|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Table S4: Bond length distances and interatomic angles of the different cationic sites in tourmalines from Minas Gerais. | | | | | | | | | | | | | | | | | |
| Interatomic bond length distances (Å) | | | | | | | | | | | | | | | | | |
|  | WR037 | WR044 | WR065 | KM058\_R | KM058\_V | KM066 | KM076 | KM117 | KM118 | KM119 | KM120 | KM132 | KF081 | WR045 | KM075 | U13757 | U20662 |
| B-O2  B-O8 x2  <B-O> | 1.342(4)  1.386(3)  1.364 | 1.355(4)  1.381(2)  1.368 | 1.360(4)  1.383(2)  1.372 | 1.359(4)  1.381(2)  1.370 | 1.364(6)  1.379(3)  1.372 | 1.350(5)  1.379(3)  1.365 | 1.350(5)  1.383(3)  1.367 | 1.355(5)  1.386(3)  1.376 | 1.354(7)  1.387(4)  1.371 | 1.361(4)  1.382(2)  1.372 | 1.358(4)  1.385(2)  1.372 | 1.361(9)  1.379(5)  1.370 | 1.357(4)  1.385(3)  1.371 | 1.348(4)  1.382(2)  1.365 | 1.349(6)  1.383(3)  1.366 | 1.354(4)  1.384(2)  1.374 | 1.354(4)  1.381(2)  1.368 |
| T-O4  T-O5  T-O6  T-O7  <T-O> | 1.6236(9)  1.6362(11)  1.6026(18)  1.6120(16)  1.619 | 1.6224(8)  1.6350(9)  1.6014(15)  1.6097(13)  1.617 | 1.6231(10)  1.6357(12)  1.603(2)  1.6104(15)  1.618 | 1.6220(8)  1.6350(10)  1.6077(16)  1.6115(13)  1.619 | 1.6227(12)  1.6333(15)  1.608(2)  1.604(2)  1.617 | 1.6201(11)  1.6347(13)  1.606(2)  1.6092(18)  1.618 | 1.6244(12)  1.6382(14)  1.599(2)  1.6115(19)  1.618 | 1.623(12)  1.636(14)  1.605(2)  1.612(19)  1.619 | 1.6181(16)  1.6317(18)  1.600(3)  1.606(3)  1.614 | 1.6226(10)  1.6380(12)  1.605(2)  1.6139(15)  1.620 | 1.6228(9)  1.6358(10)  1.6040(17)  1.6113(14)  1.618 | 1.6229(19)  1.635(2)  1.604(4)  1.615(3)  1.619 | 1.6214(10)  1.6352(12)  1.607(2)  1.6136(16)  1.619 | 1.6254(10)  1.6390(11)  1.6009(18)  1.6115(15)  1.619 | 1.6234(12)  1.6369(14)  1.603(2)  1.614(2)  1.619 | 1.6188(9)  1.6321(11)  1.6000(19)  1.607(15)  1.615 | 1.6230(8)  1.6352(9)  1.6046(15)  1.6118(13)  1.619 |
| X-O2 x3  X-O4 x3  X-O5 x3  <X-O> | 2.440(3)  2.822(3)  2.764(3)  2.675 | 2.444(3)  2.816(2)  2.754(2)  2.671 | 2.452(4)  2.810(3)  2.748(3)  2.670 | 2.454(4)  2.817(3)  2.756(3)  2.676 | 2.442(5)  2.815(4)  2.757(4)  2.671 | 2.466(4)  2.811(3)  2.745(3)  2.674 | 2.444(4)  2.821(3)  2.759(3)  2.675 | 2.453(4)  2.819(3)  2.749(3)  2.673 | 2.449(6)  2.810(5)  2.738(5)  2.666 | 2.455(4)  2.821(3)  2.754(3)  2.677 | 2.455(4)  2.812(3)  2.748(3)  2.672 | 2.521(13)  2.834(8)  2.781(7)  2.712 | 2.463(5)  2.814(3)  2.749(3)  2.675 | 2.451(3)  2.803(3)  2.752(2)  2.669 | 2.447(4)  2.820(3)  2.759(3)  2.670 | 2.447(4)  2.808(3)  2.745(3)  2.667 | 2.437(3)  2.820(2)  2.758(2)  2.672 |
| Y-O1  Y-O2 x2  Y-O3  Y-O6 x2  <Y-O> | 2.037(3)  1.9806(17)  2.165(3)  2.0254(17)  2.036 | 2.013(2)  1.9683(15)  2.154(2)  2.0002(15)  2.017 | 2.003(3)  1.967(2)  2.153(3)  1.975(2)  2.007 | 1.982(2)  1.9656(17)  2.144(3)  1.9713(17)  2.000 | 2.005(4)  1.969(3)  2.155(4)  1.988(3)  2.012 | 1.963(3)  1.962(2)  2.173(3)  1.980(2)  2.003 | 2.015(4)  1.972(2)  2.163(3)  2.017(2)  2.026 | 1.992(2)  1.966(2)  2.147(4)  1.999(3)  2.012 | 1.989(5)  1.964(3)  2.156(5)  1.976(3)  2.004 | 1.978(3)  1.962(2)  2.137(3)  1.972(2)  1.997 | 1.984(3)  1.9660(18)  2.148(3)  1.9727(18)  2.002 | 2.030(6)  1.966(3)  2.149(5)  2.043(3)  2.033 | 1.964(3)  1.958(2)  2.134(3)  1.962(2)  1.990 | 2.027(3)  1.9949(18)  2.175(3)  2.0243(17)  2.040 | 2.030(4)  1.978(2)  2.168(3)  2.024(2)  2.034 | 1.981(3)  1.9621(19)  2.153(3)  1.9725(19)  2.001 | 2.019(2)  1.9728(15)  2.157(2)  2.0039(15)  2.022 |
| Z-O3  Z-O6  Z-O7a  Z-O7b  Z-O8a  Z-O8b  <Z-O> | 1.9660(12)  1.8469(18)  1.8777(16)  1.9537(17)  1.8845(17)  1.9103(17)  1.907 | 1.9624(10)  1.8546(15)  1.8786(14)  1.9508(13)  1.8865(14)  1.9059(14)  1.906 | 1.9578(12)  1.8529(18)  1.8830(17)  1.9511(16)  1.8890(17)  1.9024(17)  1.906 | 1.9656(11)  1.8591(15)  1.8842(15)  1.9455(14)  1.8903(15)  1.9035(15)  1.908 | 1.9630(16)  1.854(2)  1.883(2)  1.952(2)  1.886(2)  1.907(2)  1.908 | 1.9579(14)  1.853(2)  1.883(2)  1.9486(18)  1.887(2)  1.9040(19)  1.906 | 1.9681(15)  1.855(2)  1.878(2)  1.953(2)  1.889(2)  1.907(2)  1.908 | 1.9654(15)  1.858(2)  1.883(2)  1.946(2)  1.888(2)  1.906(2)  1.908 | 1.959(2)  1.861(3)  1.885(3)  1.944(3)  1.892(3)  1.896(3)  1.906 | 1.9669(13)  1.8625(18)  1.8801(17)  1.9448(16)  1.8892(17)  1.9021(17)  1.908 | 1.9611(11)  1.8594(16)  1.8833(15)  1.9492(15)  1.8902(15)  1.9007(15)  1.907 | 1.976(3)  1.860(4)  1.874(4)  1.960(4)  1.888(4)  1.918(3)  1.913 | 1.9655(13)  1.8624(19)  1.8794(18)  1.9436(17)  1.8863(18)  1.8997(18)  1.906 | 1.9680(12)  1.8514(18)  1.8817(17)  1.9558(16)  1.8845(17)  1.9151(17)  1.909 | 1.9681(15)  1.850(2)  1.877(2)  1.951(2)  1.887(2)  1.911(2)  1.907 | 1.9570(12)  1.8571(18)  1.8809(16)  1.9457(16)  1.8874(17)  1.8988(17)  1.905 | 1.9641(10)  1.8529(15)  1.8794(14)  1.9504(14)  1.8851(14)  1.9090(14)  1.907 |
|  | Interatomic angles (°) | | | | | | | | | | | | | | | | |
| O4-T-O5  O6-T-O4  O6-T-O5  O6-T-O7  O7-T-O4  O7-T-O5  <O-T-O> | 104.16(12)  111.99(10)  110.90(9)  110.09(8)  110.03(11)  109.53(10)  109.450 | 104.25(10)  111.92(9)  110.83(8)  110.50(7)  109.78(9)  109.37(9)  109.442 | 104.22(12)  110.76(9)  111.90(11)  110.86(10)  109.71(11)  109.19(11)  109.440 | 104.72(10)  111.82(9)  110.75(9)  110.61(7)  109.72(9)  109.04(9)  109.443 | 104.42(16)  111.88(14)  110.66(13)  110.54(11)  109.77(14)  109.38(14)  109.442 | 104.67(14)  111.91(12)  110.79(11)  110.65(10)  109.60(12)  109.04(12)  109.443 | 104.35(14)  111.97(13)  110.99(12)  110.29(10)  109.75(13)  109.32(13)  109.445 | 104.37(15)  111.82(13)  110.85(12)  110.35(11)  109.78(13)  109.51(14)  109.447 | 104.4(2)  111.34(18)  110.74(16)  110.52(15)  110.09(17)  109.62(18)  109.452 | 104.75(12)  111.93(11)  110.88(10)  110.65(9)  109.54(11)  108.90(11)  109.442 | 104.36(11)  111.89(10)  110.85(9)  110.68(8)  109.70(10)  109.16(10)  109.440 | 105.9(2)  111.4(2)  110.5(2)  109.50(18)  109.9(2)  109.6(2)  109.467 | 104.80(12)  112.09(11)  110.79(10)  110.75(9)  109.44(11)  108.77(12)  109.440 | 103.56(12)  111.90(10)  110.18(8)  110.98(10)  110.38(10)  109.66(10)  109.443 | 104.14(15)  112.03(13)  110.88(12)  110.08(11)  110.00(14)  109.56(14)  109.448 | 104.39(12)  111.69(10)  110.78(10)  110.67(8)  109.85(10)  109.26(11)  109.440 | 104.28(10)  111.98(9)  110.84(8)  110.41(7)  109.80(9)  109.34(9)  109.442 |
| O2-B-O8 x2  O8-B-O8  <O-B-O> | 121.14(15)  117.7(3)  119.993 | 121.10(12)  117.8(2)  120.000 | 121.21(14)  117.5(3)  119.973 | 121.24(12)  117.5(2)  119.993 | 121.10(19)  117.8(4)  120.000 | 121.43(17)  117.1(3)  119.987 | 121.22(18)  117.5(4)  119.980 | 121.43(17)  117.1(3)  119.985 | 121.4(2)  117.1(5)  119.967 | 121.30(15)  117.3(3)  119.967 | 121.38(13)  117.2(3)  119.987 | 120.5(3)  118.9(6)  119.967 | 121.51(15)  116.9(3)  119.973 | 120.96(15)  118.1(3)  120.007 | 121.0(2)  118.0(4)  120.000 | 121.53(14)  116.9(3)  119.987 | 121.10(13)  117.8(3)  120.000 |