Electronic Supporting Information

Crystal Structure of $Li_2B_3PO_8$ with 2D-Linkage of BO_3, BO_4 and PO_4 Groups

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Table S1. Crystal data and refinement results for $Li_2B_3PO_8$.

Chemical formula	$Li_2B_3PO_8$	
Formula weight, M_r	205.28 g·mol^{-1}	
Temperature, T	293(2) K	
Crystal system	Triclinic	
Space group	$P\bar{1}$ (No.2)	
Unit cell dimensions	a = 8.6965(3) Å	α = 90.8057(14) °
	b = 10.7354(5) Å	β = 90.6311(12) °
	c = 12.8282(5) Å	γ = 90.0940(13) °
Unit cell volume, V	1197.45(8) Å^3	
Z	8	
Calculated density, D_{cal}	2.277 Mg·m^{-3}	
Radiation wavelength, λ	0.71075 Å (Mo$K\alpha$)	
Crystal form, color	Colorless	
Absorption correction	Numerical	
Absorption coefficient, μ	0.464 mm^{-1}	
Crystal size	0.146×0.105×0.070 mm^3	
Limiting indices	$-11 \le h \le 10$	
	$-13 \le k \le 13$	
	$-16 \le l \le 16$	
F_{000}	800	
θ range for data collection	3.01°–27.49°	
Reflections collected / unique	5417 / 4094	
R_{int}	0.0313	
Data / restraints / parameters	5417 / 0 / 505	
Weight parameters, a, b	0.0256, 3.1989	
Goodness-of-fit on F^2, S	1.100	
$R1$, $wR2$ ($I > 2\sigma(I)$)	0.0396, 0.0891	
$R1$, $wR2$ (all data)	0.0599, 0.1033	
Largest diff. peak and hole, $\Delta\rho$	0.491, −0.516 e·Å^{-3}	

$R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. $wR2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma(wF_o^2)^2]^{1/2}$, $w = 1/[\sigma^2(F_o^2)+(aP)^2+bP]$, where F_o is the observed structure factor, F_c is the calculated structure factor, σ is the standard deviation of F_c2, and $P = (F_o^2+2F_c2)/3$. $S = [\Sigma w(F_o^2-F_c^2)^2/(n-p)]^{1/2}$, where n is the number of reflections and p is the total number of parameters refined.

Table S2. Atomic coordinates and isotropic and equivalent isotropic displacement parameter (U_{eq}) for $Li_2B_3PO_8$.

Atom	Site	*x*	*y*	*z*	U_{eq}* / Å^2
Li1	2*i*	0.1194(7)	0.3435(6)	0.7149(5)	0.0269(13)
Li2	2*i*	0.1349(7)	0.7728(5)	0.2632(5)	0.0229(12)
Li3	2*i*	0.2177(7)	0.2781(5)	0.0384(5)	0.0248(13)
Li4	2*i*	0.2550(7)	0.5441(5)	0.3297(5)	0.0256(13)
Li5	2*i*	0.2578(7)	0.0611(5)	0.8284(5)	0.0253(13)
Li6	2*i*	0.3636(6)	0.5413(5)	0.0092(4)	0.0191(11)
Li7	2*i*	0.4378(9)	0.0430(6)	0.4145(6)	0.0411(18)
Li8	2*i*	0.7620(7)	0.1693(5)	0.3954(5)	0.0267(13)
B1	2*i*	0.2584(5)	0.9615(4)	0.2316(4)	0.0108(6)
B2	2*i*	0.1188(4)	0.1104(3)	0.4252(3)	0.0129(7)
B3	2*i*	0.1895(4)	0.0114(3)	0.1454(3)	0.0132(7)
B4	2*i*	0.1998(4)	0.5544(3)	0.6125(3)	0.0142(7)
B5	2*i*	0.3018(4)	0.2599(3)	0.3506(3)	0.0134(7)
B6	2*i*	0.3936(4)	0.3953(3)	0.6465(3)	0.0131(7)
B7	2*i*	0.4455(4)	0.0863(3)	0.1207(3)	0.0126(7)
B8	2*i*	0.5442(4)	0.3815(3)	0.3393(3)	0.0138(7)
B9	2*i*	0.5910(4)	0.1150(3)	0.7927(3)	0.0135(7)
B10	2*i*	0.6894(4)	0.1961(3)	0.0760(3)	0.0137(7)
B11	2*i*	0.9067(4)	0.3404(3)	0.0575(3)	0.0138(7)
B12	2*i*	0.9459(4)	0.1200(3)	0.1009(3)	0.0142(7)
P1	2*i*	0.07737(9)	0.52997(7)	0.12829(6)	0.01285(17)
P2	2*i*	0.09892(9)	0.06616(7)	0.63710(6)	0.01323(17)
P3	2*i*	0.59107(9)	0.20738(7)	0.59192(6)	0.01129(16)
P4	2*i*	0.59190(9)	0.69182(7)	0.14312(6)	0.01225(17)
O1	2*i*	0.0035(2)	0.20989(19)	0.41305(18)	0.0173(5)
O2	2*i*	0.0035(2)	0.2347(2)	0.09068(18)	0.0172(5)
O3	2*i*	0.0345(2)	0.0188(2)	0.12575(18)	0.0171(5)
O4	2*i*	0.0416(2)	0.6339(2)	0.04828(17)	0.0171(5)
O5	2*i*	0.0474(2)	0.5746(2)	0.59950(19)	0.0196(5)
O6	2*i*	0.0622(2)	0.9913(2)	0.38834(18)	0.0173(5)
O7	2*i*	0.0688(3)	0.1807(2)	0.70236(19)	0.0229(5)
O8	2*i*	0.0690(2)	0.5546(2)	0.87040(17)	0.0166(5)
O9	2*i*	0.0853(2)	0.5941(2)	0.23411(17)	0.0170(5)
O10	2*i*	0.1744(3)	0.1019(2)	0.53217(18)	0.0214(5)
O11	2*i*	0.1994(2)	0.35617(19)	0.36482(18)	0.0167(5)

O12	2*i*	0.2173(2)	0.4567(2)	0.09794(18)	0.0173(5)
O13	2*i*	0.2449(2)	0.90717(19)	0.18980(17)	0.0141(4)
O14	2*i*	0.2486(2)	0.43693(19)	0.59977(17)	0.0149(4)
O15	2*i*	0.2600(2)	0.14049(19)	0.36507(17)	0.0145(4)
O16	2*i*	0.2673(2)	0.7189(2)	0.38041(17)	0.0168(5)
O17	2*i*	0.2883(2)	0.2233(2)	0.90071(17)	0.0177(5)
O18	2*i*	0.2885(2)	0.10564(19)	0.11519(17)	0.0162(5)
O19	2*i*	0.3444(2)	0.3478(2)	0.74722(17)	0.0185(5)
O20	2*i*	0.4371(2)	0.76109(19)	0.16470(17)	0.0154(5)
O21	2*i*	0.4502(2)	0.28156(19)	0.32196(18)	0.0162(5)
O22	2*i*	0.4518(2)	0.29727(19)	0.57872(17)	0.0159(5)
O23	2*i*	0.4941(2)	0.50111(19)	0.34115(17)	0.0156(5)
O24	2*i*	0.4954(2)	0.0189(2)	0.83939(17)	0.0157(5)
O25	2*i*	0.5336(2)	0.1806(2)	0.08336(18)	0.0173(5)
O26	2*i*	0.5529(2)	0.11031(19)	0.67929(17)	0.0153(5)
O27	2*i*	0.5538(3)	0.5799(2)	0.07765(18)	0.0204(5)
O28	2*i*	0.5978(2)	0.1265(2)	0.49453(17)	0.0160(5)
O29	2*i*	0.6991(2)	0.35095(19)	0.35728(18)	0.0173(5)
O30	2*i*	0.7430(2)	0.31136(19)	0.05801(18)	0.0166(5)
O31	2*i*	0.7890(2)	0.09640(19)	0.08840(18)	0.0157(5)
O32	2*i*	0.7960(3)	0.0252(2)	0.30972(18)	0.0190(5)

* $U_{\mathrm{eq}} = (\sum_i \sum_j U_{ij}\, a_i^* a_j^*\, \boldsymbol{a}_i \cdot \boldsymbol{a}_j)/3$

Table S3. Anisotropic displacement parameters (U_{ij} / Å) for $Li_2B_3PO_8$.

Atom	Site	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Li1	2*i*	0.019(3)	0.022(3)	0.040(4)	−0.005(3)	0.007(3)	−0.006(2)
Li2	2*i*	0.019(3)	0.018(3)	0.031(3)	−0.001(2)	−0.001(2)	−0.004(2)
Li3	2*i*	0.023(3)	0.023(3)	0.029(3)	−0.002(2)	0.011(2)	−0.003(2)
Li4	2*i*	0.025(3)	0.015(3)	0.036(4)	0.001(2)	−0.008(3)	0.002(2)
Li5	2*i*	0.030(3)	0.019(3)	0.026(3)	0.001(2)	−0.005(2)	−0.007(2)
Li6	2*i*	0.010(2)	0.021(3)	0.026(3)	−0.003(2)	0.001(2)	0.000(2)
Li7	2*i*	0.046(4)	0.026(3)	0.050(4)	−0.009(3)	−0.031(4)	0.009(3)
Li8	2*i*	0.029(3)	0.018(3)	0.034(3)	0.000(2)	0.009(3)	0.002(2)
B1	2*i*	0.0145(17)	0.0151(17)	0.0178(18)	−0.0011(14)	−0.0011(13)	0.0006(14)
B2	2*i*	0.0105(16)	0.0108(15)	0.0175(17)	−0.0004(13)	0.0045(13)	−0.0014(13)
B3	2*i*	0.0122(16)	0.0115(15)	0.0158(17)	−0.0001(13)	0.0037(13)	−0.0030(13)
B4	2*i*	0.0116(16)	0.0152(17)	0.0160(17)	0.0023(13)	0.0013(13)	−0.0038(13)
B5	2*i*	0.0117(16)	0.0133(16)	0.0151(17)	0.0004(13)	−0.0011(13)	0.0020(13)
B6	2*i*	0.0128(16)	0.0092(15)	0.0173(17)	−0.0001(13)	−0.0009(13)	−0.0003(13)
B7	2*i*	0.0121(16)	0.0125(16)	0.0130(17)	−0.0014(13)	0.0005(13)	−0.0019(13)
B8	2*i*	0.0116(16)	0.0145(16)	0.0155(17)	0.0015(13)	0.0011(13)	0.0011(13)
B9	2*i*	0.0116(16)	0.0118(16)	0.0173(18)	0.0012(13)	0.0022(13)	−0.0008(13)
B10	2*i*	0.0157(17)	0.0136(16)	0.0118(17)	0.0032(13)	−0.0020(13)	−0.0019(13)
B11	2*i*	0.0108(16)	0.0080(15)	0.0226(19)	0.0031(13)	−0.0010(13)	−0.0039(12)
B12	2*i*	0.0158(17)	0.0141(16)	0.0127(17)	0.0018(13)	−0.0006(13)	−0.0011(13)
P1	2*i*	0.0124(4)	0.0108(4)	0.0153(4)	−0.0014(3)	0.0002(3)	−0.0011(3)
P2	2*i*	0.0120(4)	0.0113(4)	0.0163(4)	−0.0015(3)	0.0004(3)	−0.0020(3)
P3	2*i*	0.0112(4)	0.0085(3)	0.0142(4)	−0.0006(3)	0.0000(3)	0.0003(3)
P4	2*i*	0.0117(4)	0.0111(4)	0.0139(4)	−0.0014(3)	0.0005(3)	0.0002(3)
O1	2*i*	0.0132(11)	0.0107(10)	0.0281(13)	0.0015(9)	0.0033(9)	−0.0005(8)
O2	2*i*	0.0101(10)	0.0123(10)	0.0292(13)	0.0042(9)	−0.0025(9)	0.0007(8)
O3	2*i*	0.0085(10)	0.0143(11)	0.0285(13)	0.0055(9)	−0.0019(9)	0.0006(8)
O4	2*i*	0.0168(11)	0.0151(11)	0.0196(12)	0.0010(9)	0.0046(9)	0.0006(9)
O5	2*i*	0.0124(11)	0.0111(10)	0.0354(14)	0.0002(10)	−0.0029(10)	0.0022(9)
O6	2*i*	0.0121(11)	0.0114(10)	0.0283(13)	−0.0019(9)	−0.0018(9)	−0.0015(8)
O7	2*i*	0.0199(12)	0.0177(12)	0.0308(14)	−0.0091(10)	0.0039(10)	−0.0043(9)
O8	2*i*	0.0132(11)	0.0138(11)	0.0230(12)	−0.0020(9)	0.0038(9)	−0.0025(9)
O9	2*i*	0.0180(11)	0.0157(11)	0.0172(11)	−0.0016(9)	0.0012(9)	−0.0024(9)
O10	2*i*	0.0161(12)	0.0280(13)	0.0200(12)	0.0032(10)	−0.0021(9)	−0.0062(10)
O11	2*i*	0.0114(10)	0.0111(10)	0.0278(13)	0.0016(9)	0.0017(9)	−0.0004(8)
O12	2*i*	0.0136(11)	0.0146(11)	0.0237(12)	−0.0016(9)	0.0032(9)	−0.0004(9)

O13	2*i*	0.0114(10)	0.0097(10)	0.0214(12)	0.0037(8)	0.0014(8)	0.0000(8)
O14	2*i*	0.0134(11)	0.0113(10)	0.0200(12)	−0.0002(9)	−0.0032(9)	0.0006(8)
O15	2*i*	0.0109(10)	0.0097(10)	0.0230(12)	0.0006(9)	0.0052(9)	−0.0014(8)
O16	2*i*	0.0141(11)	0.0142(11)	0.0221(12)	−0.0011(9)	−0.0003(9)	−0.0022(9)
O17	2*i*	0.0164(11)	0.0161(11)	0.0206(12)	0.0000(9)	0.0042(9)	−0.0022(9)
O18	2*i*	0.0121(11)	0.0127(10)	0.0239(12)	0.0063(9)	0.0005(9)	0.0009(8)
O19	2*i*	0.0154(11)	0.0220(12)	0.0181(12)	0.0031(9)	−0.0004(9)	−0.0012(9)
O20	2*i*	0.0118(10)	0.0129(10)	0.0213(12)	−0.0018(9)	0.0022(9)	−0.0003(8)
O21	2*i*	0.0121(10)	0.0115(10)	0.0252(12)	−0.0014(9)	0.0048(9)	−0.0014(8)
O22	2*i*	0.0154(11)	0.0125(10)	0.0197(12)	−0.0019(9)	−0.0024(9)	0.0036(9)
O23	2*i*	0.0108(10)	0.0104(10)	0.0256(12)	0.0000(9)	−0.0013(9)	0.0012(8)
O24	2*i*	0.0103(10)	0.0156(11)	0.0214(12)	0.0038(9)	0.0012(8)	−0.0011(8)
O25	2*i*	0.0108(10)	0.0154(11)	0.0258(12)	0.0065(9)	0.0005(9)	0.0001(9)
O26	2*i*	0.0193(11)	0.0107(10)	0.0159(11)	0.0006(8)	−0.0022(9)	−0.0005(9)
O27	2*i*	0.0181(12)	0.0172(11)	0.0256(13)	−0.0097(10)	−0.0019(9)	0.0010(9)
O28	2*i*	0.0167(11)	0.0146(11)	0.0166(11)	−0.0034(9)	0.0010(9)	−0.0004(9)
O29	2*i*	0.0107(10)	0.0100(10)	0.0314(13)	0.0010(9)	0.0016(9)	0.0005(8)
O30	2*i*	0.0135(11)	0.0109(10)	0.0255(12)	0.0032(9)	−0.0014(9)	−0.0004(8)
O31	2*i*	0.0081(10)	0.0124(10)	0.0269(12)	0.0046(9)	0.0006(9)	0.0012(8)
O32	2*i*	0.0188(12)	0.0180(11)	0.0202(12)	0.0010(9)	−0.0033(9)	−0.0008(9)

Table S4. Selected bond lengths and bond valence sums (V_i) for $Li_2B_3PO_8$.

Li1–O7	1.806(6)	Li2–O7^{i}	1.896(6)
Li1–O19	1.995(6)	Li2–O16	1.978(6)
Li1–O9^{i}	2.016(6)	Li2–O13	1.984(6)
Li1–O14	2.127(7)	Li2–O9	1.995(6)
V_{Li1}	1.03	V_{Li2}	1.05
Li3–O17^{ii}	1.959(6)	Li4–O16	1.980(6)
Li3–O2	2.042(6)	Li4–O9	1.987(6)
Li3–O12	2.054(6)	Li4–O11	2.129(6)
Li3–O18	2.195(6)	Li4–O23	2.135(6)
V_{Li3}	0.82	V_{Li4}	0.82
Li5–O17	1.978(6)	Li6–O27^{iv}	1.852(6)
Li5–O32^{iii}	2.037(6)	Li6–O27	1.906(6)
Li5–O31^{iii}	2.055(6)	Li6–O12	1.949(6)
Li5–O24	2.119(7)	Li6–O30^{iv}	2.032(6)
V_{Li5}	0.84	V_{Li6}	1.14
Li7–O28	1.933(7)	Li8–O32	1.910(6)
Li7–O15	1.972(7)	Li8–O28	1.980(6)
Li7–O26^{iii}	2.027(7)	Li8–O29	2.089(6)
Li7–O28^{iii}	2.200(8)	Li8–O1^{v}	2.154(7)
V_{Li7}	0.89	V_{Li8}	0.89
B1–O1	1.346(4)	B2–O6^{vi}	1.440(4)
B1–O5^{i}	1.347(4)	B2–O10	1.454(4)
B1–O11	1.403(4)	B2–O1	1.475(4)
V_{B1}	3.05	B2–O15	1.495(4)
		V_{B2}	3.10
B3–O13^{vi}	1.350(4)	B4–O14	1.339(4)
B3–O3	1.371(4)	B4–O5	1.352(4)
B3–O18	1.389(4)	B4–O29^{vii}	1.391(4)
V_{B3}	3.01	V_{B4}	3.09

B5–O15	1.347(4)	B6–O22	1.452(4)
B5–O21	1.366(4)	B6–O14	1.464(4)
B5–O11	1.377(4)	B6–O19	1.464(4)
V_{B5}	3.06	B6–O23^{vii}	1.484(4)
		V_{B6}	3.10
B7–O24^{iii}	1.348(4)	B8–O23	1.357(4)
B7–O25	1.364(4)	B8–O21	1.362(4)
B7–O18	1.382(4)	B8–O29	1.404(4)
V_{B7}	3.06	V_{B8}	2.98
B9–O20^{vii}	1.453(4)	B10–O30	1.346(4)
B9–O24	1.463(4)	B10–O25	1.369(4)
B9–O13^{vi}	1.463(4)	B10–O31	1.387(4)
B9–O26	1.488(4)	V_{B10}	3.03
V_{B9}	3.09		
B11–O30	1.457(4)	B12–O2^{v}	1.338(4)
B11–O8^{vii}	1.461(4)	B12–O3^{v}	1.372(4)
B11–O4^{iv}	1.463(4)	B12–O31	1.394(4)
B11–O2^{v}	1.479(4)	V_{B12}	3.03
V_{B11}	3.10		
P1–O12	1.502(2)	P2–O7	1.503(2)
P1–O9	1.514(2)	P2–O32^{iii}	1.506(2)
P1–O4	1.556(2)	P2–O10	1.557(2)
P1–O8^{i}	1.563(2)	P2–O6^{i}	1.560(2)
V_{P1}	5.02	V_{P2}	5.05
P3–O16^{vii}	1.499(2)	P4–O27	1.491(2)
P3–O28	1.513(2)	P4–O17^{vii}	1.502(2)
P3–O22	1.559(2)	P4–O20	1.565(2)
P3–O26	1.579(2)	P4–O19^{vii}	1.571(2)
V_{P3}	4.98	V_{P4}	5.05

Symmetry codes: (i) $-x$, $-y+1$, $-z+1$; (ii) x, y, $z-1$; (iii) $-x+1$, $-y$, $-z+1$;(iv) $-x+1$, $-y+1$, $-z$; (v)$x+1$, y, z; (vi) x, $y-1$, z; (vii) $-x+1$, $-y+1$, $-z+1$.

Bond valence parameters: Li^{+}: 1.466 Å, B^{3+}: 1.371 Å, P^{5+}: 1.617 Å.

Table S5. Borophosphates reported in the literatures since 2007.

compounds	B:P	M/T	
$(NH_4)[B_3PO_6(OH)_3]\cdot 0.5H_2O$	3:1	M	Acta Cryst. E 63, i185 (2007)
$Na_3B_6PO_{13}$	1:2	M	J. Solid State Chem., 180, 233-239 (2007)
$Na_3BP_2O_8$	1:2	T	J. Solid State Chem., 180, 233-239 (2007)
$(C_4H_{12}N_2)_3(Fe_6(H_2O)_4)(B_6P_{12}O_{50}(OH)_2)(H_2O)_2$	1:2	T	Sci. Technol. Adv. Mat., 8, 399-405 (2007)
$Ca_{0.5}(Ni(H_2O)_2)(BP_2O_8)(H_2O)$	1:2	T	Z. Krist.-New Cyst. St., 222, 1-2 (2007)
$CsSc(B_2P_3O_{11}(OH)_3)$	2:3	M	Inorg. Chem., 46, 7503-7508 (2007)
$(NH_4)(B_3PO_6(OH)_3)(H_2O)_{0.5}$	3:1	M	Acta Cryst. E., 63, i185 (2007)
$Zn[BPO_4(OH)_2]$	1:1	T	Chem.-Eur. J., 14, 1757-1761 (2008)
$Na_8[Cr_4B_{12}P_8O_{44}(OH)_4][P_2O_7]\ (H_2O)_n$	6:5	M	Chem.-Eur. J., 14, 7212-7217 (2008)
$Ca_{0.5}Fe(H_2O)_2[BP_2O_8]\ H_2O$	1:2	T	Z. Krist.-New Cyst. St., 223, 9-10 (2008)
$KV[BP_2O_8(OH)]$	1:2	T	Z. Krist.-New Cyst. St., 223, 323-324 (2008)
$LiCo(H_2O)_2[BP_2O_8]\ H_2O$	1:2	T	Z. Krist.-New Cyst. St., 223, 333-334 (2008)
$CaFe[BP_2O_8(OH)_3]$	1:2	T	Z. Krist.-New Cyst. St., 223, 335-336 (2008)
$BaFe(BP_2O_8(OH))$	1:2	T	Z. Krist.-New Cyst. St., 223, 337-338 (2008)
$BaCo[BP_2O_8(OH)]$	1:2	T	Z. Krist.-New Cyst. St., 223, 339-340 (2008)
$M BPO_4(OH)_2$ M=Mg, Ni	1:1	T	J. Solid State Chem., 181, 1110-1115 (2008)
$LiMg(H_2O)_2[BP_2O_8]H_2O$	1:2	T	Acta Cryst. E, 64, I39-U126 (2008)
$Na_3Pb(II)[B(O_3POH)_4]$	1:1	T	Inorg. Chem., 47, 10193-10195 (2008)
$Na_5(NH_4)Mn_3[B_9P_6O_{33}(OH)_3]\ (H_2O)_{1.5}$	3:2	M	Acta Cryst. E, 64, I82-U28 (2008)
$Na_2(VB_3P_2O_{12}(OH))(H_2O)_{2.92}$	3:2	M	Chem. Mater., 20, 4900-4905 (2008)
$(CH_3NH_3)_4[N(CH_3)_4](CoPO_4)_4[B_5O_6(OH)_4]$	5:4	M	Dalton Trans., 5287-5289 (2009)
$(C_4N_3H_{16})(C_4N_3H_{15})_{0.5}[Fe_2B_4P_7O_26(OH)_4]$	4:7	T	J. Mater. Chem., 19, 4523-4528 (2009)
$CaCo(H_2O)[BP_2O_8(OH)]\cdot H_2O$	1:2	T	Z. Anorg. Allg. Chem., 635, 614-617 (2009)
$SrFe[BP_2O_8(OH)_2]$	1:2	T	Z. Anorg. Allg. Chem., 635, 1153-1156 (2009)
$Cs_2Co_3(H_2O)_2[B_4P_6O_{24}(OH)_2]$	2:3	T	Z. Krist.-New Cyst. St., 224, 1-2 (2009)
$(Co_{0.6}Mn_{0.4})_2(H_2O)[BP_3O_9(OH)_4]$	1:3	T	Z. Krist.-New Cyst. St., 224, 371-372 (2009)
$LiCu_2BP_2O_8(OH)_2$	1:2	T	Acta Cryst. E, 65, i40 (2009)
$LiNi(H_2O)_2[BP_2O_8]H_2O$	1:2	T	Acta Cryst. E, 65, i42 (2009)
$KMBP_2O_8$ (M = Sr, Ba)	1:2	T	Inorg. Chem., 48, 6623-6629 (2009)
$KNi_5[P_6B_6O_{23}(OH)_{13}]$	1:1	T	Acta Cryst. C, 65, i94-i98 (2009)

$Na(H_2O)Mn(H_2O)_2(BP_2O_8)$	1:2	T	Cystallogr. Rrep., 54(1), 13-18 (2009)
$(NH_4)_4[H_2B_2P_4O_{16}]$	1:2	T	Dalton Trans., 39, 1713-1715 (2010)
$[Na_{11}K_5Cr_8B_4P_{12}O_{70}H_8]^{15-}$	1:3	T	Dalton Trans., 39, 7262-7265 (2010)
$(NH_4)_7Co_4(H_2O)[B_2P_4O_{15}(OH)_2]_2[H_2PO_4][HPO_4]$	2:5	T	Dalton Trans., 39, 10571-10573 (2010)
$NaSc[BP_2O_6(OH)_3][(HO)PO_3]$	1:3	T	Z. Anorg. Allg. Chem., 636, 19-22 (2010)
$Pb_4\{Co_2[B(OH)_2P_2O_8](PO_4)_2\}Cl$	1:4	T	Z. Anorg. Allg. Chem., 636, 1454-1460 (2010)
$Li_3V_2[BP_3O_{12}(OH)][HPO_4]$	1:4	T	Z. Krist.-New Cyst. St., 225, 3-4 (2010)
$(Ga_{0.71}B_{0.29})PO_4$	0.29:1	T	Acta Cryst. E, 66, i4 (2010)
$Sr_{10}P_{5.50}B_{1.50}O_{26}$	1.5:5.5	T,L	J. Solid State Chem., 183, 658-661 (2010)
$M_2B(PO_4)_3$ *M*=Fe, In	1:3	M	Acta Cryst. E., 66, i63-i63 (2010)
			J. Solid State Chem., 183, 1108-1113 (2010)
$Fe_2[BP_3O_{12}]$	1:3	M	Acta Cryst. E, 66, I63-U103 (2010)
K(Fe,Al)$[BP_2O_8(OH)]$,	1:2	T	Cystallogr. Rrep., 55, 760-768 (2010)
Rb(Al,Fe)$[BP_2O_8(OH)]$	1:2	T	
M(II)$(H_2O)_2[B_2P_2O_8(OH)_2]H_2O$ (*M*(II) = Fe, Co, Ni)	1:1	T	Inorg. Chim. Acta, 363, 4299-4306 (2010)
$Cs_2Cr_3(BP_4O_{14})(P_4O_{13})$	1:8	T	Inorg. Chem., 49, 2550-2556 (2010)
$CsFe(BP_3O_{11})$	1:3	T	Inorg. Chem., 49, 2550-2556 (2010)
$Zn_3(BO_3)(PO_4)$	1:1	M	Acta Cryst. E, 67, i3 (2011)
$(NH_4)_6[Mn_3B_6P_9O_{36}(OH)_3]\cdot 4H_2O$	2:3	T	Dalton T., 40, 2549-2554 (2011)
$Ti[BP_2O_7(OH)_3]$	1:2	T	Crystengcomm, 13, 7185-7188 (2011)
$Na_6H_2Co_3B_2P_5O_{22}Cl$	2:5	T	Inorg. Chem., 50, 1073-1078 (2011)
$K_5H_2Mn_2B_2P_5O_{21}$	2:5	T	Inorg. Chem., 50, 1073-1078 (2011)
$N_8H_{36}Co_2B_4P_8O_{34}$	1:2	T	Inorg. Chem., 50, 1073-1078 (2011)
$C_3H_{13}N_2MnB_2P_3O_{13}$	2:3	T	Solid State Sci., 13, 757-761 (2011)
$C_3H_{13}N_2FeB_2P_3O_{13}$	2:3	T	Solid State Sci., 13, 757-761 (2011)
$C_4H_{13}N_2FeB_2P_3O_{13}$	2:3	T	Solid State Sci., 13, 757-761 (2011)
$AgMg(H_2O)_2[BP_2O_8]H_2O$	1:2	T	Acta Cryst. E, 67, i39 (2011)
$K_3Ln[OB(OH)_2]_2[HOPO_3]_2$ (*Ln*=Yb, Lu)	1:1	M	J. Solid State Chem., 184, 1517-1522 (2011)
$(Ag_{0.57}Ni_{0.22})Ni(H_2O)_2[BP_2O_8]$	1:2	T	Acta Cryst. E, 67, i44 (2011)
$C_4H_{24}B_4Co_2N_4O_{27}P_6$	2:3	T	J. Solid State Chem., 184, 2538-2542 (2011)
$Th_2[BO_4][PO_4]$	1:1	T	Can. Mineral., 49, 1211-1220 (2011)
$LiZn(H_2O)_2(BP_2O_8)(H_2O)$	1:2	T	Journal of Henan Polytechnic University (Natural Science) (2011), 30(1), 100-103

$(H_3O)Mg(H_2O)_2(BP_2O_8)(H_2O)$	1:2	T	Journal of Henan Polytechnic University (Natural Science) (2011), 30(1), 100-103
$H_{37}B_4Mn_4N_7O_{43}P_{10}$	2:5	T	Micropor. Mesopor. Mater. 147, 73-78 (2012)
$(Ag_{0.79}Co_{0.11})Co(H_2O)_2[BP_2O_8]0.67H_2O$	1:2	T	Acta Cryst. E, 68, i3 (2012)
$Ba_5[(UO_2)(PO_4)_3(B_5O_9)]nH_2O$	5:3	M	Chem. Commun., 48, 3479-3481 (2012)
$KMnBP_2O_7(OH)_2$	1:2	T	Eur. J. Inorg. Chem., 3032-3038 (2012)
$KCo(H_2O)_2BP_2O_8\_0.48H_2O$	1:2	T	Acta Cryst. C, 68, i55 (2012)
$K_{0.17}Ca_{0.42}Co(H_2O)_2BP_2O_8\_H_2O$	1:2	T	Acta Cryst. C, 68, i55 (2012)
$BiM_2BP_2O_{10}$ (M = Co, Ni)	1:2	T	Inorg. Chem., 51, 8842-8847 (2012)
$Li_2Cs_2B_2P_4O_{15}$	1:2	T	Chem.-Eur. J., 18, 12046-12051 (2012)
$LiK_2BP_2O_8$	1:2	T	Chem.-Eur. J., 18, 12046-12051 (2012)
$Li_3M_2BP_4O_{14}$ (M=K, Rb)	1:4	T	Chem.-Eur. J., 18, 12046-12051 (2012)
$Na_3Cd_3B(PO_4)_4$	1:4	T	Inorg. Chem., 51, 10870-10875 (2012)
$K(Mn(H_2O)_2(BP_2O_8))(H_2O)$	1:2	T	Z. Krist.-New Cyst. St., 227(1), 3-4 (2012)
$Na_{13}(H_3O)_2[B_6P_{11}O_{42}(OH)_2]Cl_2\ \ H_2O$	6:11	T	Crystengcomm. 15, 2048-2051 (2013)
$LiCu_2[BP_2O_8(OH)_2]$	1:2	T	Dalton Trans., 42, 6298-6301 (2013)
$RbPbBP_2O_8$	1:2	T	Crystengcomm., 15, 4956-4962 (2013)
$KPbBP_2O_8$	1:2	T	Eur. J. Inorg. Chem., 3185-3190 (2013)
$Ba_{11}B_{26}O_{44}(PO_4)_2(OH)_6$	13:1	M	J. Solid State Chem., 203, 166-173 (2013)
$Mn_3(OH_2)[B(OH)_4][PO_4]$	1:1	T	Z. Kristallogr., 228, 509-519 (2013)
$KNi_5[P_6B_6O_{23}(OH)_{13}]$	1:1	T	Z. Kristallogr., 228, 509-519 (2013)
$Na_{0.45}K(MgNi,Al)Ni_2(Ni,Al,Mg_2)_2[P_6B_6O_{24}(OH)_{12}]$	1:1	T	Z. Kristallogr., 228, 509-519 (2013)
$Li_3BP_2O_8$	1:2	T	Dalton Trans., 43, 2294-2300 (2014)
$Cu_3[B_2P_3O_{12}(OH)_3]$	1:2	T	J. Solid State Chem., 210, 60-64 (2014)

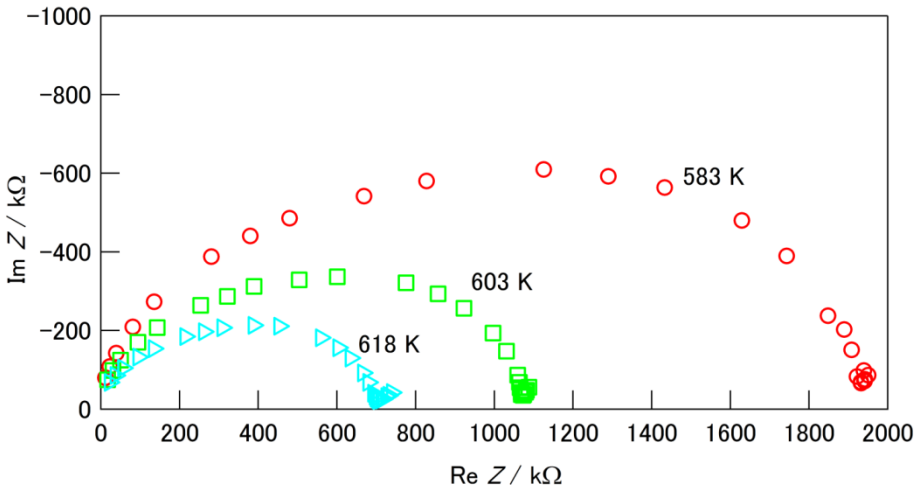

Fig. S1 Complex impedance plots for a polycrystalline $Li_2B_3PO_8$ sample at 583, 603, and 618 K.

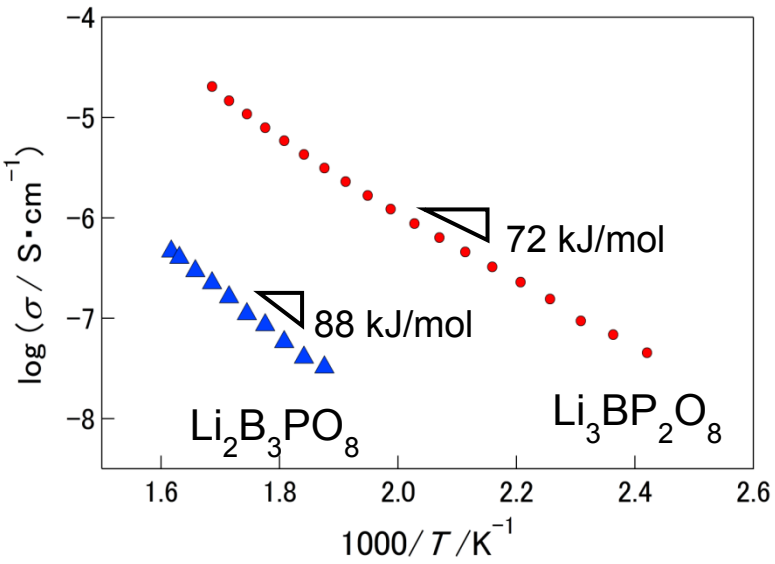

Fig. S2 Arrhenius plots of the conductivities of $Li_2B_3PO_8$ and $Li_3BP_2O_8$ [S2] measured by the AC impedance method

(S2) T. Hasegawa and H.Yamane, *Dalton. Trans.*, 2014, **43**, 2294.