Table S1. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å2) of Na3Sm(BO3)2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Na3Sm(BO3)2 | *x* | *y* | *z* | *U*iso\*/*U*eq |
| Sm1 | 0.15904 (2) | 0.88633 (2) | 0.14639 (2) | 0.00614 (9) |
| O1 | 0.3190 (4) | 0.4208 (3) | 0.1176 (2) | 0.0179 (6) |
| O2 | 0.1929 (4) | 0.6546 (3) | 0.0211 (3) | 0.0174 (5) |
| O3 | 0.2579 (4) | 0.6362 (2) | 0.2508 (2) | 0.0099 (5) |
| O4 | 0.5137 (4) | 0.8968 (3) | 0.1309 (3) | 0.0158 (5) |
| O5 | 0.8280 (4) | 0.7894 (3) | 0.2053 (3) | 0.0140 (5) |
| O6 | 0.8331 (4) | 1.0176 (3) | 0.0816 (2) | 0.0113 (5) |
| Na1 | 0.5215 (2) | 1.18834 (16) | 0.10228 (13) | 0.0128 (3) |
| Na2 | 0.5223 (2) | 0.76316 (17) | 0.34440 (14) | 0.0146 (3) |
| Na3 | 0.2828 (4) | 0.4391 (2) | −0.10694 (18) | 0.0433 (6) |
| B1 | 0.7194 (6) | 0.9004 (4) | 0.1380 (4) | 0.0080 (7) |
| B2 | 0.2548 (6) | 0.5692 (4) | 0.1274 (4) | 0.0091 (7) |

Table S2. Atomic displacement parameters (Å2) of Na3Sm(BO3)2

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Na3Sm(BO3)2 | *U*11 | *U*22 | *U*33 | *U*12 | *U*13 | *U*23 |
| Sm1 | 0.00584 (11) | 0.00574 (11) | 0.00682 (11) | −0.00005 (5) | −0.00063 (6) | 0.00036 (5) |
| O1 | 0.0347 (16) | 0.0102 (12) | 0.0088 (12) | 0.0092 (11) | −0.0008 (11) | 0.0009 (9) |
| O2 | 0.0323 (15) | 0.0094 (11) | 0.0104 (12) | 0.0058 (11) | −0.0055 (10) | 0.0004 (10) |
| O3 | 0.0124 (12) | 0.0075 (11) | 0.0096 (12) | 0.0014 (9) | −0.0029 (9) | 0.0003 (9) |
| O4 | 0.0073 (12) | 0.0196 (14) | 0.0204 (14) | 0.0007 (9) | −0.0004 (10) | 0.0065 (10) |
| O5 | 0.0078 (11) | 0.0156 (13) | 0.0186 (13) | 0.0006 (9) | −0.0016 (9) | 0.0087 (10) |
| O6 | 0.0089 (11) | 0.0112 (11) | 0.0140 (12) | −0.0005 (9) | 0.0004 (9) | 0.0038 (9) |
| Na1 | 0.0128 (6) | 0.0137 (7) | 0.0118 (6) | 0.0008 (5) | 0.0002 (5) | −0.0030 (5) |
| Na2 | 0.0158 (7) | 0.0153 (7) | 0.0124 (7) | −0.0043 (5) | −0.0065 (5) | 0.0011 (5) |
| Na3 | 0.0920 (17) | 0.0209 (9) | 0.0166 (9) | 0.0128 (10) | −0.0109 (10) | −0.0049 (7) |
| B1 | 0.0088 (16) | 0.0095 (17) | 0.0056 (16) | 0.0009 (12) | 0.0007 (12) | −0.0005 (12) |
| B2 | 0.0097 (16) | 0.0075 (16) | 0.0100 (17) | 0.0010 (13) | −0.0006 (13) | 0.0011 (13) |