# Supporting information

***Synthesis and crystal structure of a neodymium borosilicate Nd3BSi2O10***

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Computing details

Data collection: *XRD commander* (Kienle & Jacob, 2003); program used to solve and refine structure: *TOPAS* (Bruker, 2009); molecular graphics: *VESTA* (Momma & Izumi, 2011); software used to prepare materials for publication: *publ*CIF (Westrip, 2010).

*Crystal data*

|  |  |
| --- | --- |
| Nd3BSi2O10 | *V* = 1606.47(5) Å3 |
| *Mr*= 659.7 | *Z* = 8 |
| Orthorhombic, *Pbca* | *Dx* = 5.4547 Mg m-3 |
| Hall symbol: -P 2ac 2ab | Cu *K*α1, *K*α2, λ = 1.540562, 1.544390 Å |
| *a* = 9.7889(2) Å | *T* = 295 K |
| *b* = 7.10770(10) Å | blue-violet |
| *c* = 23.0893(4) Å | cylinder, 25 × 1 mm |

*Data collection*

|  |  |
| --- | --- |
| Bruker AXS D8 Advance diffractometer | Data collection mode: reflection |
| Radiation source: sealed X-ray tube, BrukerAXS D8 | scan method: step |
| Specimen mounting: standard PMMA Ø 25 mm back loading holder | 2θmin = 14.5, 2θmax = 90, 2θstep = 0.014 |

*Refinement*

|  |  |
| --- | --- |
| *R*p = 0.030 | *R*Bragg = 0.013 |
| *R*wp = 0.040 | 82 parameters |
| *R*exp = 0.011 | Background function: Chebyshev polynomial |
|  |  |

Table S1. Atomic coordinates. Displacement parameters (Beq) were fixed as 1 Å2 during refinement.

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | *x* | y | z |
| Nd1 | 0.4909(2) | 0.3621(3) | 0.42810(6) |
| Nd2 | 0.1338(2) | 0.3296(4) | 0.33652(7) |
| Nd3 | 0.2655(2) | 0.0934(3) | 0.18257(7) |
| B1 | 0.249(4) | 0.387(7) | 0.9703(13) |
| Si1 | 0.3810(10) | 0.3516(16) | 0.0787(3) |
| Si2 | 0.4381(9) | 0.3240(17) | 0.2814(4) |
| O1 | 0.2558(17) | 0.254(3) | 0.9191(7) |
| O2 | 0.1165(18) | 0.399(3) | 0.9903(7) |
| O3 | 0.3697(19) | 0.348(3) | 0.0088(6) |
| O4 | 0.4525(17) | 0.170(3) | 0.1055(7) |
| O5 | 0.2286(15) | 0.346(3) | 0.1083(7) |
| O6 | 0.4662(17) | 0.537(3) | 0.0938(8) |
| O7 | 0.6028(18) | 0.293(2) | 0.2773(7) |
| O8 | 0.4151(15) | 0.369(2) | 0.2120(7) |
| O9 | 0.3903(18) | 0.466(2) | 0.3239(7) |
| O10 | 0.3481(15) | 0.138(3) | 0.2880(6) |

Table S2. Bond lengths and angles.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Geometric parameters (Å, º) | | | | |
| Nd1-O1i | 2.454(17) |  | O1i-Nd1-O2ii | 83.2(6) |
| Nd1-O2ii | 2.460(19) |  | O1i-Nd1-O2iii | 128.2(6) |
| Nd1-O2iii | 2.265(17) |  | O1i-Nd1-O4iv | 119.9(6) |
| Nd1-O4iv | 2.39(2) |  | O1i-Nd1-O6v | 79.8(6) |
| Nd1-O5v | 2.40(2) |  | O2ii-Nd1-O2iii | 70.5(6) |
| Nd2-O1i | 2.327(17) |  | O2ii-Nd1-O4iv | 69.9(6) |
| Nd2-O8vi | 2.432(15) |  | O2ii-Nd1-O6 | 149.5(6) |
| Nd2-O10vii | 2.47(2) |  | O2iii-Nd1-O4iv | 92.2(7) |
| Nd3-Nd3vii | 3.567(3) |  | O2iii-Nd1-O6v | 101.0(7) |
| Nd3-Nd3viii | 3.567(3) |  | O4iv-Nd1-O6v | 140.6(6) |
| Nd3-O5 | 2.457(19) |  | O1i-Nd2-O8vi | 149.1(6) |
| Nd3-O7vi | 2.325(16) |  | O1i-Nd2-O10vii | 124.2(6) |
| B1-O2 | 1.38(4) |  | O8vi-Nd2-O10vii | 75.6(5) |
| Si1-O3 | 1.618(16) |  | Nd3viii-Nd3-Nd3vii | 170.24(8) |
| Si1-O4 | 1.59(2) |  | Nd3viii-Nd3-O5viii | 44.7(4) |
| Si1-O5 | 1.641(18) |  | Nd3viii-Nd3-O7vi | 123.3(4) |
| Si1-O6 | 1.60(2) |  | Nd3vii-Nd3-O5viii | 135.7(4) |
| Si2-O7 | 1.63(2) |  | Nd3vii-Nd3-O7vi | 48.2(4) |
| Si2-O8 | 1.649(19) |  | O5viii-Nd3-O7vi | 137.0(5) |
| Si2-O9 | 1.483(19) |  | O3-Si1-O4 | 113.9(11) |
| Si2-O10 | 1.60(2) |  | O3-Si1-O5 | 110.7(10) |
|  |  |  | O3-Si1-O6 | 105.4(11) |
|  |  |  | O4-Si1-O5 | 102.6(11) |
|  |  |  | O4-Si1-O6 | 110.7(11) |
|  |  |  | O5-Si1-O6 | 113.8(11) |
|  |  |  | O7-Si2-O8 | 96.0(9) |
|  |  |  | O7-Si2-O9 | 116.3(11) |
|  |  |  | O7-Si2-O10 | 116.1(11) |
|  |  |  | O8-Si2-O9 | 117.9(11) |
|  |  |  | O8-Si2-O10 | 100.3(9) |
|  |  |  | O9-Si2-O10 | 109.0(10) |
|  |  |  | Nd1ix-O1-Nd2ix | 117.7(7) |
|  |  |  | Nd1x-O2-Nd1xi | 109.5(7) |
|  |  |  | Nd1x-O2-B1 | 104(2) |
|  |  |  | Nd1xi-O2-B1 | 141.4(17) |
|  |  |  | Nd1v-O4-Si1 | 135.9(10) |
|  |  |  | Nd3vii-O5-Si1 | 104.6(9) |
|  |  |  | Nd1iv-O6-Si1 | 147.0(11) |
|  |  |  | Nd3xii-O7-Si2 | 137.5(9) |
|  |  |  | Nd2xii-O8-Si2 | 107.8(8) |
|  |  |  | Nd2viii-O10-Si2 | 137.7(9) |

Symmetry codes: (i) x,-y+1/2,z-1/2; (ii) -x+1/2,-y+1,z-1/2; (iii) x+1/2,y,-z+3/2; (iv) -x+1,y+1/2,-z+1/2; (v) x+1/2,y,-z+1/2; (vi) x-1/2,y,-z+1/2; (vii) -x+1/2,y-1/2,z; (viii) -x+1/2,y+1/2,z; (ix) x,-y+1/2,z+1/2; (x) -x+1/2,-y+1,z+1/2; (xi) x-1/2,y,-z+3/2; (xii) x+1/2,y,-z+1/2

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