Figure S1: X-ray powder diffraction pattern of the synthesized $Li_6CuB_4O_{10}$ sample before melting.



Figure S2: Calculated X-ray powder diffraction pattern of $Li_6CuB_4O_{10}$ based on single crystal data.



Figure S3: Transmission spectrum of $Li_6CuB_4O_{10}$. The peak around 610 nm is absorbance from $Li_6CuB_4O_{10}$. The peak at ~800 nm is due to changing the grating on the spectrophotometer. The peak at ~870 nm is due to KBr.



Figure S4: The linear temperature dependence of the reciprocal susceptibility for $Li_6CuB_4O_{10}$.



Figure S5. The mid-infrared spectra of $Li_6CuB_4O_{10}$.



Figure S6. XRD pattern of the solidified $Li_6CuB_4O_{10}$ sample after melting.



Figure S7. DTA curve of the solidified melt of $Li_6CuB_4O_{10}$ after melting.



Atoms	Distances	Atoms	Angle
Li(1)-O(6)#1	1.865(17)	O(6)#1-Li(1)-O(7)	119.6(8)
Li(1)-O(7)	1.988(14)	O(6)#1-Li(1)-O(3)	106.3(7)
Li(1)-O(3)	2.037(14)	O(7)-Li(1)-O(3)	122.6(7)
Li(1)-O(8)#2	2.037(15)	O(6)#1-Li(1)-O(8)#2	105.4(8)
		O(7)-Li(1)-O(8)#2	94.3(6)
		O(3) -Li(1)-O(8)#2	105.2(7)
Li(2)-O(10)	1.832(16)	O(10)-Li(2)-O(2)	107.4(7)
Li(2)-O(2)	1.920(16)	O(10)-Li(2)-O(3)	139.7(9)
Li(2)-O(3)	2.037(15)	O(2)-Li(2)-O(3)	84.8(6)
Li(2)-O(8)	2.066(16)	O(10)-Li(2)-O(8)	108.3(8)
		O(2)-Li(2)-O(8)	101.9(7)
		O(3)-Li(2)-O(8)	106.3(7)
Li(3)-O(4)#7	1.85(2)	O(4)#7-Li(3)-O(1)	91.5(10)
Li(3)-O(1)	1.89(2)	O(4)#7-Li(3)-O(6)	96.0(10)
Li(3)-O(6)	2.07(2)	O(1) -Li(3)-O(6)	130.6(13)
Li(3)-O(10)#7	2.36(3)	O(4)#7-Li(3)-O(10)#7	102.0(11)
		O(1) -Li(3)-O(10)#7	98.6(9)
		O(6)-Li(3)-O(10)#7	126.9(11)
Li(4)-O(10)	1.75(2)	O(10)-Li(4)-O(8)#1	127.5(12)
Li(4)-O(8) #1	1.977(19)	O(10)-Li(4)-O(7)#8	105.7(11)
Li(4)-O(7)#8	2.07(2)	O(8)#1-Li(4)-O(7)#8	93.7(8)
Li(4)-O(6)#8	2.22(3)	O(10)-Li(4)-O(6)#8	112.0(11)
		O(8)#1-Li(4)-O(6)#8	113.9(9)
		O(7)#8-Li(4)-O(6)#8	95.9(8)
Li(5)-O(5)	1.96(2)	O(5)-Li(5)-O(8)#9	136.5(13)

Table S1. Selected bond lengths (Å) and angles (degree) for $Li_6CuB_4O_{10}$.

Li(5)-O(8)#9	1.98(2)	O(5)-Li(5)-O(9)#3	129.8(13)
Li(5)-O(9)#3	2.00(2)	O(8)#9-Li(5)-O(9)#3	71.5(8)
Li(5)-O(2)#9	2.08(3)	O(5)-Li(5)-O(2)#9	108.3(11)
		O(8)#9-Li(5)-O(2)#9	99.6(10)
		O(9)#3-Li(5)-O(2)#9	103.6(10)
Li(6)-O(7)#8	1.89(3)	O(7)#8-Li(6)-O(9)	134.9(15)
Li(6)-O(9)	1.96(2)	O(7)#8-Li(6)-O(1)#1	106.6(11)
Li(6)-O(1)#1	2.11(3)	O(9)-Li(6)-O(1)#1	118.1(12)
Li(6)-O(10)	2.12(3)	O(7)#8-Li(6)-O(10)	98.7(12)
		O(9)-Li(6)-O(10)	69.3(9)
		O(1)#1-Li(6)-O(10)	99.7(11)
Cu(1)-O(2)#10	1.883(12)	O(2)#10-Cu(1)-O(3)#10	88.7(5)
Cu(1)-O(3)#10	1.933(10)	O(2)#10-Cu(1)-O(4)	170.9(7)
Cu(1)-O(4)	1.936(12)	O(3)#10-Cu(1)-O(4)	94.6(5)
Cu(1)-O(1)#1	2.008(10)	O(2)#10-Cu(1)-O(1)#1	91.2(5)
		O(3)#10-Cu(1)-O(1)#1	178.5(5)
		O(4)-Cu(1)-O(1)#1	85.7(5)
B(1)-O(6)	1.32(2)	O(6)-B(1)-O(3)	126.2(12)
B(1)-O(3)	1.413(14)	O(6)-B(1)-O(5)#6	117.1(11)
B(1)-O(5)#6	1.426(16)	O(3)-B(1)-O(5)#6	116.6(12)
B(2)-O(7)	1.33(2)	O(7)-B(2)-O(5)	122.1(13)
B(2)-O(5)	1.38(2)	O(7)-B(2)-O(4)	119.1(15)
B(2)-O(4)	1.389(19)	O(5)-B(2)-O(4)	118.6(14)
B(3)-O(1)	1.30(2)	O(1)-B(3)-O(10)	121.6(15)
B(3)-O(10)	1.38(2)	O(1)-B(3)-O(9)	126.8(14)
B(3)-O(9)	1.43(2)	O(10)-B(3)-O(9)	111.5(14)
B(4)-O(2) #11	1.327(18)	O(2)#11-B(4)-O(8)#10	127.7(13)

B(4)-O(8)#10	1.356(18)	O(2)#11-B(4)-O(9)	121.6(13)	
B(4)-O(9)	1.473(18)	O(8)#10-B(4)-O(9)	110.5(12)	
Note. Symmetry transformations used to generate equivalent atoms:				

#1 x+1,y,z #2 x,y+1,z #3 x-1,y+1,z

#4 x+1,y,z-1 #5 x+1,y-1,z-1 #6 x,y,z-1

#7 x-1,y,z #8 x+1,y-1,z #9 x-1,y+1,z+1

#10 x,y,z+1 #11 x-1,y,z+1 #12 x,y-1,z

Atom	01	O2	03	O4	05	O6	O7	08	09	O10	\sum_{cations}
Li1			0.214			0.340	0.244	0.214			1.012
Li2		0.293	0.214					0.198		0.371	1.076
Li3	0.318			0.354		0.195				0.089	0.956
Li4						0.130	0.195	0.251		0.464	1.040
Li5		0.190			0.263			0.249	0.230		0.932
Li6	0.171						0.318		0.263	0.171	0.923
Cu1	0.411	0.576	0.503	0.499							1.989
B1			0.900		0.864	1.148					2.912
B2				0.955	0.976		1.117				3.048
B3	1.212								0.853	1.003	3.068
B4		1.123						1.044	0.759		2.926
$\Sigma_{ m anios}$	2.112	2.182	1.831	1.808	2.103	1.813	1.874	1.956	2.105	2.098	

Table S2. Bond valence analysis of the $Li_6CuB_4O_{10}^{a,b}$

Bond valences calculated with the program Bond Valence Calculator Version 2.00,
 Hormillosa, C., Healy, S., Stephen, T. McMaster University (1993).

b Valence sums calculated with the formula: $S_i = \exp[(R_0 - R_i)/B]$, where $S_i =$ valence of bond "*i*" and B = 0.37.

Temperature (K)	Inverse Molar Susceptibility			
	(mol.Oe/emu)			
1.84	11.08033			
2	11.48501			
2.3	12.21747			
2.5	12.7421			
2.7	13.25205			
3	14.02131			
3.3	14.79728			
3.5	15.32332			
3.71	15.8705			
4	16.64447			
4.3	17.37619			
4.5	18.0018			
4.7	18.50824			
5	19.2864			
5	19.28268			
5.5	20.59308			
6	21.94908			
6.5	23.35357			
7	24.73411			
7.5	26.13696			
8	21.57963			
8.5	28.93519			
9	30.30303			
9.5	31.69572			
10	33.07972			
10.51	34.44712			
11.02	35.91954			
12.02	38.58025			
13.05	41.30525			
14.09	44.09171			
15	46.55493			
17	58.41121			
19	57.47126			
20.96	62.77464			
23	68.25939			
25	73.74631			
27	78.80221			
28.99	84.10429			

Table S3. Numerical Temperature and Inverse Molar Suseptability Data for $\rm Li_6CuB_4O_{10}.$

31.01	89.44544
33.17	94.51796
35.04	99.10803
37.05	104.60251
39.05	109.40919
41.31	114.94253
43.03	119.33174
45.19	124.06948
47.3	128.5347
49.47	132.80212
51.3	137.17421
55.44	146.62757
59.2	157.72871
63.37	167.50419
69.27	180.83183
75.44	195.3125
81.32	208.76827
87.01	220.75055
93.11	234.19204
99.14	246.91358
105.14	259.06736
115.19	280.89888
125.29	301.20482
128.01	303.95137
149.99	350.87719
155.24	358.42294
160.24	371.74721
165.24	380.22814
170.26	389.10506
175.28	398.40637
180.28	409.83607
185.26	416.66667
190.27	429.18455
195.29	440.52863
200.29	450.45045
205.29	456.621
210.3	469.48357
215.29	478.4689
220.29	485.43689
225.28	495.0495
230.3	507.61421
235.29	518.13472
240.27	523.56021

245.29	537.63441
250.3	546.44809
255.3	558.65922
260.28	568.18182
265.3	581.39535
270.29	588.23529
275.28	602.40964
280.29	609.7561
285.28	621.11801
290.29	628.93082
295.28	641.02564
300.28	657.89474
305.28	666.66667
310.29	684.93151
315.28	684.93151
320.31	709.21986
325.29	724.63768
330.27	735.29412
335.28	746.26866
340.26	769.23077