Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.


# Supporting Information

## Inducing Large Birefringence by Increasing Asymmetric Electron Distribution of Y-O Polyhedra

Mengen Gao[a], Qiang Bian*[b], Hongping Wu *[a] , Hongwei Yu[a] , Zhanggui Hu[a], Jiyang Wang[a] and Yicheng Wu[a]

[a] Tianjin Key Laboratory of Functional Crystal Materials, Institute of Functional Crystal, Tianjin University of Technology, Tianjin 300384, China
E-mail: wuhp@ms.xjb.ac.cn
[b] School of Materials and Energy, Guangdong University of Technology
E-mail: bianqiang2006@126.com

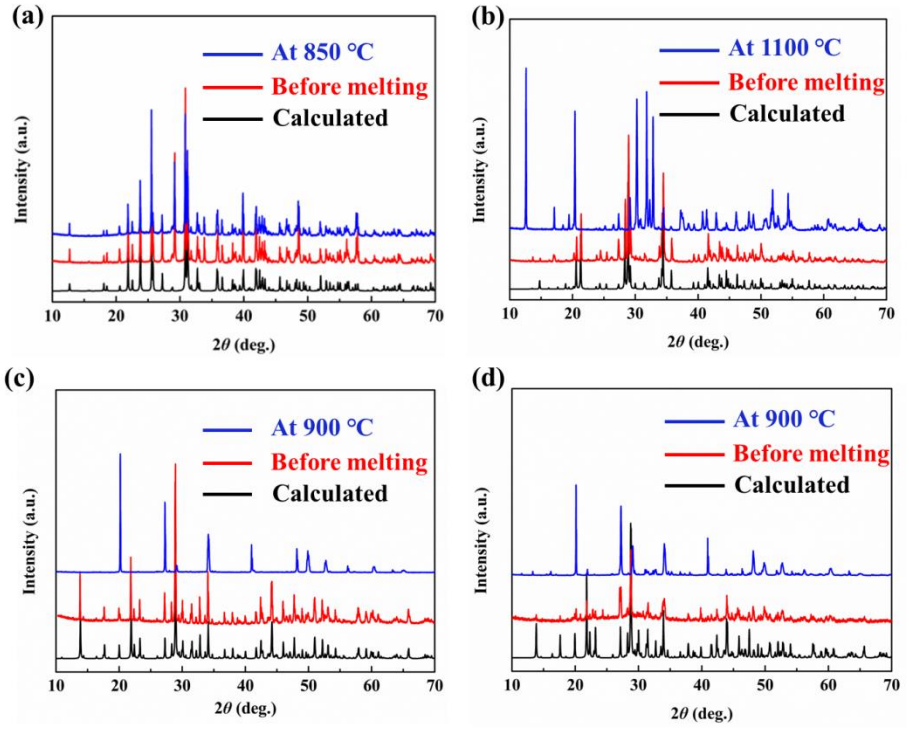


**Fig. S1** Powder XRD patterns for $LiRb_2YB_2O_6$ (a), $CaRbYB_2O_6$ (b), $Li_2RbY_4B_5O_{15}$ (c) and $Li_2CsY_4B_5O_{15}$ (d).

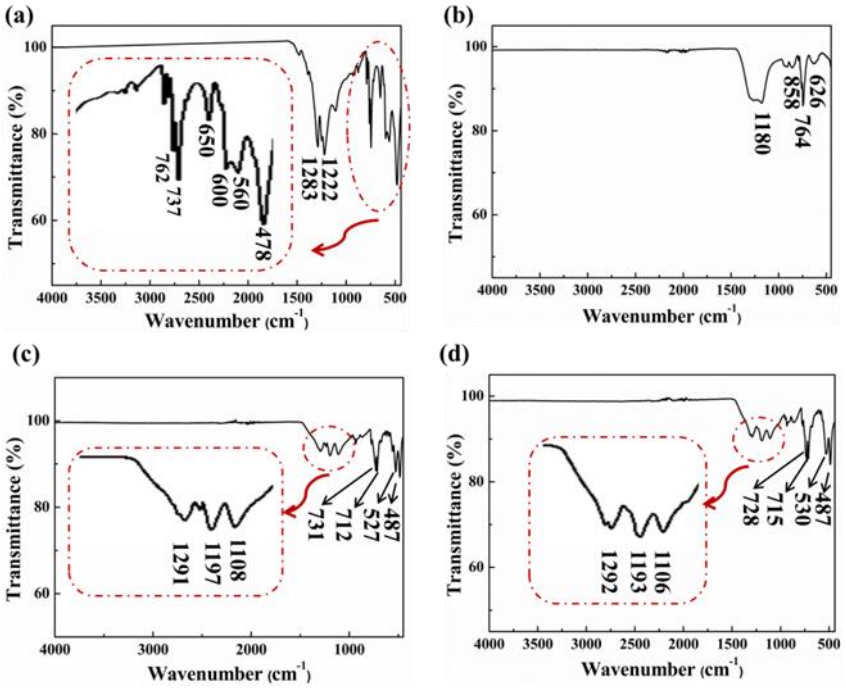


**Fig. S2** Infrared spectra of $LiRb_2YB_2O_6$ (a), $CaRbYB_2O_6$ (b), $Li_2RbY_4B_5O_{15}$ (c) and $Li_2CsY_4B_5O_{15}$ (d).

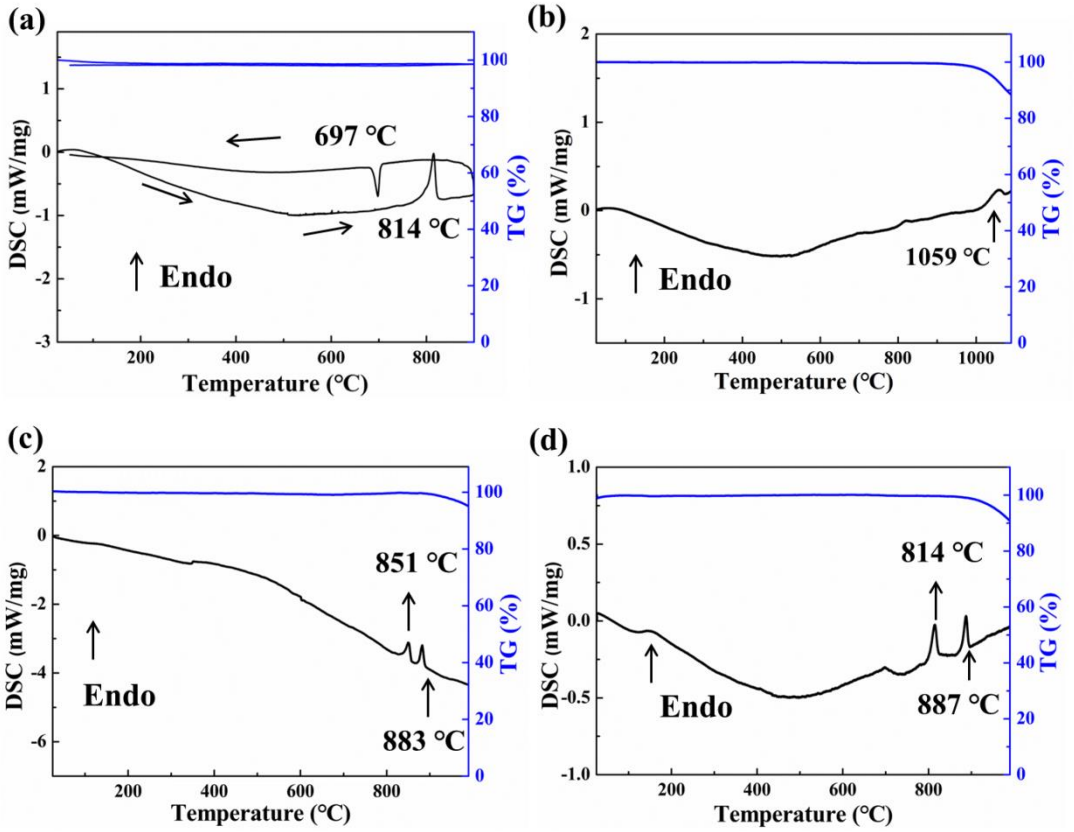


**Fig. S3** TG-DSC curves for (a) $LiRb_2YB_2O_6$, (b) $CaRbYB_2O_6$, (c) $Li_2RbY_4B_5O_{15}$ and (d) $Li_2CsY_4B_5O_{15}$.

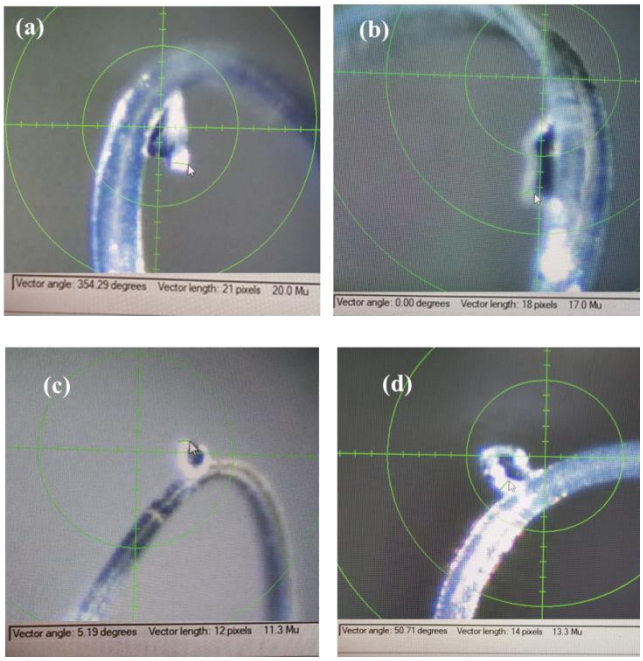


**Fig. S4** Photograph of crystal size for (a) $LiRb_2YB_2O_6$, (b) $CaRbYB_2O_6$, (c) $Li_2RbY_4B_5O_{15}$ and (d) $Li_2CsY_4B_5O_{15}$.

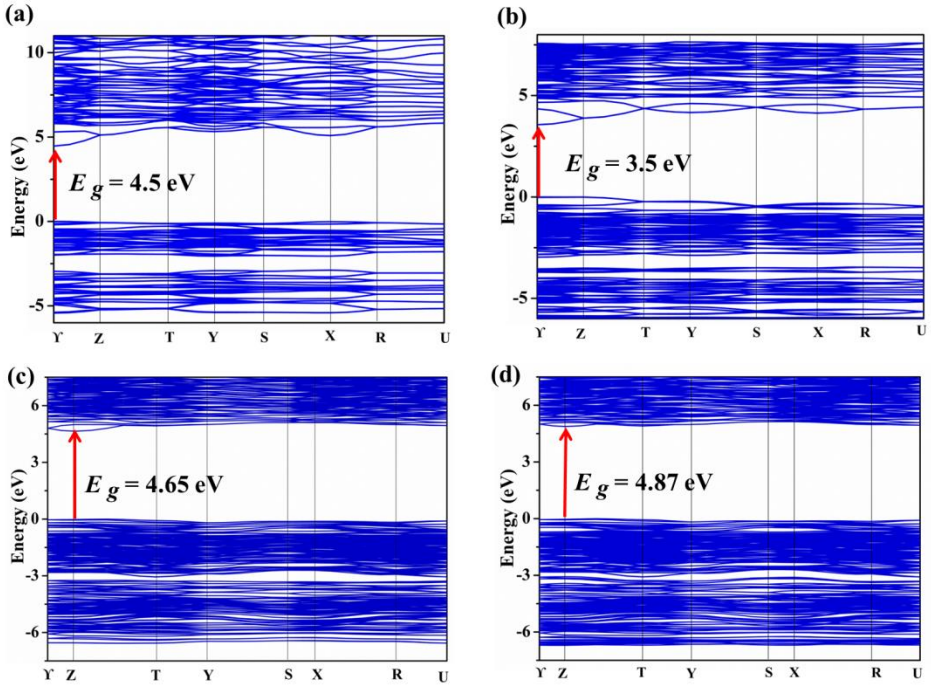


**Fig. S5** Calculated band gaps for (a) $LiRb_2YB_2O_6$, (b) $CaRbYB_2O_6$, (c) $Li_2RbY_4B_5O_{15}$, (d) $Li_2CsY_4B_5O_{15}$. They are all direct band gap compounds with the band gaps of 4.5, 3.5, 4.87 and 4.65 eV, respectively.

**Table S1.** Crystallographic data and structure refinements for four compounds.

| Empirical formula | $LiRb_2YB_2O_6$ | $CaRbYB_2O_6$ | $Li_2RbY_4B_5O_{15}$ | $Li_2CsY_4B_5O_{15}$ |
|---|---|---|---|---|
| Formula weight | 384.41 | 332.08 | 749.04 | 796.48 |
| Crystal system | Orthorhombic | Orthorhombic | Monoclinic | Monoclinic |
| Space group | *Pbcm* | *Pbca* | *P*2/*n* | *P*2/*n* |
| Unit cell (Å) | *a* = 6.962(2)<br>*b* = 9.556(3)<br>*c* = 9.995(3) | *a* =10.0405(8)<br>*b* = 9.1393(5)<br>*c* = 13.0367(8) | *a* = 10.5033(10)<br>*b* = 6.3799(8)<br>*c* = 19.735(2)<br>*β* = 105.339(5)° | *a* = 10.5584(5)<br>*b* = 6.3942(3)<br>*c* = 19.8267(9)<br>*β* = 105.267(2)° |
| Z, Volume ($Å^3$) | 4, 665.0(3) | 8, 1196.29(14) | 4, 1275.3(2) | 4, 1291.31(10) |
| Density (g $cm^{-3}$) | 3.840 | 3.688 | 3.901 | 4.097 |
| Absorption coefficient ($mm^{-1}$) | 23.286 | 18.657 | 21.901 | 20.663 |
| Goodness-of-fit on $F_2$ | 1.072 | 1.120 | 1.090 | 1.063 |
| Final *R* indices $[F_0^2>2s(F_0^2)]^a$ | $R_1$ = 0.0410<br>$wR_2$ = 0.0911 | $R_1$ = 0.0743<br>$wR_2$ = 0.2106 | $R_1$ = 0.0483<br>$wR_2$ = 0.0977 | $R_1$ = 0.0214<br>$wR_2$ = 0.0440 |
| *R* indices (all data) | $R_1$ = 0.0677<br>$wR_2$ = 0.1033 | $R_1$ = 0.0898<br>$wR_2$ = 0.2262 | $R_1$ = 0.0769<br>$wR_2$ = 0.1105 | $R_1$ = 0.0266<br>$wR_2$ = 0.0456 |

**Table S2.** Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($A^2 \times 10^3$), $U_{eq}$ is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor

| Atoms | x | y | z | U(eq) | BVS |
|---|---|---|---|---|---|
| **$LiRb_2YB_2O_6$** | | | | | |
| Rb(1) | 7792(1) | 4141(1) | 4453(1) | 26(1) | 1.13 |
| Li(1) | 490(30) | 6492(19) | 2500 | 21(5) | 1.23 |
| Y(1) | 6369(2) | 7590(1) | 2500 | 14(1) | 2.73 |
| B(1) | 3501(16) | 5566(12) | 2500 | 8(2) | 2.92 |
| B(2) | 7993(18) | 7500 | 5000 | 17(3) | 2.97 |
| O(1) | 3196(11) | 7011(7) | 2500 | 19(2) | 2.16 |
| O(2) | 5345(11) | 5055(8) | 2500 | 21(2) | 1.98 |
| O(3) | 8907(8) | 6962(5) | 3901(6) | 18(1) | 2.21 |
| O(4) | 6003(12) | 7500 | 5000 | 22(2) | 1.75 |
| O(5) | 1948(12) | 4681(8) | 2500 | 29(2) | 1.81 |
| **$CaRbYB_2O_6$** | | | | | |
| Rb(1) | 3540(1) | 5683(1) | 4103(1) | 20(1) | 1.13 |
| Ca(1) | 6224(2) | 7557(3) | 2812(2) | 10(1) | 2.11 |
| Y(001) | 9129(1) | 5975(1) | 3870(1) | 13(1) | 2.97 |
| B(1) | 6247(11) | 7636(12) | 5035(9) | 6(2) | 2.98 |
| B(2) | 6374(10) | 4198(11) | 2660(9) | 4(2) | 3.03 |
| O(1) | 5436(9) | 8608(9) | 4509(7) | 16(2) | 1.88 |
| O(2) | 7604(9) | 4763(10) | 2904(7) | 19(2) | 2.03 |
| O(3) | 6244(8) | 2703(9) | 2596(6) | 14(2) | 2.02 |
| O(4) | 7198(8) | 6881(9) | 4514(6) | 15(2) | 1.97 |
| O(5) | 5353(9) | 5126(9) | 2475(7) | 18(2) | 2.04 |
| O(6) | 6017(10) | 7487(10) | 6068(6) | 20(2) | 2.09 |
| **$Li_2RbY_4B_5O_{15}$** | | | | | |
| Rb(1) | 5596(1) | -873(2) | 3641(1) | 16(1) | 0.81 |
| Li(1) | 6422(12) | 10230(20) | 1530(6) | 7(3) | 1.23 |
| Li(2) | 2228(14) | 200(20) | 3419(6) | 11(3) | 1.32 |
| Y(1) | 7500 | 14144(2) | 2500 | 6(1) | 2.80 |
| Y(2) | 6428(1) | -3580(1) | 5537(1) | 5(1) | 3.17 |
| Y(3) | 4557(1) | 6609(1) | 1500(1) | 6(1) | 3.23 |
| Y(4) | 8432(1) | 3536(1) | 4539(1) | 6(1) | 3.06 |
| Y(5) | 2500 | 14059(2) | 2500 | 11(1) | 2.72 |

| | | | | | |
|---|---|---|---|---|---|
| B(1) | 2500 | 8330(20) | 2500 | 5(2) | 3.08 |
| B(2) | 7500 | 8450(20) | 2500 | 9(3) | 2.94 |
| B(3) | 4509(9) | 12190(16) | 1481(4) | 8(2) | 2.94 |
| B(4) | 5434(9) | 4126(16) | 3243(5) | 8(2) | 2.96 |
| B(5) | 3442(9) | -1939(16) | 4499(4) | 7(2) | 2.96 |
| B(6) | 8577(9) | -2000(16) | 4571(4) | 8(2) | 2.93 |
| O(1) | 5598(5) | 13319(9) | 1403(3) | 6(1) | 2.08 |
| O(2) | 9672(5) | -3197(9) | 4528(3) | 8(1) | 2.01 |
| O(3) | 6696(5) | 3435(9) | 3567(3) | 12(1) | 1.87 |
| O(4) | 2773(5) | 7239(9) | 1965(2) | 7(1) | 2.12 |
| O(5) | 2309(5) | -3090(9) | 4479(3) | 7(1) | 2.07 |
| O(6) | 3366(5) | 13303(9) | 1482(2) | 6(1) | 2.10 |
| O(7) | 3461(5) | 92(9) | 4304(3) | 8(1) | 1.99 |
| O(8) | 8405(5) | 43(9) | 4403(3) | 10(1) | 2.06 |
| O(9) | 4341(5) | 3635(10) | 3469(3) | 13(1) | 1.94 |
| O(10) | 7500 | 10592(13) | 2500 | 9(2) | 2.07 |
| O(11) | 4584(5) | -3129(9) | 4703(3) | 10(1) | 2.12 |
| O(12) | 5270(6) | 5155(10) | 2616(3) | 16(1) | 1.78 |
| O(13) | 6831(5) | 7332(9) | 1912(2) | 6(1) | 2.04 |
| O(14) | 2500 | 10477(13) | 2500 | 16(2) | 2.14 |
| O(15) | 7611(5) | -3206(9) | 4753(3) | 11(1) | 2.04 |
| O(16) | 4585(5) | 10101(10) | 1583(3) | 13(1) | 2.19 |
| **$Li_2CsY_4B_5O_{15}$** | | | | | |
| Cs(1) | 552(1) | 931(1) | 3590(1) | 12(1) | 1.13 |
| Li(1) | 3610(6) | -225(9) | 3479(3) | 11(1) | 1.21 |
| Li(2) | 2773(6) | 172(9) | 6565(3) | 10(1) | 1.29 |
| Y(1) | 5438(1) | 3413(1) | 3504(1) | 5(1) | 3.19 |
| Y(2) | 1432(1) | 3588(1) | 5538(1) | 4(1) | 3.12 |
| Y(3) | -2500 | -4051(1) | 2500 | 9(1) | 2.68 |
| Y(4) | 3440(1) | -3544(1) | 4544(1) | 5(1) | 3.03 |
| Y(5) | 2500 | 5863(1) | 2500 | 6(1) | 2.76 |
| B(1) | -448(4) | 4095(6) | 6766(2) | 6(1) | 2.96 |
| B(2) | 7500 | 1640(8) | 2500 | 5(1) | 3.01 |
| B(3) | 1566(4) | -1907(6) | 5481(2) | 6(1) | 2.95 |
| B(4) | 2500 | 11556(8) | 2500 | 6(1) | 2.96 |
| B(5) | 5489(3) | -2185(6) | 3516(2) | 6(1) | 2.95 |
| B(6) | 3576(4) | 1988(6) | 4586(2) | 6(1) | 2.90 |
| O(1) | 3369(2) | 3285(4) | 6482(1) | 7(1) | 2.07 |

| | | | | | |
|---|---|---|---|---|---|
| O(2) | 658(2) | 3725(4) | 6532(1) | 12(1) | 1.90 |
| O(3) | 4419(2) | -3293(3) | 3615(1) | 7(1) | 2.07 |
| O(4) | 1701(2) | -3518(4) | 3584(1) | 11(1) | 1.90 |
| O(5) | 5324(2) | -3198(4) | 5465(1) | 6(1) | 1.96 |
| O(6) | 3178(2) | 2661(4) | 3077(1) | 6(1) | 2.07 |
| O(7) | 2717(2) | -3085(4) | 5535(1) | 6(1) | 2.01 |
| O(8) | 2500 | 9399(5) | 2500 | 10(1) | 1.96 |
| O(9) | 4707(3) | 4971(4) | 2405(1) | 14(1) | 1.84 |
| O(10) | -446(2) | 3100(4) | 4745(1) | 10(1) | 2.13 |
| O(11) | 7182(2) | 2764(4) | 3021(1) | 9(1) | 2.08 |
| O(12) | 1568(2) | 100(4) | 5686(1) | 8(1) | 2.13 |
| O(13) | 2634(2) | 3195(4) | 4775(1) | 9(1) | 2.08 |
| O(14) | 5413(2) | -98(4) | 3418(1) | 10(1) | 2.17 |
| O(15) | 3420(2) | -47(4) | 4409(1) | 8(1) | 2.06 |
| O(16) | 7500 | -500(5) | 2500 | 10(1) | 2.03 |

**Table S3.** Selected bond distances (Å) and angles (deg.)

| **$LiRb_2YB_2O_6$** | | | |
|---|---|---|---|
| Rb(1)-O(2) | 2.735(5) | O(3)-Rb(1)-O(1)#3 | 123.20(17) |
| Rb(1)-O(3) | 2.860(5) | O(1)#1-Rb(1)-O(1)#3 | 109.65(10) |
| Rb(1)-O(1)#1 | 2.903(5) | O(3)#2-Rb(1)-O(1)#3 | 62.65(18) |
| Rb(1)-O(3)#2 | 3.016(6) | O(4)#3-Rb(1)-O(1)#3 | 59.73(13) |
| Rb(1)-O(4)#3 | 3.120(7) | O(3)#4-Rb(1)-O(1)#3 | 95.35(17) |
| Rb(1)-O(3)#4 | 3.150(5) | B(1)#3-Rb(1)-O(1)#3 | 24.7(2) |
| Rb(1)-O(5)#3 | 3.252(3) | O(5)#3-Rb(1)-O(1)#3 | 42.71(17) |
| Rb(1)-O(1)#3 | 3.310(3) | O(3)#6-Li(1)-O(3)#7 | 99.1(10) |
| Li(1)-O(3)#6 | 1.839(14) | O(3)#6-Li(1)-O(1) | 121.2(6) |
| Li(1)-O(3)#7 | 1.839(14) | O(3)#7-Li(1)-O(1) | 121.2(6) |
| Li(1)-O(1) | 1.95(2) | O(3)#6-Li(1)-O(5) | 121.0(6) |
| Li(1)-O(5) | 2.00(2) | O(3)#7-Li(1)-O(5) | 121.0(6) |
| Y(1)-O(1) | 2.277(8) | O(1)-Li(1)-O(5) | 74.4(8) |
| Y(1)-O(5)#8 | 2.316(8) | O(1)-Y(1)-O(5)#8 | 134.4(3) |
| Y(1)-O(3) | 2.332(6) | O(1)-Y(1)-O(3) | 132.24(18) |
| Y(1)-O(3)#9 | 2.332(6) | O(5)#8-Y(1)-O(3) | 80.7(2) |
| Y(1)-O(4)#9 | 2.5132(11) | O(1)-Y(1)-O(3)#9 | 132.24(18) |
| Y(1)-O(4) | 2.5132(11) | O(5)#8-Y(1)-O(3)#9 | 80.7(2) |
| Y(1)-O(2) | 2.525(8) | O(5)#8-Y(1)-O(2) | 166.0(3) |
| Y(1)-O(2)#8 | 2.641(8) | O(3)-Y(1)-O(2) | 88.13(18) |
| B(1)-O(5) | 1.372(14) | O(3)#9-Y(1)-O(2) | 88.13(18) |
| B(1)-O(2) | 1.373(13) | O(4)#9-Y(1)-O(2) | 86.48(6) |
| B(1)-O(1) | 1.397(13) | O(4)-Y(1)-O(2) | 86.48(6) |
| B(2)-O(3) | 1.370(8) | O(1)-Y(1)-O(2)#8 | 77.2(2) |
| B(2)-O(3)#10 | 1.370(8) | O(5)#8-Y(1)-O(2)#8 | 57.2(3) |
| B(2)-O(4) | 1.386(15) | O(3)-Y(1)-O(2)#8 | 124.86(17) |
| O(2)-Rb(1)-O(3) | 74.3(2) | O(3)#9-Y(1)-O(2)#8 | 124.86(17) |
| O(2)-Rb(1)-O(1)#1 | 66.17(19) | O(4)#9-Y(1)-O(2)#8 | 89.12(9) |
| O(3)-Rb(1)-O(1)#1 | 126.54(16) | O(4)-Y(1)-O(2)#8 | 89.12(9) |
| O(2)-Rb(1)-O(3)#2 | 167.34(16) | O(2)-Y(1)-O(2)#8 | 136.73(6) |
| O(3)-Rb(1)-O(3)#2 | 103.18(13) | O(5)-B(1)-O(2) | 121.1(9) |
| O(1)#1-Rb(1)-O(3)#2 | 107.60(17) | O(5)-B(1)-O(1) | 119.3(9) |
| O(2)-Rb(1)-O(4)#3 | 75.99(17) | O(2)-B(1)-O(1) | 119.6(9) |
| O(3)-Rb(1)-O(4)#3 | 137.51(14) | O(3)-Y(1)-O(3)#9 | 73.8(3) |

| | | | |
|---|---|---|---|
| O(1)#1-Rb(1)-O(4)#3 | 64.20(14) | O(1)-Y(1)-O(4)#9 | 83.87(18) |
| O(3)#2-Rb(1)-O(4)#3 | 111.96(13) | O(5)#8-Y(1)-O(4)#9 | 94.63(10) |
| O(2)-Rb(1)-O(3)#4 | 122.72(16) | O(3)-Y(1)-O(4)#9 | 131.7(2) |
| O(3)-Rb(1)-O(3)#4 | 113.03(9) | O(3)#9-Y(1)-O(4)#9 | 58.1(2) |
| O(1)#1-Rb(1)-O(3)#4 | 65.90(18) | O(1)-Y(1)-O(4) | 83.87(18) |
| O(3)#2-Rb(1)-O(3)#4 | 46.3(2) | O(5)#8-Y(1)-O(4) | 94.63(10) |
| O(4)#3-Rb(1)-O(3)#4 | 108.45(12) | O(3)-Y(1)-O(4) | 58.1(2) |
| O(2)-Rb(1)-O(5)#3 | 126.35(19) | O(3)#9-Y(1)-O(4) | 131.7(2) |
| O(3)-Rb(1)-O(5)#3 | 80.75(18) | O(4)#9-Y(1)-O(4) | 167.7(4) |
| O(1)#1-Rb(1)-O(5)#3 | 152.35(16) | O(1)-Y(1)-O(2) | 59.5(2) |
| O(3)#2-Rb(1)-O(5)#3 | 64.40(18) | O(3)-B(2)-O(3)#10 | 124.6(11) |
| O(4)#3-Rb(1)-O(5)#3 | 93.27(14) | O(3)-B(2)-O(4) | 117.7(5) |
| O(3)#4-Rb(1)-O(5)#3 | 110.65(18) | O(3)#10-B(2)-O(4) | 117.7(5) |
| O(2)-Rb(1)-O(1)#3 | 129.31(19) | | |
| **$CaRbYB_2O_6$** | | | |
| Rb(1)-O(5) | 2.841(9) | O(6)#5-Ca(1)-O(2)#6 | 96.4(3) |
| Rb(1)-O(3)#1 | 2.890(8) | O(6)#5-Ca(1)-O(5) | 76.8(3) |
| Rb(1)-O(2)#2 | 2.904(9) | O(2)#6-Ca(1)-O(5) | 168.5(3) |
| Rb(1)-O(6)#3 | 2.939(9) | O(6)#5-Ca(1)-O(4) | 156.1(4) |
| Rb(1)-O(6)#4 | 3.044(11) | O(2)#6-Ca(1)-O(4) | 88.3(3) |
| Rb(1)-O(4)#3 | 3.048(8) | O(5)-Ca(1)-O(4) | 94.3(3) |
| Rb(1)-O(4)#4 | 3.166(9) | O(6)#5-Ca(1)-O(3)#1 | 72.8(3) |
| Rb(1)-O(1) | 3.324(9) | O(2)#6-Ca(1)-O(3)#1 | 117.2(3) |
| Ca(1)-O(6)#5 | 2.283(9) | O(5)-Ca(1)-O(3)#1 | 70.0(3) |
| Ca(1)-O(2)#6 | 2.338(9) | O(4)-Ca(1)-O(3)#1 | 125.5(3) |
| Ca(1)-O(5) | 2.427(9) | O(6)#5-Ca(1)-O(1) | 147.8(4) |
| Ca(1)-O(4) | 2.503(9) | O(2)#6-Ca(1)-O(1) | 77.6(3) |
| Ca(1)-O(3)#1 | 2.538(8) | O(5)-Ca(1)-O(1) | 113.0(3) |
| Ca(1)-O(1) | 2.539(9) | O(4)-Ca(1)-O(1) | 56.1(3) |
| Ca(1)-O(3)#6 | 2.561(8) | O(3)#1-Ca(1)-O(1) | 81.8(3) |
| Ca(1)-O(5)#1 | 2.857(10) | O(6)#5-Ca(1)-O(3)#6 | 88.9(3) |
| Ca(1)-O(2) | 2.907(10) | O(2)#6-Ca(1)-O(3)#6 | 57.4(3) |
| Y(001)-O(4) | 2.269(8) | O(5)-Ca(1)-O(3)#6 | 112.7(3) |
| Y(001)-O(2) | 2.271(8) | O(4)-Ca(1)-O(3)#6 | 73.9(3) |
| Y(001)-O(5)#7 | 2.278(9) | O(3)#1-Ca(1)-O(3)#6 | 160.64(14) |
| Y(001)-O(3)#6 | 2.323(8) | O(1)-Ca(1)-O(3)#6 | 112.7(3) |
| Y(001)-O(1)#8 | 2.359(8) | O(6)#5-Ca(1)-O(5)#1 | 80.4(3) |
| Y(001)-O(6)#9 | 2.362(9) | O(2)#6-Ca(1)-O(5)#1 | 65.0(3) |

| | | | |
|---|---|---|---|
| Y(001)-O(1)#9 | 2.517(9) | O(5)-Ca(1)-O(5)#1 | 121.93(10) |
| B(1)-O(4) | 1.360(14) | O(4)-Ca(1)-O(5)#1 | 122.4(3) |
| B(1)-O(6) | 1.373(14) | O(3)#1-Ca(1)-O(5)#1 | 52.3(2) |
| B(1)-O(1) | 1.387(14) | O(1)-Ca(1)-O(5)#1 | 68.3(3) |
| B(2)-O(5) | 1.352(13) | O(3)#6-Ca(1)-O(5)#1 | 119.5(2) |
| B(2)-O(2) | 1.376(13) | O(6)#5-Ca(1)-O(2) | 94.0(3) |
| B(2)-O(3) | 1.376(13) | O(2)#6-Ca(1)-O(2) | 121.03(10) |
| O(5)-Rb(1)-O(3)#1 | 59.6(2) | O(5)-Ca(1)-O(2) | 51.4(3) |
| O(5)-Rb(1)-O(2)#2 | 58.9(2) | O(4)-Ca(1)-O(2) | 63.9(3) |
| O(3)#1-Rb(1)-O(2)#2 | 61.3(2) | O(3)#1-Ca(1)-O(2) | 121.3(3) |
| O(5)-Rb(1)-O(6)#3 | 70.7(3) | O(1)-Ca(1)-O(2) | 116.4(3) |
| O(3)#1-Rb(1)-O(6)#3 | 124.1(2) | O(3)#6-Ca(1)-O(2) | 65.0(2) |
| O(2)#2-Rb(1)-O(6)#3 | 72.3(3) | O(5)#1-Ca(1)-O(2) | 172.5(2) |
| O(5)-Rb(1)-O(6)#4 | 125.3(2) | O(4)-Y(001)-O(2) | 78.9(3) |
| O(3)#1-Rb(1)-O(6)#4 | 69.9(2) | O(4)-Y(001)-O(5)#7 | 150.5(3) |
| O(2)#2-Rb(1)-O(6)#4 | 79.9(2) | O(2)-Y(001)-O(5)#7 | 76.8(3) |
| O(6)#3-Rb(1)-O(6)#4 | 131.4(2) | O(4)-Y(001)-O(3)#6 | 83.0(3) |
| B(1)#4-Rb(1)-O(6)#4 | 26.3(3) | O(2)-Y(001)-O(3)#6 | 80.0(3) |
| O(5)-Rb(1)-O(4)#3 | 117.4(2) | O(5)#7-Y(001)-O(3)#6 | 76.6(3) |
| O(3)#1-Rb(1)-O(4)#3 | 164.2(2) | O(4)-Y(001)-O(1)#8 | 111.2(3) |
| O(2)#2-Rb(1)-O(4)#3 | 103.4(2) | O(2)-Y(001)-O(1)#8 | 82.8(3) |
| O(6)#3-Rb(1)-O(4)#3 | 47.5(2) | O(5)#7-Y(001)-O(1)#8 | 81.9(3) |
| B(1)#4-Rb(1)-O(4)#3 | 89.1(3) | O(3)#6-Y(001)-O(1)#8 | 155.0(3) |
| O(6)#4-Rb(1)-O(4)#3 | 105.3(2) | O(4)-Y(001)-O(6)#9 | 117.1(3) |
| O(5)-Rb(1)-O(4)#4 | 145.5(2) | O(2)-Y(001)-O(6)#9 | 148.3(3) |
| O(3)#1-Rb(1)-O(4)#4 | 91.1(2) | O(5)#7-Y(001)-O(6)#9 | 78.2(3) |
| O(2)#2-Rb(1)-O(4)#4 | 125.4(2) | O(3)#6-Y(001)-O(6)#9 | 75.5(3) |
| O(6)#3-Rb(1)-O(4)#4 | 143.2(2) | O(1)#8-Y(001)-O(6)#9 | 112.6(3) |
| B(1)#4-Rb(1)-O(4)#4 | 25.3(3) | O(4)-Y(001)-O(1)#9 | 94.6(3) |
| O(6)#4-Rb(1)-O(4)#4 | 45.6(2) | O(2)-Y(001)-O(1)#9 | 153.0(3) |
| O(4)#3-Rb(1)-O(4)#4 | 95.7(2) | O(5)#7-Y(001)-O(1)#9 | 114.6(3) |
| O(5)-Rb(1)-O(1) | 84.0(2) | O(3)#6-Y(001)-O(1)#9 | 125.6(3) |
| O(3)#1-Rb(1)-O(1) | 64.3(2) | O(1)#8-Y(001)-O(1)#9 | 75.3(3) |
| O(2)#2-Rb(1)-O(1) | 124.2(2) | O(6)#9-Y(001)-O(1)#9 | 57.5(3) |
| O(6)#3-Rb(1)-O(1) | 135.9(3) | O(4)-B(1)-O(6) | 123.8(10) |
| B(1)#4-Rb(1)-O(1) | 88.2(3) | O(4)-B(1)-O(1) | 119.4(10) |
| O(6)#4-Rb(1)-O(1) | 92.6(2) | O(6)-B(1)-O(1) | 116.7(10) |
| O(4)#3-Rb(1)-O(1) | 131.5(2) | O(5)-B(2)-O(2) | 119.1(9) |

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|---|---|---|---|
| O(4)#4-Rb(1)-O(1) | 65.6(2) | O(5)-B(2)-O(3) | 122.7(10) |
| B(1)#3-Rb(1)-O(1) | 131.3(2) | O(2)-B(2)-O(3) | 118.2(9) |
| **$Li_2RbY_4B_5O_{15}$** | | | |
| Rb(1)-O(7) | 2.944(5) | O(4)#4-Li(2)-O(6)#4 | 159.8(8) |
| Rb(1)-O(11) | 2.962(5) | O(10)-Y(1)-O(13)#3 | 149.72(12) |
| Rb(1)-O(8) | 2.993(5) | O(10)-Y(1)-O(13)#6 | 149.72(12) |
| Rb(1)-O(3) | 3.000(6) | O(13)#3-Y(1)-O(13)#6 | 60.6(2) |
| Rb(1)-O(15) | 3.009(6) | O(10)-Y(1)-O(12)#3 | 104.96(15) |
| Rb(1)-O(9) | 3.144(6) | O(13)#3-Y(1)-O(12)#3 | 69.95(19) |
| Rb(1)-O(12)#1 | 3.204(6) | O(13)#6-Y(1)-O(12)#3 | 84.08(19) |
| Li(1)-O(8)#3 | 1.902(13) | O(10)-Y(1)-O(12)#6 | 104.96(15) |
| Li(1)-O(16) | 1.961(13) | O(13)#3-Y(1)-O(12)#6 | 84.08(19) |
| Li(1)-O(10) | 1.962(12) | O(13)#6-Y(1)-O(12)#6 | 69.95(19) |
| Li(1)-O(13) | 2.002(15) | O(12)#3-Y(1)-O(12)#6 | 150.1(3) |
| Li(1)-O(1) | 2.138(15) | O(10)-Y(1)-O(3)#3 | 79.60(14) |
| Li(2)-O(7) | 1.880(14) | O(13)#3-Y(1)-O(3)#3 | 116.53(18) |
| Li(2)-O(16)#4 | 1.904(15) | O(13)#6-Y(1)-O(3)#3 | 82.25(18) |
| Li(2)-O(14)#1 | 1.918(12) | O(12)#3-Y(1)-O(3)#3 | 55.78(17) |
| Li(2)-O(4)#4 | 2.037(16) | O(12)#6-Y(1)-O(3)#3 | 130.96(17) |
| Li(2)-O(6)#4 | 2.099(16) | O(10)-Y(1)-O(3)#6 | 79.60(14) |
| Y(1)-O(10) | 2.266(8) | O(13)#3-Y(1)-O(3)#6 | 82.25(18) |
| Y(1)-O(13)#3 | 2.355(5) | O(13)#6-Y(1)-O(3)#6 | 116.53(18) |
| Y(1)-O(13)#6 | 2.355(5) | O(12)#3-Y(1)-O(3)#6 | 130.96(17) |
| Y(1)-O(12)#3 | 2.498(6) | O(12)#6-Y(1)-O(3)#6 | 55.78(17) |
| Y(1)-O(12)#6 | 2.498(6) | O(3)#3-Y(1)-O(3)#6 | 159.2(3) |
| Y(1)-O(3)#3 | 2.509(5) | O(10)-Y(1)-O(1)#7 | 78.23(13) |
| Y(1)-O(3)#6 | 2.509(5) | O(13)#3-Y(1)-O(1)#7 | 72.48(17) |
| Y(1)-O(1)#7 | 2.581(5) | O(13)#6-Y(1)-O(1)#7 | 130.79(18) |
| Y(1)-O(1) | 2.581(5) | O(12)#3-Y(1)-O(1)#7 | 65.98(17) |
| Y(2)-O(11) | 2.204(5) | O(12)#6-Y(1)-O(1)#7 | 120.82(16) |
| Y(2)-O(15) | 2.238(5) | O(3)#3-Y(1)-O(1)#7 | 108.01(17) |
| Y(2)-O(7)#5 | 2.246(6) | O(3)#6-Y(1)-O(1)#7 | 67.49(17) |
| Y(2)-O(9)#5 | 2.311(5) | O(10)-Y(1)-O(1) | 78.23(13) |
| Y(2)-O(11)#8 | 2.344(6) | O(13)#3-Y(1)-O(1) | 130.79(18) |
| Y(2)-O(6)#9 | 2.376(5) | O(13)#6-Y(1)-O(1) | 72.48(17) |
| Y(2)-O(5)#8 | 2.508(6) | O(12)#3-Y(1)-O(1) | 120.82(16) |
| Y(3)-O(16) | 2.234(6) | O(12)#6-Y(1)-O(1) | 65.98(17) |
| Y(3)-O(12) | 2.322(5) | O(3)#3-Y(1)-O(1) | 67.49(17) |

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| Y(3)-O(4) | 2.328(5) | O(3)#6-Y(1)-O(1) | 108.02(17) |
| Y(3)-O(13) | 2.356(5) | O(1)#7-Y(1)-O(1) | 156.5(3) |
| Y(3)-O(5)#11 | 2.368(5) | O(11)-Y(2)-O(15) | 90.5(2) |
| Y(3)-O(2)#3 | 2.379(5) | O(11)-Y(2)-O(7)#5 | 88.7(2) |
| Y(3)-O(1)#1 | 2.398(6) | O(15)-Y(2)-O(7)#5 | 88.5(2) |
| Y(3)-O(6)#1 | 2.447(6) | O(11)-Y(2)-O(9)#5 | 101.5(2) |
| Y(4)-O(8) | 2.244(6) | O(15)-Y(2)-O(9)#5 | 166.1(2) |
| Y(4)-O(3) | 2.271(5) | O(7)#5-Y(2)-O(9)#5 | 85.0(2) |
| Y(4)-O(5)#5 | 2.290(5) | O(11)-Y(2)-O(11)#8 | 72.8(2) |
| Y(4)-O(15)#6 | 2.331(6) | O(15)-Y(2)-O(11)#8 | 105.1(2) |
| Y(4)-O(2)#12 | 2.338(5) | O(7)#5-Y(2)-O(11)#8 | 156.84(19) |
| Y(4)-O(1)#2 | 2.348(5) | O(9)#5-Y(2)-O(11)#8 | 85.2(2) |
| Y(4)-O(2)#6 | 2.461(6) | O(11)-Y(2)-O(6)#9 | 167.9(2) |
| Y(5)-O(14) | 2.285(9) | O(15)-Y(2)-O(6)#9 | 91.01(19) |
| Y(5)-O(4)#11 | 2.340(6) | O(7)#5-Y(2)-O(6)#9 | 79.31(19) |
| Y(5)-O(4)#6 | 2.340(6) | O(9)#5-Y(2)-O(6)#9 | 75.75(19) |
| Y(5)-O(9)#11 | 2.348(6) | O(11)#8-Y(2)-O(6)#9 | 118.29(19) |
| Y(5)-O(9)#6 | 2.348(6) | O(11)-Y(2)-O(5)#8 | 117.68(19) |
| Y(5)-O(6) | 2.462(5) | O(15)-Y(2)-O(5)#8 | 71.94(19) |
| Y(5)-O(6)#14 | 2.462(5) | O(7)#5-Y(2)-O(5)#8 | 146.38(18) |
| B(1)-O(4)#14 | 1.358(9) | O(9)#5-Y(2)-O(5)#8 | 107.60(19) |
| B(1)-O(4) | 1.358(9) | O(11)#8-Y(2)-O(5)#8 | 56.78(18) |
| B(1)-O(14) | 1.368(15) | O(6)#9-Y(2)-O(5)#8 | 74.15(18) |
| B(2)-O(10) | 1.367(16) | O(16)-Y(3)-O(12) | 109.5(2) |
| B(2)-O(13)#7 | 1.385(9) | O(16)-Y(3)-O(4) | 78.2(2) |
| B(2)-O(13) | 1.385(9) | O(12)-Y(3)-O(4) | 77.72(19) |
| B(3)-O(16) | 1.347(12) | O(16)-Y(3)-O(13) | 77.70(19) |
| B(3)-O(1) | 1.394(11) | O(12)-Y(3)-O(13) | 73.05(19) |
| B(3)-O(6) | 1.395(10) | O(4)-Y(3)-O(13) | 132.75(17) |
| B(4)-O(12) | 1.370(10) | O(16)-Y(3)-O(5)#11 | 88.3(2) |
| B(4)-O(9) | 1.375(10) | O(12)-Y(3)-O(5)#11 | 142.69(19) |
| B(4)-O(3) | 1.383(10) | O(4)-Y(3)-O(5)#11 | 74.24(17) |
| B(5)-O(7) | 1.354(11) | O(13)-Y(3)-O(5)#11 | 144.10(17) |
| B(5)-O(11) | 1.386(10) | O(16)-Y(3)-O(2)#3 | 90.53(19) |
| B(5)-O(5) | 1.390(10) | O(12)-Y(3)-O(2)#3 | 137.08(19) |
| B(6)-O(8) | 1.345(11) | O(4)-Y(3)-O(2)#3 | 144.85(18) |
| B(6)-O(15) | 1.393(10) | O(13)-Y(3)-O(2)#3 | 74.99(17) |
| B(6)-O(2) | 1.402(10) | O(5)#11-Y(3)-O(2)#3 | 72.22(17) |

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| O(7)-Rb(1)-O(11) | 47.88(15) | O(16)-Y(3)-O(1)#1 | 151.82(19) |
| O(7)-Rb(1)-O(8) | 120.09(15) | O(12)-Y(3)-O(1)#1 | 71.75(19) |
| O(11)-Rb(1)-O(8) | 103.31(15) | O(4)-Y(3)-O(1)#1 | 127.89(19) |
| O(7)-Rb(1)-O(3) | 100.28(15) | O(13)-Y(3)-O(1)#1 | 75.92(18) |
| O(11)-Rb(1)-O(3) | 134.01(15) | O(5)#11-Y(3)-O(1)#1 | 107.60(18) |
| O(8)-Rb(1)-O(3) | 60.30(16) | O(2)#3-Y(3)-O(1)#1 | 73.27(18) |
| O(7)-Rb(1)-O(15) | 104.54(14) | O(16)-Y(3)-O(6)#1 | 149.04(19) |
| O(11)-Rb(1)-O(15) | 63.80(15) | O(12)-Y(3)-O(6)#1 | 72.85(19) |
| O(8)-Rb(1)-O(15) | 47.19(15) | O(4)-Y(3)-O(6)#1 | 72.13(19) |
| O(3)-Rb(1)-O(15) | 106.44(15) | O(13)-Y(3)-O(6)#1 | 129.89(19) |
| O(7)-Rb(1)-O(9) | 60.65(15) | O(5)#11-Y(3)-O(6)#1 | 75.43(18) |
| O(11)-Rb(1)-O(9) | 107.59(15) | O(2)#3-Y(3)-O(6)#1 | 108.68(18) |
| O(8)-Rb(1)-O(9) | 101.84(16) | O(1)#1-Y(3)-O(6)#1 | 59.11(19) |
| O(3)-Rb(1)-O(9) | 46.58(15) | O(14)-Y(5)-O(4)#11 | 150.12(12) |
| O(15)-Rb(1)-O(9) | 136.48(15) | O(14)-Y(5)-O(4)#6 | 150.12(12) |
| O(7)-Rb(1)-O(12)#1 | 118.63(15) | O(4)#11-Y(5)-O(4)#6 | 59.8(2) |
| O(11)-Rb(1)-O(12)#1 | 93.67(15) | O(14)-Y(5)-O(9)#11 | 83.38(15) |
| O(8)-Rb(1)-O(12)#1 | 113.46(15) | O(4)#11-Y(5)-O(9)#11 | 107.16(19) |
| O(3)-Rb(1)-O(12)#1 | 132.22(15) | O(4)#6-Y(5)-O(9)#11 | 84.54(19) |
| O(15)-Rb(1)-O(12)#1 | 90.37(15) | O(14)-Y(5)-O(9)#6 | 83.38(15) |
| O(9)-Rb(1)-O(12)#1 | 133.10(15) | O(4)#11-Y(5)-O(9)#6 | 84.54(19) |
| O(8)#3-Li(1)-O(16) | 113.3(6) | O(4)#6-Y(5)-O(9)#6 | 107.16(19) |
| O(8)#3-Li(1)-O(10) | 140.7(7) | O(9)#11-Y(5)-O(9)#6 | 166.8(3) |
| O(16)-Li(1)-O(10) | 106.0(6) | O(14)-Y(5)-O(6) | 78.71(13) |
| O(8)#3-Li(1)-O(13) | 103.8(6) | O(4)#11-Y(5)-O(6) | 130.85(18) |
| O(16)-Li(1)-O(13) | 93.2(6) | O(4)#6-Y(5)-O(6) | 71.67(18) |
| O(10)-Li(1)-O(13) | 74.3(5) | O(9)#11-Y(5)-O(6) | 73.46(18) |
| O(8)#3-Li(1)-O(1) | 94.9(6) | O(9)#6-Y(5)-O(6) | 103.86(18) |
| O(16)-Li(1)-O(1) | 70.9(5) | O(14)-Y(5)-O(6)#14 | 78.71(13) |
| O(10)-Li(1)-O(1) | 96.8(6) | O(4)#11-Y(5)-O(6)#14 | 71.67(18) |
| O(13)-Li(1)-O(1) | 159.3(7) | O(4)#6-Y(5)-O(6)#14 | 130.85(18) |
| O(7)-Li(2)-O(16)#4 | 116.3(7) | O(9)#11-Y(5)-O(6)#14 | 103.86(18) |
| O(7)-Li(2)-O(14)#1 | 130.1(8) | O(9)#6-Y(5)-O(6)#14 | 73.46(18) |
| O(16)#4-Li(2)-O(14)#1 | 113.6(7) | O(6)-Y(5)-O(6)#14 | 157.4(3) |
| O(7)-Li(2)-O(4)#4 | 104.1(7) | O(7)-B(5)-O(11) | 122.0(8) |
| O(16)#4-Li(2)-O(4)#4 | 93.8(6) | O(7)-B(5)-O(5) | 125.1(8) |
| O(14)#1-Li(2)-O(4)#4 | 73.6(5) | O(11)-B(5)-O(5) | 112.8(8) |
| O(7)-Li(2)-O(6)#4 | 95.6(6) | O(8)-B(6)-O(15) | 122.7(7) |

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| O(16)#4-Li(2)-O(6)#4 | 73.2(5) | O(8)-B(6)-O(2) | 124.8(8) |
| O(14)#1-Li(2)-O(6)#4 | 97.1(6) | O(15)-B(6)-O(2) | 112.3(8) |
| **$Li_2CsY_4B_5O_{15}$** | | | |
| Cs(1)-O(12)#1 | 3.033(2) | O(14)-Y(1)-O(5)#5 | 90.43(8) |
| Cs(1)-O(10) | 3.090(2) | O(11)-Y(1)-O(5)#5 | 145.42(8) |
| Cs(1)-O(4) | 3.094(2) | O(9)-Y(1)-O(5)#5 | 136.06(8) |
| Cs(1)-O(15) | 3.100(2) | O(7)#5-Y(1)-O(5)#5 | 72.21(8) |
| Cs(1)-O(13) | 3.120(3) | O(6)-Y(1)-O(5)#5 | 76.06(8) |
| Cs(1)-O(9)#2 | 3.217(3) | O(14)-Y(1)-O(3)#6 | 152.27(8) |
| Cs(1)-O(2)#1 | 3.224(2) | O(11)-Y(1)-O(3)#6 | 128.06(8) |
| Li(1)-O(15) | 1.910(6) | O(9)-Y(1)-O(3)#6 | 70.45(8) |
| Li(1)-O(14) | 1.940(6) | O(7)#5-Y(1)-O(3)#6 | 107.43(8) |
| Li(1)-O(8)#4 | 2.000(6) | O(6)-Y(1)-O(3)#6 | 77.11(8) |
| Li(1)-O(6) | 2.014(7) | O(5)#5-Y(1)-O(3)#6 | 73.28(8) |
| Li(1)-O(3) | 2.128(6) | O(14)-Y(1)-O(1)#7 | 148.69(8) |
| Li(2)-O(12) | 1.867(7) | O(11)-Y(1)-O(1)#7 | 72.46(8) |
| Li(2)-O(14)#5 | 1.907(6) | O(9)-Y(1)-O(1)#7 | 71.72(9) |
| Li(2)-O(16)#5 | 1.962(6) | O(7)#5-Y(1)-O(1)#7 | 75.76(8) |
| Li(2)-O(11)#5 | 2.045(6) | O(6)-Y(1)-O(1)#7 | 130.26(8) |
| Li(2)-O(1) | 2.107(6) | O(5)#5-Y(1)-O(1)#7 | 109.08(8) |
| Y(1)-O(14) | 2.251(2) | O(3)#6-Y(1)-O(1)#7 | 59.03(8) |
| Y(1)-O(11) | 2.326(2) | O(10)-Y(2)-O(13) | 93.76(9) |
| Y(1)-O(9) | 2.335(2) | O(10)-Y(2)-O(12) | 88.11(9) |
| Y(1)-O(7)#5 | 2.348(2) | O(13)-Y(2)-O(12) | 87.04(8) |
| Y(1)-O(6) | 2.361(2) | O(10)-Y(2)-O(2) | 99.14(9) |
| Y(1)-O(5)#5 | 2.390(2) | O(13)-Y(2)-O(2) | 165.70(9) |
| Y(1)-O(3)#6 | 2.401(2) | O(12)-Y(2)-O(2) | 87.22(8) |
| Y(1)-O(1)#7 | 2.455(2) | O(10)-Y(2)-O(10)#3 | 72.55(10) |
| Y(2)-O(10) | 2.205(2) | O(13)-Y(2)-O(10)#3 | 103.52(8) |
| Y(2)-O(13) | 2.230(2) | O(12)-Y(2)-O(10)#3 | 158.33(8) |
| Y(2)-O(12) | 2.249(2) | O(2)-Y(2)-O(10)#3 | 86.34(8) |
| Y(2)-O(2) | 2.325(2) | O(10)-Y(2)-O(1) | 166.17(8) |
| Y(2)-O(10)#3 | 2.361(2) | O(13)-Y(2)-O(1) | 89.97(9) |
| Y(2)-O(1) | 2.388(2) | O(12)-Y(2)-O(1) | 78.78(8) |
| Y(2)-O(7)#6 | 2.524(2) | O(2)-Y(2)-O(1) | 76.06(8) |
| Y(3)-O(16)#8 | 2.271(3) | O(10)#3-Y(2)-O(1) | 119.46(8) |
| Y(3)-O(11)#9 | 2.347(2) | O(10)-Y(2)-O(7)#6 | 120.04(8) |
| Y(3)-O(11)#10 | 2.347(2) | O(13)-Y(2)-O(7)#6 | 71.99(8) |

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|---|---|---|---|
| Y(3)-O(2)#1 | 2.355(3) | O(12)-Y(2)-O(7)#6 | 145.11(8) |
| Y(3)-O(2)#11 | 2.355(3) | O(2)-Y(2)-O(7)#6 | 106.25(8) |
| Y(3)-O(1)#1 | 2.477(2) | O(10)#3-Y(2)-O(7)#6 | 56.44(8) |
| Y(3)-O(1)#11 | 2.477(2) | O(1)-Y(2)-O(7)#6 | 73.77(8) |
| Y(4)-O(15) | 2.251(2) | O(16)#8-Y(3)-O(11)#9 | 150.19(5) |
| Y(4)-O(4) | 2.271(3) | O(16)#8-Y(3)-O(11)#10 | 150.19(5) |
| Y(4)-O(7) | 2.305(2) | O(11)#9-Y(3)-O(11)#10 | 59.61(11) |
| Y(4)-O(5) | 2.329(2) | O(16)#8-Y(3)-O(2)#1 | 84.93(6) |
| Y(4)-O(13)#4 | 2.343(2) | O(11)#9-Y(3)-O(2)#1 | 104.61(8) |
| Y(4)-O(3) | 2.343(2) | O(11)#10-Y(3)-O(2)#1 | 84.33(8) |
| Y(4)-O(5)#12 | 2.461(2) | O(16)#8-Y(3)-O(2)#11 | 84.93(6) |
| Y(5)-O(8) | 2.261(3) | O(11)#9-Y(3)-O(2)#11 | 84.33(8) |
| Y(5)-O(6) | 2.363(2) | O(11)#10-Y(3)-O(2)#11 | 104.61(8) |
| Y(5)-O(6)#2 | 2.363(2) | O(2)#1-Y(3)-O(2)#11 | 169.86(12) |
| Y(5)-O(9) | 2.454(2) | O(16)#8-Y(3)-O(1)#1 | 78.60(5) |
| Y(5)-O(9)#2 | 2.454(2) | O(11)#9-Y(3)-O(1)#1 | 131.05(8) |
| Y(5)-O(4)#6 | 2.537(2) | O(11)#10-Y(3)-O(1)#1 | 71.72(7) |
| Y(5)-O(4)#13 | 2.537(2) | O(2)#1-Y(3)-O(1)#1 | 73.84(8) |
| Y(5)-O(3)#6 | 2.632(2) | O(2)#11-Y(3)-O(1)#1 | 104.08(8) |
| Y(5)-O(3)#13 | 2.632(2) | O(16)#8-Y(3)-O(1)#11 | 78.60(5) |
| B(1)-O(9)#15 | 1.371(4) | O(11)#9-Y(3)-O(1)#11 | 71.72(7) |
| B(1)-O(4)#1 | 1.373(4) | O(11)#10-Y(3)-O(1)#11 | 131.05(8) |
| B(1)-O(2) | 1.385(4) | O(2)#1-Y(3)-O(1)#11 | 104.08(8) |
| B(2)-O(16) | 1.368(6) | O(2)#11-Y(3)-O(1)#11 | 73.84(8) |
| B(2)-O(11)#16 | 1.370(3) | O(1)#1-Y(3)-O(1)#11 | 157.20(11) |
| B(2)-O(11) | 1.370(3) | O(15)-Y(4)-O(4) | 84.98(9) |
| B(3)-O(12) | 1.346(5) | O(15)-Y(4)-O(7) | 88.88(8) |
| B(3)-O(10)#1 | 1.379(4) | O(4)-Y(4)-O(7) | 109.73(8) |
| B(3)-O(7) | 1.410(4) | O(15)-Y(4)-O(5) | 88.77(9) |
| B(4)-O(6)#6 | 1.375(3) | O(4)-Y(4)-O(5) | 172.55(8) |
| B(4)-O(6)#13 | 1.375(3) | O(7)-Y(4)-O(5) | 74.12(8) |
| B(4)-O(8) | 1.379(6) | O(15)-Y(4)-O(13)#4 | 156.17(8) |
| B(5)-O(14) | 1.348(5) | O(4)-Y(4)-O(13)#4 | 85.14(9) |
| B(5)-O(3) | 1.390(4) | O(7)-Y(4)-O(13)#4 | 74.20(8) |
| B(5)-O(1)#5 | 1.395(4) | O(5)-Y(4)-O(13)#4 | 102.16(8) |
| B(6)-O(15) | 1.347(5) | O(15)-Y(4)-O(3) | 80.24(8) |
| B(6)-O(13) | 1.387(4) | O(4)-Y(4)-O(3) | 76.51(8) |
| B(6)-O(5)#5 | 1.421(4) | O(7)-Y(4)-O(3) | 167.04(8) |

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|---|---|---|---|
| O(12)#1-Cs(1)-O(10) | 46.24(6) | O(5)-Y(4)-O(3) | 98.45(8) |
| O(12)#1-Cs(1)-O(4) | 98.11(6) | O(13)#4-Y(4)-O(3) | 118.22(8) |
| O(10)-Cs(1)-O(4) | 128.76(6) | O(6)#2-Y(5)-O(9) | 86.23(8) |
| O(12)#1-Cs(1)-O(15) | 116.68(6) | O(8)-Y(5)-O(9)#2 | 103.44(6) |
| O(10)-Cs(1)-O(15) | 100.31(6) | O(6)-Y(5)-O(9)#2 | 86.23(8) |
| O(4)-Cs(1)-O(15) | 59.09(6) | O(6)#2-Y(5)-O(9)#2 | 70.31(8) |
| O(12)#1-Cs(1)-O(13) | 101.86(6) | O(9)-Y(5)-O(9)#2 | 153.13(12) |
| O(10)-Cs(1)-O(13) | 62.84(6) | O(8)-Y(5)-O(4)#6 | 81.02(6) |
| O(4)-Cs(1)-O(13) | 103.30(6) | O(6)-Y(5)-O(4)#6 | 81.43(7) |
| O(15)-Cs(1)-O(13) | 45.70(6) | O(6)#2-Y(5)-O(4)#6 | 114.80(8) |
| O(12)#1-Cs(1)-O(9)#2 | 120.70(6) | O(9)-Y(5)-O(4)#6 | 129.45(8) |
| O(10)-Cs(1)-O(9)#2 | 95.94(6) | O(9)#2-Y(5)-O(4)#6 | 55.74(8) |
| O(4)-Cs(1)-O(9)#2 | 134.90(6) | O(8)-Y(5)-O(4)#13 | 81.02(6) |
| O(15)-Cs(1)-O(9)#2 | 113.36(6) | O(6)-Y(5)-O(4)#13 | 114.80(8) |
| O(13)-Cs(1)-O(9)#2 | 91.06(6) | O(6)#2-Y(5)-O(4)#13 | 81.43(7) |
| O(12)#1-Cs(1)-O(2)#1 | 60.49(6) | O(9)-Y(5)-O(4)#13 | 55.74(8) |
| O(10)-Cs(1)-O(2)#1 | 105.31(6) | O(9)#2-Y(5)-O(4)#13 | 129.45(8) |
| O(4)-Cs(1)-O(2)#1 | 45.46(6) | O(4)#6-Y(5)-O(4)#13 | 162.05(11) |
| O(15)-Cs(1)-O(2)#1 | 99.54(6) | O(8)-Y(5)-O(3)#6 | 78.17(5) |
| O(13)-Cs(1)-O(2)#1 | 132.17(6) | O(6)-Y(5)-O(3)#6 | 72.70(7) |
| O(9)#2-Cs(1)-O(2)#1 | 136.71(7) | O(6)#2-Y(5)-O(3)#6 | 130.75(8) |
| O(15)-Li(1)-O(14) | 114.3(3) | O(9)-Y(5)-O(3)#6 | 64.89(7) |
| O(15)-Li(1)-O(8)#4 | 139.5(3) | O(9)#2-Y(5)-O(3)#6 | 121.31(7) |
| O(14)-Li(1)-O(8)#4 | 106.2(3) | O(4)#6-Y(5)-O(3)#6 | 67.09(7) |
| O(15)-Li(1)-O(6) | 104.9(3) | O(4)#13-Y(5)-O(3)#6 | 108.98(7) |
| O(14)-Li(1)-O(6) | 93.5(3) | O(8)-Y(5)-O(3)#13 | 78.17(5) |
| O(8)#4-Li(1)-O(6) | 73.3(2) | O(6)-Y(5)-O(3)#13 | 130.75(8) |
| O(15)-Li(1)-O(3) | 94.2(3) | O(6)#2-Y(5)-O(3)#13 | 72.70(7) |
| O(14)-Li(1)-O(3) | 71.3(2) | O(9)-Y(5)-O(3)#13 | 121.31(7) |
| O(8)#4-Li(1)-O(3) | 97.2(3) | O(9)#2-Y(5)-O(3)#13 | 64.89(7) |
| O(6)-Li(1)-O(3) | 159.5(3) | O(4)#6-Y(5)-O(3)#13 | 108.98(7) |
| O(12)-Li(2)-O(14)#5 | 116.8(3) | O(4)#13-Y(5)-O(3)#13 | 67.09(7) |
| O(12)-Li(2)-O(16)#5 | 130.6(3) | O(3)#6-Y(5)-O(3)#13 | 156.33(10) |
| O(14)#5-Li(2)-O(16)#5 | 112.5(3) | O(9)#15-B(1)-O(4)#1 | 116.6(3) |
| O(12)-Li(2)-O(11)#5 | 106.9(3) | O(9)#15-B(1)-O(2) | 118.6(3) |
| O(14)#5-Li(2)-O(11)#5 | 93.1(3) | O(4)#1-B(1)-O(2) | 124.8(3) |
| O(16)#5-Li(2)-O(11)#5 | 73.2(2) | O(16)-B(2)-O(11)#16 | 121.6(2) |
| O(12)-Li(2)-O(1) | 95.4(3) | O(16)-B(2)-O(11) | 121.6(2) |

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|---|---|---|---|
| O(14)#5-Li(2)-O(1) | 72.9(2) | O(11)#16-B(2)-O(11) | 116.8(4) |
| O(16)#5-Li(2)-O(1) | 95.4(3) | O(12)-B(3)-O(10)#1 | 124.0(3) |
| O(11)#5-Li(2)-O(1) | 157.4(3) | O(12)-B(3)-O(7) | 123.6(3) |
| O(14)-Y(1)-O(11) | 77.62(8) | O(10)#1-B(3)-O(7) | 112.2(3) |
| O(14)-Y(1)-O(9) | 111.13(9) | O(6)#6-B(4)-O(6)#13 | 118.2(4) |
| O(11)-Y(1)-O(9) | 78.15(9) | O(6)#6-B(4)-O(8) | 120.9(2) |
| O(14)-Y(1)-O(7)#5 | 87.89(9) | O(6)#13-B(4)-O(8) | 120.9(2) |
| O(11)-Y(1)-O(7)#5 | 74.98(8) | O(14)-B(5)-O(3) | 120.3(3) |
| O(9)-Y(1)-O(7)#5 | 142.67(8) | O(14)-B(5)-O(1)#5 | 121.2(3) |
| O(14)-Y(1)-O(6) | 77.24(8) | O(3)-B(5)-O(1)#5 | 118.4(3) |
| O(11)-Y(1)-O(6) | 130.60(8) | O(15)-B(6)-O(13) | 124.1(3) |
| O(9)-Y(1)-O(6) | 72.42(8) | O(15)-B(6)-O(5)#5 | 123.6(3) |
| O(7)#5-Y(1)-O(6) | 144.74(8) | O(13)-B(6)-O(5)#5 | 112.0(3) |

Symmetry transformations used to generate equivalent atoms:

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

#4 -x+2,y-1/2,z #5 x,-y+1/2,-z+1 #6 x-1,y,-z+1/2

#7 x-1,y,z #8 -x+1,y+1/2,-z+1/2 #9 x,y,-z+1/2

#10 x,-y+3/2,-z+1 #11 -x+1,-y+1,z-1/2 #12 -x+1,y+1/2,z
#13 x,-y+3/2,z+1/2 #14 -x+2,y+1/2,z #15 x+1,y,z ($LiRb_2YB_2O_6$)

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

#4 x-1/2,-y+3/2,-z+1 #5 x,-y+3/2,z-1/2 #6 -x+3/2,y+1/2,z

#7 x+1/2,y,-z+1/2 #8 -x+3/2,y-1/2,z #9 x+1/2,-y+3/2,-z+1
#10 -x+2,-y+1,-z+1 #11 -x+1,y-1/2,-z+1/2 #12 x,-y+3/2,z+1/2 ($CaRbYB_2O_6$)

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

#4 -x+1/2,y-1,-z+1/2 #5 -x+1,-y,-z+1 #6 x,y+1,z

#7 -x+3/2,y,-z+1/2 #8 -x+1,-y-1,-z+1 #9 x+1/2,-y+1,z+1/2

#10 -x+1,-y+1,-z+1 #11 -x+1/2,y+1,-z+1/2 #12 -x+2,-y,-z+1
#13 -x+2,-y+1,-z+1 #14 -x+1/2,y,-z+1/2 #15 x-1/2,-y+1,z-1/2 ($Li_2RbY_4B_5O_{15}$)

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

#4 x,y-1,z #5 -x+1,-y,-z+1 #6 x,y+1,z #7 -x+1,-y+1,-z+1

#8 x-1,y,z #9 -x+1/2,y-1,-z+1/2 #10 x-1,y-1,z

#11 x-1/2,-y,z-1/2 #12 -x+1,-y-1,-z+1 #13 -x+1/2,y+1,-z+1/2

#14 x+1/2,-y+1,z-1/2 #15 x-1/2,-y+1,z+1/2 #16 -x+3/2,y,-z+1/2
#17 x+1/2,-y,z-1/2 #18 x+1,y+1,z #19 x+1,y,z ($Li_2CsY_4B_5O_{15}$)