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**Supporting information for article:**

# Orientational order-disorder *γ* ↔ *β* ↔ *α′* ↔ *α* phase transitions in Sr2B2O5 pyroborate and crystal structures of *β* and *α* phases

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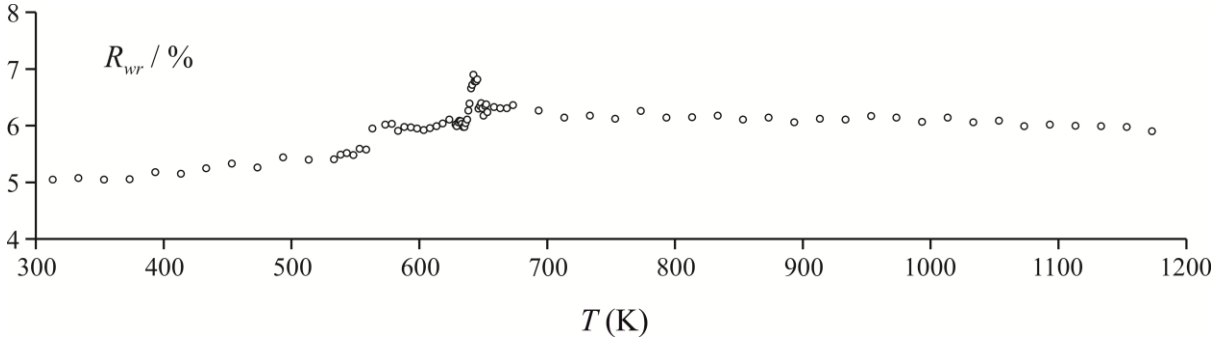


**Figure S1**

**Table S1** Experimental details of the measurement at 568 K.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $Sr_2B_2O_5$ |
| $M_r$ | 276.9 |
| Crystal system, space group | Triclinic, *P*–1 |
| Temperature (K) | 568 |
| | |
| *a*, *b*, *c* (Å) | 9.4593 (7), 13.2461 (4), 11.8639 (11) |
| α, β, γ (°) | 88.674 (7), 91.928 (7), 91.682 (7) |
| *V* (Å$^3$) | 1484.69 (18) |
| *Z* | 12 |
| Radiation type | Mo *K*α |
| μ (mm$^{-1}$) | 21.41 |
| Crystal size (mm) | 0.22 × 0.08 × 0.01 |
| | |
| Data collection | |
| Diffractometer | Xcalibur, AtlasS2, Gemini ultra |
| Absorption correction | Analytical<br>(Clark & Reid, 1995) |
| | |
| No. of measured, independent and observed [$I > 3\sigma(I)$] reflections | 21046, 5429, 1466 |
| $R_{int}$ | 0.106 |
| $(\sin \theta/\lambda)_{max}$ (Å$^{-1}$) | 0.661 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.147, 0.194, 2.83 |
| No. of reflections | 5429 |
| No. of parameters | 285 |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 6.37, -4.65 |

Computer programs: *CrysAlis PRO* 1.171.38.41 (Rigaku OD, 2015).

**Table S2** Atomic coordinates, displacement parameters (Å2) and site-occupancy factors (SOFs) in the structure of Sr2B2O5 modifications in 3D description

| Atom | Occ. | *x* | *y* | *z* | *U* iso/eq |
|---|---|---|---|---|---|
| | | | $\gamma$-$Sr_2B_2O_5$ | | |
| Sr1 | 1 | 0.62327(6) | 0.90996(8) | 0.34035(4) | 0.00756(15) |
| Sr2 | 1 | 0.11787(6) | 0.95066(9) | 0.36761(4) | 0.00801(15) |
| O1 | 1 | 0.6437(5) | 0.3478(7) | 0.6483(3) | 0.0116(11) |
| O2 | 1 | 0.0987(5) | 0.4070(7) | 0.6692(3) | 0.0125(12) |
| O3 | 1 | 0.3928(5) | 0.2876(7) | 0.8593(3) | 0.0125(12) |
| O4 | 1 | 0.8542(4) | 0.2998(6) | 0.9285(3) | 0.0097(11) |
| O5 | 1 | 0.7462(5) | 0.6012(6) | 0.4932(3) | 0.0137(12) |
| B1 | 1 | 0.6599(8) | 0.5697(11) | 0.5953(5) | 0.0081(17) |
| B2 | 1 | 0.1611(8) | 0.5489(11) | 0.5841(5) | 0.0089(17) |
| | | | $\beta$-$Sr_2B_2O_5$ | | |
| Sr1 | 1 | 0.70892(8) | 0.09510(6) | 0.34759(6) | 0.0209(2) |
| Sr2 | 1 | 0.04720(8) | 0.92415(5) | 0.36218(6) | 0.0196(2) |
| Sr3 | 1 | 0.37774(8) | 0.75776(6) | 0.35632(7) | 0.0267(3) |
| Sr4 | 1 | 0.71458(8) | 0.60563(6) | 0.35623(6) | 0.0235(2) |
| Sr5 | 1 | 0.04627(8) | 0.43538(6) | 0.36293(6) | 0.0219(2) |
| Sr6 | 1 | 0.38104(8) | 0.27060(6) | 0.36092(7) | 0.0245(2) |
| Sr7 | 1 | 0.38232(8) | 0.00104(5) | 0.16754(6) | 0.0209(2) |
| Sr8 | 1 | 0.73464(8) | 0.84858(6) | 0.12191(6) | 0.0208(2) |
| Sr9 | 1 | 0.06011(8) | 0.67659(6) | 0.12282(6) | 0.0210(2) |
| Sr10 | 1 | 0.38921(8) | 0.50987(5) | 0.13384(6) | 0.0200(2) |
| Sr11 | 1 | 0.71972(8) | 0.34256(5) | 0.15101(6) | 0.0197(2) |
| Sr12 | 1 | 0.05373(8) | 0.17209(5) | 0.15907(6) | 0.0195(2) |
| O1 | 1 | 0.5581(6) | 0.9116(4) | 0.6442(5) | 0.0310(19) |
| O2 | 1 | 0.8883(5) | 0.7460(4) | 0.6484(4) | 0.0233(18) |
| O3 | 1 | 0.2175(5) | 0.5739(4) | 0.6596(4) | 0.0266(18) |
| O4 | 1 | 0.5506(6) | 0.4317(4) | 0.6725(4) | 0.0283(19) |
| O5 | 1 | 0.8863(6) | 0.2686(4) | 0.6840(4) | 0.0273(18) |
| O6 | 1 | 0.2079(6) | 0.1227(5) | 0.6777(5) | 0.044(2) |
| O7 | 1 | 0.5487(6) | 0.1842(4) | 0.8312(5) | 0.039(2) |
| O8 | 1 | 0.8972(6) | 0.0181(4) | 0.8283(4) | 0.0244(18) |
| O9 | 1 | 0.2075(5) | 0.8379(4) | 0.8451(4) | 0.0200(17) |

| | | | | | |
|---|---|---|---|---|---|
| O10 | 1 | 0.5555(6) | 0.6722(4) | 0.8354(5) | 0.038(2) |
| O11 | 1 | 0.8780(6) | 0.5053(4) | 0.8305(4) | 0.0284(19) |
| O12 | 1 | 0.2140(6) | 0.3378(4) | 0.8372(4) | 0.033(2) |
| O13 | 1 | 0.3640(6) | 0.9772(4) | 0.8592(5) | 0.033(2) |
| O14 | 1 | 0.6912(6) | 0.8194(4) | 0.8830(6) | 0.050(3) |
| O15 | 1 | 0.6794(6) | 0.3142(4) | 0.9254(5) | 0.042(2) |
| O16 | 1 | 0.0047(5) | 0.1471(4) | 0.9471(4) | 0.0223(17) |
| O17 | 0.5 | 0.0242(14) | 0.6417(10) | 0.8702(11) | 0.027(3)* |
| O18 | 0.5 | 0.3560(13) | 0.4746(9) | 0.8905(10) | 0.017(3)* |
| O19 | 0.5 | 0.0179(14) | 0.6484(10) | 0.9076(11) | 0.027(4)* |
| O20 | 0.5 | 0.3481(14) | 0.4793(10) | 0.9267(10) | 0.024(3)* |
| O21 | 1 | 0.6921(6) | 0.5570(4) | 0.5724(5) | 0.039(2) |
| O22 | 1 | 0.0258(5) | 0.3911(3) | 0.5769(4) | 0.0255(18) |
| O23 | 1 | 0.3692(5) | 0.2274(4) | 0.5711(4) | 0.0274(18) |
| O24 | 1 | 0.6843(6) | 0.0673(4) | 0.6140(5) | 0.034(2) |
| O25 | 1 | 0.0218(6) | 0.9003(4) | 0.6167(5) | 0.033(2) |
| O26 | 1 | 0.3476(6) | 0.7279(4) | 0.6336(5) | 0.037(2) |
| O27 | 1 | 0.7022(6) | 0.9434(4) | 0.4807(4) | 0.037(2) |
| O28 | 1 | 0.0499(6) | 0.7702(4) | 0.4961(4) | 0.040(2) |
| O29 | 1 | 0.3570(7) | 0.6122(4) | 0.4948(5) | 0.050(2) |
| O30 | 1 | 0.4843(7) | 0.2314(6) | 0.0032(5) | 0.088(4) |
| O31 | 1 | 0.7923(6) | 0.0515(4) | 0.9979(4) | 0.0329(19) |
| O32 | 0.5 | 0.8428(13) | 0.5561(10) | 0.0030(11) | 0.045(4)* |
| O33 | 0.5 | 0.1556(13) | 0.3912(9) | 0.0057(10) | 0.036(3)* |
| B1 | 1 | 0.6430(9) | 0.9751(7) | 0.5839(8) | 0.023(3) |
| B2 | 1 | 0.9808(9) | 0.8046(7) | 0.5889(7) | 0.016(3) |
| B3 | 1 | 0.3034(9) | 0.6363(6) | 0.5995(7) | 0.015(3) |
| B4 | 1 | 0.6285(10) | 0.4676(7) | 0.5849(7) | 0.021(3) |
| B5 | 1 | 0.9570(9) | 0.3032(6) | 0.5922(7) | 0.017(3) |
| B6 | 1 | 0.2945(10) | 0.1412(6) | 0.5899(7) | 0.018(3) |
| B7 | 1 | 0.2588(9) | 0.9162(7) | 0.9012(8) | 0.019(3) |
| B8 | 1 | 0.5902(9) | 0.7493(6) | 0.9022(7) | 0.015(3) |
| B9 | 1 | 0.9167(9) | 0.5767(7) | 0.9018(7) | 0.018(3) |
| B10 | 1 | 0.2447(9) | 0.4102(6) | 0.9114(7) | 0.018(3) |
| B11 | 1 | 0.5785(10) | 0.2440(7) | 0.9194(7) | 0.018(3) |
| B12 | 1 | 0.9062(9) | 0.0735(6) | 0.9230(7) | 0.016(3) |
| | | | $\alpha$-$Sr_2B_2O_5$ | | |
| Sr | 1 | 1.23349(13) | 0.90193(10) | 0.35875(5) | 0.0300(2) |
| O1 | 1 | 1.2538(11) | 0.4053(8) | 0.6668(4) | 0.0435(16) |
| O2 | 0.5 | 0.763(7) | 0.325(5) | 0.8816(15) | 0.044(6) |
| O2' | 0.5 | 0.731(6) | 0.312(5) | 0.9255(13) | 0.030(5) |
| O3 | 0.5 | 0.527(5) | 0.5691(16) | 0.4976(13) | 0.058(4) |
| B | 1 | 1.3272(17) | 0.5774(12) | 0.5902(6) | 0.024(2) |

*isotropical ADP

**Table S3** Anisotropic parameters of atomic displacements the structure of $Sr_2B_2O_5$ modifications in 3D description.

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| | | | $\gamma$-$Sr_2B_2O_5$ | | | |
| Sr1 | 0.0070(3) | 0.0069(3) | 0.0088(3) | 0.00038(18) | 0.00040(18) | 0.00015(16) |
| Sr2 | 0.0072(3) | 0.0087(3) | 0.0083(3) | 0.00064(19) | 0.00160(18) | 0.00128(17) |
| O1 | 0.012(2) | 0.0101(19) | 0.013(2) | 0.0008(15) | 0.0034(15) | 0.0022(14) |
| O2 | 0.015(2) | 0.014(2) | 0.009(2) | -0.0023(16) | 0.0028(15) | 0.0013(14) |
| O3 | 0.014(2) | 0.009(2) | 0.015(2) | 0.0004(15) | 0.0054(15) | 0.0013(14) |
| O4 | 0.0094(19) | 0.0082(19) | 0.0116(19) | 0.0017(15) | 0.0004(14) | -0.0004(13) |
| O5 | 0.020(2) | 0.010(2) | 0.011(2) | 0.0050(16) | 0.0075(16) | 0.0025(14) |
| B1 | 0.007(3) | 0.011(3) | 0.006(3) | -0.001(2) | -0.001(2) | 0.002(2) |
| B2 | 0.005(3) | 0.013(3) | 0.009(3) | 0.000(2) | 0.000(2) | 0.000(2) |
| | | | $\beta$-$Sr_2B_2O_5$ | | | |
| Sr1 | 0.0176(4) | 0.0190(4) | 0.0260(4) | 0.0004(3) | 0.0014(3) | 0.0043(3) |
| Sr2 | 0.0190(4) | 0.0143(4) | 0.0255(4) | 0.0015(3) | 0.0031(3) | 0.0014(3) |
| Sr3 | 0.0195(4) | 0.0142(4) | 0.0464(5) | 0.0021(3) | 0.0031(4) | 0.0038(3) |
| Sr4 | 0.0196(4) | 0.0202(4) | 0.0308(4) | 0.0029(3) | 0.0034(3) | 0.0002(3) |
| Sr5 | 0.0175(4) | 0.0173(4) | 0.0311(4) | 0.0031(3) | 0.0035(3) | 0.0003(3) |
| Sr6 | 0.0201(4) | 0.0211(4) | 0.0324(4) | 0.0025(3) | 0.0055(3) | 0.0062(3) |
| Sr7 | 0.0174(4) | 0.0164(4) | 0.0290(4) | 0.0001(3) | -0.0003(3) | -0.0042(3) |
| Sr8 | 0.0211(4) | 0.0186(4) | 0.0232(4) | 0.0023(3) | 0.0010(3) | -0.0046(3) |
| Sr9 | 0.0219(4) | 0.0190(4) | 0.0222(4) | 0.0025(3) | -0.0023(3) | -0.0018(3) |
| Sr10 | 0.0199(4) | 0.0169(4) | 0.0235(4) | 0.0039(3) | -0.0005(3) | -0.0028(3) |
| Sr11 | 0.0210(4) | 0.0165(4) | 0.0216(4) | 0.0017(3) | -0.0011(3) | -0.0032(3) |
| Sr12 | 0.0181(4) | 0.0190(4) | 0.0214(4) | 0.0020(3) | -0.0002(3) | -0.0018(3) |
| O1 | 0.031(3) | 0.025(3) | 0.037(3) | 0.002(3) | 0.005(3) | -0.001(3) |
| O2 | 0.021(3) | 0.026(3) | 0.023(3) | -0.001(3) | 0.004(2) | -0.005(2) |
| O3 | 0.026(3) | 0.025(3) | 0.029(3) | 0.001(3) | 0.005(3) | 0.007(2) |
| O4 | 0.024(3) | 0.042(4) | 0.019(3) | 0.003(3) | -0.001(2) | 0.000(3) |
| O5 | 0.031(3) | 0.036(3) | 0.015(3) | -0.002(3) | 0.006(2) | -0.007(2) |
| O6 | 0.031(4) | 0.072(5) | 0.029(3) | -0.015(3) | 0.011(3) | -0.007(3) |
| O7 | 0.057(4) | 0.023(3) | 0.035(4) | -0.001(3) | -0.014(3) | -0.012(3) |
| O8 | 0.033(3) | 0.024(3) | 0.017(3) | -0.003(3) | 0.007(2) | -0.002(2) |
| O9 | 0.023(3) | 0.014(3) | 0.023(3) | 0.001(2) | 0.001(2) | -0.003(2) |
| O10 | 0.050(4) | 0.027(3) | 0.036(4) | -0.006(3) | -0.012(3) | -0.007(3) |
| O11 | 0.032(3) | 0.013(3) | 0.040(4) | -0.002(3) | -0.011(3) | -0.009(3) |
| O12 | 0.041(4) | 0.027(3) | 0.032(3) | 0.005(3) | -0.004(3) | -0.009(3) |
| O13 | 0.020(3) | 0.022(3) | 0.056(4) | -0.005(3) | 0.004(3) | -0.003(3) |
| O14 | 0.027(4) | 0.015(3) | 0.107(6) | -0.006(3) | -0.002(4) | 0.006(3) |
| O15 | 0.033(4) | 0.014(3) | 0.077(5) | -0.005(3) | -0.005(3) | 0.006(3) |
| O16 | 0.020(3) | 0.019(3) | 0.028(3) | -0.005(2) | -0.003(2) | -0.005(2) |
| O21 | 0.035(4) | 0.028(3) | 0.052(4) | -0.004(3) | -0.001(3) | 0.005(3) |
| O22 | 0.027(3) | 0.011(3) | 0.039(3) | -0.003(2) | 0.009(3) | -0.002(2) |
| O23 | 0.023(3) | 0.025(3) | 0.034(3) | -0.006(3) | 0.000(2) | 0.000(2) |
| O24 | 0.030(3) | 0.011(3) | 0.061(4) | -0.005(3) | 0.006(3) | -0.013(3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O25 | 0.033(4) | 0.021(3) | 0.047(4) | 0.003(3) | 0.000(3) | -0.009(3) |
| O26 | 0.032(4) | 0.014(3) | 0.066(4) | -0.009(3) | 0.000(3) | -0.010(3) |
| O27 | 0.057(4) | 0.024(3) | 0.031(3) | -0.007(3) | 0.019(3) | -0.005(3) |
| O28 | 0.052(4) | 0.039(4) | 0.029(3) | -0.009(3) | 0.020(3) | -0.010(3) |
| O29 | 0.080(5) | 0.037(4) | 0.034(4) | 0.004(4) | 0.018(3) | -0.014(3) |
| O30 | 0.073(6) | 0.146(8) | 0.048(5) | 0.026(6) | 0.037(4) | -0.008(5) |
| O31 | 0.035(4) | 0.038(3) | 0.025(3) | -0.016(3) | 0.006(3) | -0.013(3) |
| B1 | 0.014(5) | 0.026(5) | 0.030(5) | 0.006(4) | -0.005(4) | -0.003(4) |
| B2 | 0.021(5) | 0.017(5) | 0.010(4) | 0.006(4) | 0.000(4) | 0.000(3) |
| B3 | 0.014(5) | 0.013(4) | 0.018(4) | -0.001(4) | -0.002(4) | 0.001(3) |
| B4 | 0.023(5) | 0.024(5) | 0.016(5) | 0.005(4) | -0.003(4) | -0.002(4) |
| B5 | 0.021(5) | 0.011(4) | 0.019(4) | 0.006(4) | -0.004(4) | -0.002(4) |
| B6 | 0.027(5) | 0.012(4) | 0.016(4) | 0.007(4) | 0.000(4) | -0.008(4) |
| B7 | 0.012(5) | 0.017(5) | 0.028(5) | -0.004(4) | 0.006(4) | -0.005(4) |
| B8 | 0.009(4) | 0.019(5) | 0.017(4) | 0.003(4) | -0.008(3) | -0.003(4) |
| B9 | 0.018(5) | 0.019(5) | 0.018(4) | -0.007(4) | -0.001(4) | -0.002(4) |
| B10 | 0.020(5) | 0.013(4) | 0.022(5) | 0.005(4) | 0.007(4) | 0.000(4) |
| B11 | 0.023(5) | 0.023(5) | 0.010(4) | 0.006(4) | 0.004(4) | 0.001(4) |
| B12 | 0.021(5) | 0.006(4) | 0.022(5) | 0.002(4) | -0.006(4) | -0.002(3) |
| | | | $\alpha$-$Sr_2B_2O_5$ | | | |
| Sr | 0.0193(4) | 0.0256(4) | 0.0449(5) | -0.0020(2) | 0.0004(3) | 0.0076(3) |
| O1 | 0.044(3) | 0.040(3) | 0.046(3) | -0.015(2) | 0.001(2) | 0.014(2) |
| O2 | 0.033(7) | 0.015(5) | 0.084(16) | 0.001(4) | 0.015(12) | 0.015(11) |
| O2' | 0.024(8) | 0.022(6) | 0.043(9) | 0.000(5) | -0.002(7) | 0.010(7) |
| O3 | 0.090(9) | 0.048(8) | 0.039(5) | -0.008(9) | 0.044(5) | -0.003(8) |
| B | 0.019(3) | 0.025(3) | 0.027(4) | 0.003(3) | 0.002(3) | 0.002(3) |

**Table S4** Atomic coordinates, displacement parameters (Å$^2$) and site-occupancy factors (SOFs) in the structure of $Sr_2B_2O_5$ modifications in 4D superspace description

| Atom | Occ. | *x* | *y* | *z* | *U* iso/eq |
|---|---|---|---|---|---|
| | | | $\gamma$-$Sr_2B_2O_5$ | | |
| Sr | 1 | 1.24116(9) | 0.93026(6) | 0.35395(3) | 0.00779(12) |
| O1 | 1 | 1.2466(7) | 0.3746(5) | 0.6577(2) | 0.0120(8) |
| O2 | 0.5 | 0.7856(9) | 0.2875(7) | 0.8593(3) | 0.0125(12) |
| O2' | 0.5 | 0.7084(9) | 0.2997(6) | 0.9285(3) | 0.0098(11) |
| O3 | 0.5 | 0.4923(10) | 0.6013(6) | 0.4932(3) | 0.0137(12) |
| B | 1 | 1.3213(11) | 0.5581(8) | 0.5890(4) | 0.0084(12) |
| | | | $\beta$-$Sr_2B_2O_5$ | | |
| Sr1 | 1 | 1.22906(9) | 0.90884(7) | 0.35769(3) | 0.02280(11) |
| Sr2 | 1 | 0.76227(9) | 0.40663(6) | 0.14340(3) | 0.02036(11) |
| O1a | 1 | 1.2515(6) | 0.4030(5) | 0.66439(19) | 0.0289(8) |
| O1b | 1 | 0.7483(7) | 0.8992(6) | 0.8355(2) | 0.0308(9) |
| O2a | 0.3333 | 0.7471(14) | 0.3294(9) | 0.8807(5) | 0.050(2) |
| O2a' | 0.3333 | 0.7177(12) | 0.2994(8) | 0.9445(4) | 0.0263(14) |
| O2a'' | 0.1667 | 0.766(3) | 0.306(2) | 0.8874(8) | 0.022(2)* |
| O2a''' | 0.1667 | 0.740(3) | 0.308(2) | 0.9229(9) | 0.024(2)* |
| O2b | 0.5 | 1.2759(9) | 0.8149(6) | 0.5728(3) | 0.0293(11) |
| O2b' | 0.5 | 1.2372(9) | 0.8119(6) | 0.6238(3) | 0.0345(12) |
| O3a | 0.5 | 0.5130(9) | 0.5857(7) | 0.4911(3) | 0.0405(13) |
| O3b | 0.3333 | 0.4959(13) | -0.0735(10) | 0.0013(4) | 0.067(2) |
| O3b' | 0.1667 | 0.549(3) | -0.0540(16) | 0.0042(9) | 0.045(2)* |
| B1 | 1 | 1.3265(10) | 0.5775(8) | 0.5898(3) | 0.0178(12) |
| B2 | 1 | 0.6755(10) | 0.0717(8) | 0.9097(3) | 0.0172(11) |

*isotropical ADP

**Table S5** Anisotropic parameters of atomic displacements the structure of $Sr_2B_2O_5$ modifications in 4D superspace description

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| | | | $\gamma$-$Sr_2B_2O_5$ | | | |
| Sr1 | 0.0070(3) | 0.0069(3) | 0.0088(3) | 0.00038(18) | 0.00040(18) | 0.00015(16) |
| Sr2 | 0.0072(3) | 0.0087(3) | 0.0083(3) | 0.00064(19) | 0.00160(18) | 0.00128(17) |
| O1 | 0.012(2) | 0.0101(19) | 0.013(2) | 0.0008(15) | 0.0034(15) | 0.0022(14) |
| O2 | 0.015(2) | 0.014(2) | 0.009(2) | -0.0023(16) | 0.0028(15) | 0.0013(14) |
| O3 | 0.014(2) | 0.009(2) | 0.015(2) | 0.0004(15) | 0.0054(15) | 0.0013(14) |
| O4 | 0.0094(19) | 0.0082(19) | 0.0116(19) | 0.0017(15) | 0.0004(14) | -0.0004(13) |
| O5 | 0.020(2) | 0.010(2) | 0.011(2) | 0.0050(16) | 0.0075(16) | 0.0025(14) |
| B1 | 0.007(3) | 0.011(3) | 0.006(3) | -0.001(2) | -0.001(2) | 0.002(2) |
| B2 | 0.005(3) | 0.013(3) | 0.009(3) | 0.000(2) | 0.000(2) | 0.000(2) |
| | | | $\beta$-$Sr_2B_2O_5$ | | | |
| Sr1 | 0.01688(19) | 0.01957(19) | 0.03197(19) | 0.00114(14) | 0.00123(13) | 0.00408(15) |
| Sr2 | 0.01757(19) | 0.01963(19) | 0.02392(17) | 0.00163(14) | 0.00149(13) | -0.00292(13) |
| O1a | 0.0305(15) | 0.0308(14) | 0.0256(13) | -0.0048(12) | 0.0049(11) | 0.0011(11) |
| O1b | 0.0358(17) | 0.0261(15) | 0.0305(15) | 0.0075(13) | 0.0002(12) | -0.0092(12) |
| O2a | 0.031(4) | 0.019(3) | 0.100(5) | 0.000(2) | -0.006(3) | 0.008(3) |
| O2a' | 0.028(2) | 0.016(2) | 0.035(3) | 0.0011(16) | -0.0035(19) | -0.0026(18) |
| O2b | 0.030(2) | 0.0173(17) | 0.041(2) | 0.0013(14) | 0.0022(15) | 0.0017(15) |
| O2b' | 0.030(2) | 0.0172(17) | 0.057(2) | 0.0056(14) | 0.0075(17) | -0.0078(16) |
| O3a | 0.055(3) | 0.0363(19) | 0.0315(19) | 0.0130(17) | 0.0214(18) | 0.0036(15) |
| O3b | 0.067(5) | 0.095(5) | 0.039(3) | -0.021(4) | 0.027(3) | 0.005(3) |
| B1 | 0.014(2) | 0.021(2) | 0.0182(18) | 0.0031(17) | -0.0006(14) | -0.0029(17) |
| B2 | 0.017(2) | 0.017(2) | 0.0182(17) | 0.0011(16) | 0.0017(14) | -0.0010(16) |

**Table S6** Selected geometric parameters (Å) in structure of $\gamma$-$Sr_2B_2O_5$

| | | | |
|---|---|---|---|
| Sr1—O1$^{i}$ | 2.497 (4) | Sr2—O2$^{ii}$ | 2.474 (4) |
| Sr1—O1$^{ii}$ | 2.633 (4) | Sr2—O3$^{ii}$ | 2.556 (4) |
| Sr2—O4$^{iii}$ | 2.574 (4) | Sr2—O4$^{v}$ | 2.551 (4) |
| Sr1—O2$^{i}$ | 2.749 (4) | B1—O1 | 1.350 (7) |
| Sr1—O3$^{i}$ | 2.593 (4) | B1—O3$^{v}$ | 1.353 (7) |
| Sr1—O3$^{ii}$ | 2.428 (4) | B1—O5 | 1.422 (7) |
| Sr1—O4$^{ii}$ | 2.557 (3) | B2—O2 | 1.369 (7) |
| Sr1—O5 | 2.600 (4) | B2—O4$^{v}$ | 1.352 (7) |
| Sr2—O1$^{i}$ | 2.456 (4) | B2—O5$^{i}$ | 1.436 (7) |
| Sr2—O2$^{iv}$ | 2.568 (4) | | |

Symmetry codes: (i) -*x*+1, -*y*+1, -*z*+1; (ii) *x*, -*y*+3/2, *z*-1/2; (iii) *x*-1, -*y*+3/2, *z*-1/2; (iv) -*x*, -*y*+1, -*z*+1; (v) -*x*+1, *y*+1/2, -*z*+3/2.

**Table S7** Selected geometric parameters (Å) in structure of $\beta$-$Sr_2B_2O_5$

| | | | |
|---|---|---|---|
| Sr1—O1$^{i}$ | 2.531 (6) | Sr10—O18$^{vii}$ | 2.941 (12) |
| Sr1—O9$^{i}$ | 2.574 (5) | Sr10—O18$^{i}$ | 2.440 (12) |
| Sr1—O13$^{i}$ | 2.718 (6) | Sr10—O20$^{vii}$ | 2.518 (12) |
| Sr1—O25$^{i}$ | 2.571 (6) | Sr10—O20$^{i}$ | 2.607 (13) |
| Sr1—O26$^{i}$ | 2.439 (5) | Sr10—O32$^{viii}$ | 2.825 (13) |
| Sr1—O27$^{ii}$ | 2.534 (5) | Sr11—O3$^{i}$ | 2.574 (5) |
| Sr2—O5$^{i}$ | 2.721 (5) | Sr11—O9$^{i}$ | 2.509 (5) |
| Sr2—O6$^{iii}$ | 2.512 (6) | Sr11—O10$^{i}$ | 2.617 (6) |
| Sr2—O8$^{i}$ | 2.440 (5) | Sr11—O15$^{vii}$ | 2.726 (6) |
| Sr2—O24$^{i}$ | 2.549 (6) | Sr11—O17$^{i}$ | 2.448 (13) |
| Sr2—O25$^{iv}$ | 2.456 (5) | Sr11—O18$^{i}$ | 2.582 (12) |
| Sr2—O28 | 2.563 (5) | Sr11—O19$^{i}$ | 2.598 (14) |

| | | | |
|---|---|---|---|
| Sr3—O4$^{i}$ | 2.654 (6) | Sr11—O20$^{i}$ | 2.609 (13) |
| Sr3—O5$^{i}$ | 2.548 (5) | Sr11—O26$^{i}$ | 2.789 (6) |
| Sr3—O7$^{i}$ | 2.454 (6) | Sr12—O2$^{i}$ | 2.589 (5) |
| Sr3—O23$^{i}$ | 2.527 (5) | Sr12—O8$^{v}$ | 2.579 (5) |
| Sr3—O24$^{i}$ | 2.445 (5) | Sr12—O9$^{iii}$ | 2.472 (5) |
| Sr3—O29 | 2.519 (6) | Sr12—O14$^{i}$ | 2.479 (6) |
| Sr4—O3$^{i}$ | 2.496 (5) | Sr12—O16$^{vii}$ | 2.571 (5) |
| Sr4—O4$^{i}$ | 2.561 (5) | Sr12—O17$^{iii}$ | 2.611 (13) |
| Sr4—O12$^{i}$ | 2.507 (5) | Sr12—O19$^{iii}$ | 2.596 (13) |
| Sr4—O21 | 2.645 (6) | Sr12—O25$^{iii}$ | 2.913 (6) |
| Sr4—O22$^{i}$ | 2.560 (5) | B1—O1 | 1.358 (11) |
| Sr4—O23$^{i}$ | 2.549 (5) | B1—O24$^{xi}$ | 1.328 (11) |
| Sr5—O2$^{i}$ | 2.509 (5) | B1—O27 | 1.437 (11) |
| Sr5—O3$^{iii}$ | 2.504 (5) | B2—O2 | 1.359 (10) |
| Sr5—O11$^{i}$ | 2.529 (5) | B2—O25$^{xii}$ | 1.364 (10) |
| Sr5—O21$^{i}$ | 2.572 (6) | B2—O28$^{xii}$ | 1.388 (10) |
| Sr5—O22 | 2.606 (5) | B3—O3 | 1.353 (10) |
| Sr5—O22$^{iii}$ | 2.542 (5) | B3—O26 | 1.343 (10) |
| Sr6—O1$^{i}$ | 2.504 (5) | B3—O29 | 1.401 (10) |
| Sr6—O2$^{i}$ | 2.553 (5) | B4—O4 | 1.363 (10) |
| Sr6—O10$^{i}$ | 2.519 (5) | B4—O21 | 1.325 (11) |
| Sr6—O21$^{i}$ | 2.555 (6) | B4—O29$^{i}$ | 1.446 (11) |
| Sr6—O23 | 2.553 (5) | B5—O5 | 1.361 (10) |
| Sr6—O26$^{i}$ | 2.567 (6) | B5—O22$^{xii}$ | 1.332 (10) |
| Sr7—O1$^{i}$ | 2.579 (5) | B5—O28$^{i}$ | 1.445 (10) |
| Sr7—O7$^{v}$ | 2.560 (6) | B6—O6 | 1.360 (10) |
| Sr7—O8$^{v}$ | 2.653 (5) | B6—O23 | 1.347 (10) |
| Sr7—O13$^{i}$ | 2.440 (5) | B6—O27$^{i}$ | 1.416 (10) |
| Sr7—O14$^{i}$ | 2.555 (5) | B7—O9 | 1.321 (10) |
| Sr7—O24$^{v}$ | 2.812 (6) | B7—O13 | 1.367 (10) |
| Sr7—O31$^{v}$ | 2.624 (5) | B7—O31$^{xiii}$ | 1.384 (10) |
| Sr8—O6$^{i}$ | 2.459 (5) | B8—O10 | 1.335 (10) |
| Sr8—O7$^{i}$ | 2.776 (6) | B8—O14 | 1.339 (10) |
| Sr8—O12$^{i}$ | 2.567 (5) | B8—O30$^{i}$ | 1.375 (11) |
| Sr8—O13$^{vi}$ | 2.533 (5) | B9—O11 | 1.322 (10) |
| Sr8—O14$^{vii}$ | 2.885 (7) | B9—O17$^{xii}$ | 1.372 (16) |
| Sr8—O16$^{i}$ | 2.621 (5) | B9—O19$^{xii}$ | 1.334 (16) |
| Sr8—O30$^{viii}$ | 2.721 (7) | B9—O32$^{xiv}$ | 1.425 (15) |
| Sr9—O5$^{i}$ | 2.454 (5) | B9—O33$^{i}$ | 1.390 (15) |
| Sr9—O11$^{i}$ | 2.545 (5) | B10—O12 | 1.338 (10) |
| Sr9—O12$^{iii}$ | 2.653 (6) | B10—O18 | 1.365 (15) |
| Sr9—O15$^{i}$ | 2.547 (6) | B10—O20 | 1.335 (15) |
| Sr9—O16$^{iii}$ | 2.551 (5) | B10—O32$^{i}$ | 1.415 (16) |
| Sr9—O19$^{vii}$ | 2.607 (13) | B10—O33$^{xiv}$ | 1.435 (15) |
| Sr9—O32$^{ix}$ | 2.927 (13) | B11—O7 | 1.346 (10) |
| Sr9—O33$^{x}$ | 2.662 (12) | B11—O15 | 1.319 (10) |
| Sr10—O4$^{i}$ | 2.486 (5) | B11—O30$^{xiv}$ | 1.360 (11) |
| Sr10—O10$^{i}$ | 2.503 (6) | B12—O8 | 1.355 (10) |
| Sr10—O11$^{i}$ | 2.579 (5) | B12—O16$^{xii}$ | 1.362 (9) |
| Sr10—O15$^{i}$ | 2.521 (5) | B12—O31 | 1.438 (10) |

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

**Table S8** Selected geometric parameters (Å) in structure of $\alpha$-$Sr_2B_2O_5$

| | | | |
|---|---|---|---|
| Sr—O1$^{i}$ | 2.532 (4) | Sr—O2$^{iv}$ | 2.58 (2) |
| Sr—O1$^{ii}$ | 2.623 (4) | Sr—O3$^{vi}$ | 2.666 (14) |
| Sr—O1$^{iii}$ | 2.506 (5) | B—O1 | 1.335 (8) |
| Sr—O2$^{iii}$ | 2.38 (3) | B—O2$^{v}$ | 1.42 (3) |
| Sr—O2$^{iv}$ | 2.54 (3) | B—O2$^{v}$ | 1.29 (3) |
| Sr—O2$^{v}$ | 2.605 (16) | B—O3$^{vi}$ | 1.371 (18) |
| Sr—O2$^{iii}$ | 2.64 (2) | B—O3$^{i}$ | 1.437 (16) |

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+3, -y+1, -z+1$; (iii) $x, -y+3/2, z-1/2$; (iv) $x+1, -y+3/2, z-1/2$; (v) $-x+2, y+1/2, -z+3/2$; (vi) $x+1, y, z$.

**Table S9** The equations of temperature dependences of unit cell parameters and volume of the $Sr_2B_2O_5$ modifications.

| |
|---|
| 313–568 K |
| $a_t$=3.8685(4)+0.0406(18)$t$+0.0340(20)$t^2$ |
| $b_t$=5.33035(65)+0.0163(30)$t$+0.0364(33)$t^2$ |
| $c_t$=11.8499(11)+0.0795(52)$t$–0.0360(58)$t^2$ |
| $\beta_t$=92.915(19)–0.775(85)$t$–0.325(94)$t^2$ |
| $V_t$=244.028(42)+5.14(19)$t$+3.14(21)$t^2$ |
| 573–636K |
| $a_t$=3.831(13)+0.160(44)$t$–0.069(36)$t^2$ |
| $b_t$=5.435(28)–0.255(93)$t$+0.243(76)$t^2$ |
| $c_t$=12.061(47)–0.80(15)$t$+0.77(13)$t^2$ |
| $\alpha_t$=90.2091(89)–0.277(15)$t$ |
| $\beta_t$=93.12(44)–2(1)$t$ |
| $\gamma_t$=90.362(21)–0.412(33)$t$ |
| $V_t$=229(4)+55(13)$t$–38(10)$t^2$ |
| 636–641K |
| $a_t$=3.9599(10)–0.088(15) |
| $b_t$=5.234(22–0.215(35)$t$ |
| $c_t$=23.12265(0)–37.03174(0)$t$+30.39616(0)$t^2$ |
| $\alpha_t$=91.36(40)–2.08(62)$t$ |
| $\beta_t$=97.94(35)–9.36(56)$t$ |
| $\gamma_t$=95.16(42)–7.96(65)$t$ |
| $V_t$=268.62990(0)–105.45020(0)$t$+116.50220$t^2$ |
| 641–646 K |
| $a_t$=3.8509(69)+0.082(11)$t$ |
| $b_t$=5.2823(90)$_+$0.141(14)$t$ |
| $c_t$=11.662(58)+0.332(90)$t$ |
| $\alpha_t$=92.54(10)–4(2)$t$ |
| $\beta_t$=94.22(31)–3.57(49)t |
| $\gamma_t$=92.62(32)–4.00(50)$t$ |
| $V_t$=237(1)+18(2)$t$ |
| 646–658 K |
| $a_t$=3.916(87)–0.17(27)$t$+0.24(21)$t^2$ |
| $b_t$=–7(2)+39(5)$t$–30(4)$t^2$ |
| $c_t$=0.72194(0)+22.99574(0)$t$+9(7)$t^2$–27(6)$t^3$ |
| $\beta_t$=106(8)–174.16000(0)$t$+435.57600(0)$t^2$–310.36200(0)$t^3$ |
| $V_t$=395(63)–257(94)$t$–266.46330(0)t$^2$+488(148)$t^3$ |
| 658–753 K |
| $a_t$=3.83746(76)+0.1040(11)$t$ |
| $b_t$=5.416(45)–0.14(13)$t$+0.121(91)t$^2$ |

| |
|---|
| $c_t$=12.042(61)–0.49(18)$t$+0.35(12)$t^2$ |
| $\beta_t$=90.06(55)+6(2)$t$–5(1)$t^2$ |
| $V_t$=240(2)+18(6)$t$–7(4)$t^2$ |
| 753–1173 K |
| $a_t$=3.86145(95)+0.0550(20)$t$+0.0228(10)$t^2$ |
| $b_t$=5.3530(12)+0.0401(25)$t$–0.0113(13)$t^2$ |
| $c_t$=11.8568(41)–0.0236(87)$t$+0.0617(45)$t^2$ |
| $\beta_t$=92.3757(10)–0.422(20 )$t$–0.390(11)$t^2$ |
| $V_t$=244.89(10)+4.87(22)$t$+2.33(11)$t^2$ |