a</sup>, Hsin-Kuan Liu,<sup>a</sup> Sue-Lein Wang,<sup>\*,b</sup> and Kwang-Hwa Lii<sup>\*,a,c</sup>

<sup>a</sup>Department of Chemistry, National Central University, Zhongli, Taiwan 320, R.O.C.

<sup>b</sup>Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan 300, R.O.C.

<sup>c</sup>Institute of Chemistry, Academia Sinica, Taipei, Taiwan 115, R.O.C.



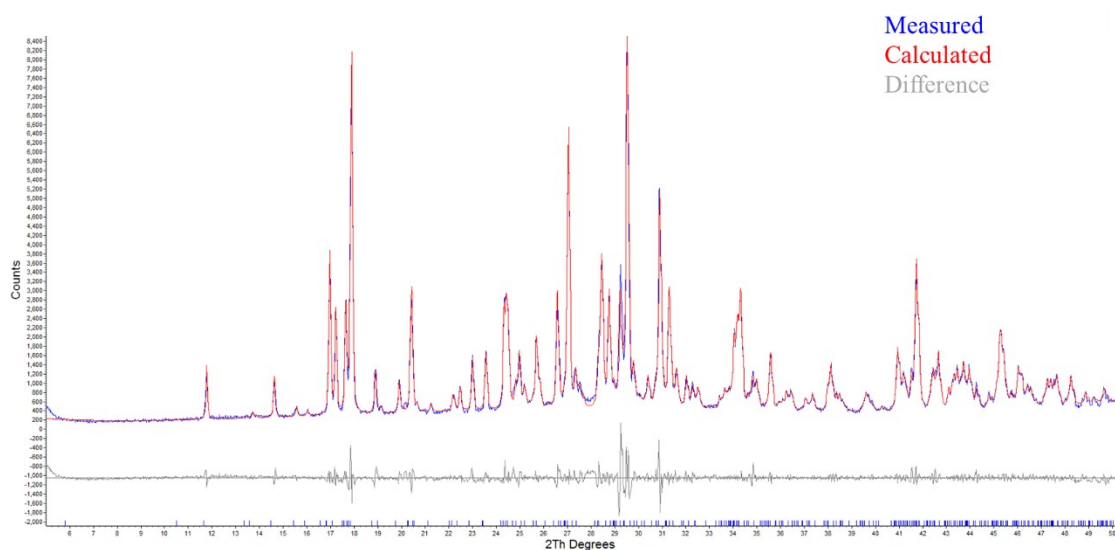
Processing option: Oxygen by stoichiometry (Normalised)  
LB-01

Spectrum	In stats.	B	Ba	Pb	O
Spectrum1	Yes	30.36	9.24	2.80	57.59
Spectrum2	Yes	22.59	13.56	8.21	55.65
Mean		26.47	11.40	5.51	56.62
Std. deviation		5.50	3.05	3.82	1.37
Mas.		30.36	13.56	8.21	57.59
Min		22.59	9.24	2.80	55.65

All results in atomic %

**Figure S1.** Results of EDS analysis on a crystal of  $[\text{Ba}_3\text{Pb}(\text{H}_2\text{O})][\text{B}_{11}\text{O}_{19}(\text{OH})_3]$ .

	Value		Use	Value	Code	Error
GOF	2.05	Use Phase	<input checked="" type="checkbox"/>			
Resp	3.29	Le Bail	<input type="checkbox"/>			
Rwp	6.77	Delete hkls on Refinement	<input checked="" type="checkbox"/>			
Rp	4.59	LP Search	<input type="checkbox"/>	0.4		
Rexp-dash	5.44	Spacegroup		P21/n		
Rwp-dash	11.18	a (Å)		6.6763254	Refine	0.0004093
Rp-dash	8.52	b (Å)		30.4410438	Refine	0.0014908
Weighted Durbin Watson	0.78	c (Å)		8.7765892	Refine	0.0004553
		beta		90.91868	Refine	0.00353863



**Figure S2.** Pawley fit of the powder diffraction data to the structure of  $[\text{Ba}_3\text{Pb}(\text{H}_2\text{O})][\text{B}_{11}\text{O}_{19}(\text{OH})_3]$ .