# Supporting Information

## Crystal growth and calculation of the electronic band structure, density of states of $Li_3Cs_2B_5O_{10}$

Yun Yang[a], Xin Su[a], Shilie Pan[a*], Min Zhang[a], Ying Wang[a], Jian Han[a], Zhihua Yang[a*]

[a] Key Laboratory of Functional Materials and Devices for Special Environments, Xinjiang Technical Institute of physics & Chemistry, Chinese Academy of Sciences,Xinjiang Key Laboratory of Electronic Information Materials and Devices, 40–1 South Beijing Road, Urumqi 830011, China

*To whom correspondence should be addressed
E-mail: slpan@ms.xjb.ac.cn (S. Pan) Tel: (86)-991-3674558
E-mail: zhyang@ms.xjb.ac.cn (Z.H. Yang) Tel: (86)-991-3859931
Fax: (86)-991-3838957

Figure S1. The measured optical absorption spectrum of $Li_3Cs_2B_5O_{10}$.

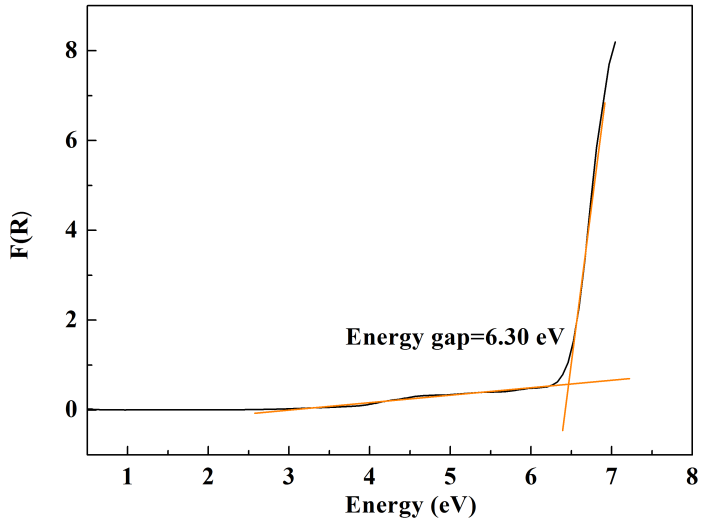

Table S1. The calculated bond lengths in comparison with experimental data, bond charge and bond order.

| bond type | experiment bond length (Å) | calculation bond length(Å) | bond charge | bond order |
|---|---|---|---|---|
| Cs(1)-O(1) | 3.047(3) | 3.009(4) | 0.61 | 0.14 |
| Cs(1)-O(1)#1 | 3.047(3) | 3.009(4) | 0.61 | 0.14 |
| Cs(1)-O(5)#2 | 3.191(3) | 3.091(1) | 0.61 | 0.14 |
| Cs(1)-O(5)#3 | 3.191(3) | 3.091(1) | 0.61 | 0.14 |
| Cs(1)-O(3)#3 | 3.343(4) | 3.384(7) | 0.61 | 0.02 |
| Cs(1)-O(3)#2 | 3.343(4) | 3.384(7) | 0.61 | 0.02 |
| Cs(1)-O(2)#1 | 3.484(3) | 3.423(2) | 0.83 | 0.02 |
| Cs(1)-O(2) | 3.484(3) | 3.423(2) | 0.83 | 0.02 |
| Cs(1)-O(4)#4 | 3.554(4) | 3.639(9) | 0.61 | -0.03 |
| Cs(1)-O(4)#5 | 3.554(4) | 3.639(9) | 0.61 | -0.03 |
| Cs(2)-O(3)#6 | 3.176(2) | 3.082(8) | 0.83 | -0.13 |
| Cs(2)-O(3)#5 | 3.176(2) | 3.082(8) | 0.83 | -0.13 |
| Cs(2)-O(1)#1 | 3.289(4) | 3.329(9) | 0.83 | 0.16 |
| Cs(2)-O(1)#7 | 3.289(4) | 3.329(9) | 0.83 | 0.16 |
| Cs(2)-O(2)#1 | 3.334(3) | 3.361(6) | 0.83 | 0 |
| Cs(2)-O(2)#7 | 3.334(3) | 3.361(6) | 0.83 | 0 |
| Cs(2)-O(5)#8 | 3.457(3) | 3.395(2) | 0.61 | -0.01 |
| Cs(2)-O(5)#9 | 3.457(3) | 3.395(2) | 0.61 | -0.01 |
| B(1)-O(3)#14 | 1.465(4) | 1.446(5) | 0.82 | 0.67 |
| B(1)-O(4)#8 | 1.474(4) | 1.467(1) | 0.82 | 0.62 |
| B(1)-O(4)#6 | 1.474(4) | 1.467(1) | 0.82 | 0.62 |
| B(1)-O(3) | 1.465(4) | 1.446(5) | 0.82 | 0.67 |
| B(2)-O(3)#2 | 1.380(6) | 1.371(4) | 0.78 | 0.79 |
| B(2)-O(2)#7 | 1.413(5) | 1.407(3) | 0.78 | 0.71 |
| B(2) -O(5) | 1.316(6) | 1.312(7) | 0.78 | 1.01 |
| B(3)-O(2)#4 | 1.410(5) | 1.394(5) | 0.71 | 0.75 |
| B(3)-O(1) | 1.319(6) | 1.319(1) | 0.71 | 0.99 |
| B(3) -O(4) | 1.391(5) | 1.375(1) | 0.71 | 0.77 |
| Li(1)-O(1)#15 | 2.010(9) | 2.002(4) | 1.20 | -0.04 |
| Li(1)-O(1)#2 | 2.020(9) | 2.021(4) | 1.20 | -0.04 |
| Li(1)-O(2)#2 | 2.141(8) | 2.138(9) | 1.20 | 0 |
| Li(1)-O(4)#2 | 2.305(8) | 2.337(4) | 1.20 | 0.01 |
| Li(1)-O(5) | 1.869(8) | 1.888(1) | 1.20 | -0.09 |
| Li(2)-O(5)#2 | 1.842(6) | 1.858(0) | 1.14 | -0.11 |
| Li(2)-O(4) | 2.133(8) | 2.130(7) | 1.14 | 0.05 |
| Li(2)-O(4)#2 | 2.133(8) | 2.130(7) | 1.14 | 0.05 |
| Li(2)-O(5) | 1.842(6) | 1.858(0) | 1.14 | -0.11 |