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## Supplementary Information

Synthesis and crystal structure of  $\text{Sr}_3\text{Bi}_2\text{O}_6$  and structure change in the strontium-bismuth-oxide system

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## Tables

Table S1 Atomic coordinates and isotropic and equivalent displacement parameters ( $U_{\text{iso}}$ ,  $U_{\text{eq}}/\text{\AA}^2$ ) for  $\text{Sr}_3\text{Bi}_2\text{O}_6$ .

| Atom | Occ. | $x$        | $y$        | $z$         | $U_{\text{iso}}$ , $U_{\text{eq}}^*$ |
|------|------|------------|------------|-------------|--------------------------------------|
| Bi1  | 1    | 0.74344(2) | 0.49796(2) | 0.79624(3)  | 0.00743(14)                          |
| Bi2  | 1    | 0.90791(3) | 0.58183(2) | 0.53710(3)  | 0.00803(14)                          |
| Bi3  | 1    | 0.50375(2) | 0.51060(3) | 0.61207(3)  | 0.00916(14)                          |
| Bi4  | 1    | 0.72692(3) | 0.73815(2) | 0.19483(3)  | 0.00915(14)                          |
| Bi5  | 1    | 0.59300(3) | 0.41892(2) | 0.46790(3)  | 0.00909(14)                          |
| Bi6  | 1    | 2/3        | 1/3        | 0.71155(5)  | 0.0104(2)                            |
| Sr7  | 1    | 2/3        | 1/3        | 1/3         | 0.0079(6)                            |
| Sr8  | 1    | 0.65335(6) | 0.57452(6) | 0.32301(8)  | 0.0093(3)                            |
| Sr9  | 1    | 3/8        | 2/3        | 2/3         | 0.0078(4)                            |
| Sr10 | 1    | 0.66241(6) | 0.57589(6) | 0.93384(8)  | 0.0093(3)                            |
| Sr11 | 1    | 0.74681(6) | 0.50252(6) | 0.61035(8)  | 0.0087(3)                            |
| Sr12 | 1    | 0.74159(6) | 0.49626(6) | 0.39317(8)  | 0.0091(3)                            |
| Sr13 | 1    | 0.57399(6) | 0.41516(6) | 0.66953(7)  | 0.0101(3)                            |
| Sr14 | 1    | 0.66415(6) | 0.83349(6) | 0.13622(8)  | 0.0100(3)                            |
| Sr15 | 1    | 2/3        | 1/3        | 0.53059(13) | 0.0106(5)                            |
| Sr16 | 1    | 0.58051(6) | 0.66317(6) | 0.04723(8)  | 0.0093(3)                            |
| O17  | 1    | 0.7337(5)  | 0.8117(5)  | 0.2537(5)   | 0.011(2)                             |
| O18  | 1    | 0.8059(5)  | 0.5738(5)  | 0.7376(6)   | 0.019(2)                             |
| O19  | 1    | 0.7342(5)  | 0.5494(5)  | 0.8784(6)   | 0.016(2)                             |
| O20  | 1    | 0.4506(5)  | 0.4357(5)  | 0.6785(5)   | 0.013(2)                             |
| O21  | 1    | 0.8417(5)  | 0.5633(5)  | 0.4591(5)   | 0.013(2)                             |
| O22  | 1    | 0.5943(5)  | 0.3509(5)  | 0.4062(6)   | 0.018(2)                             |
| O23  | 1    | 0.6826(4)  | 0.6783(5)  | 0.2807(5)   | 0.012(2)                             |
| O24  | 1    | 0.6430(5)  | 0.7212(5)  | 0.1493(5)   | 0.014(2)                             |
| O25  | 1    | 0.8537(5)  | 0.5211(5)  | 0.6138(5)   | 0.014(2)                             |
| O26  | 1    | 0.9003(5)  | 0.6547(5)  | 0.5780(6)   | 0.016(2)                             |
| O27  | 1    | 0.6762(5)  | 0.4425(5)  | 0.5145(6)   | 0.022(3)                             |
| O28  | 1    | 0.6745(5)  | 0.4862(5)  | 0.7238(5)   | 0.015(2)                             |
| O29  | 1    | 0.5850(5)  | 0.5121(5)  | 0.6311(6)   | 0.016(2)                             |
| O30  | 1    | 0.6298(5)  | 0.4812(5)  | 0.3851(6)   | 0.015(2)                             |
| O31  | 1    | 0.5980(5)  | 0.3330(5)  | 0.6485(6)   | 0.017(2)                             |
| O32  | 1    | 0.5116(5)  | 0.5725(5)  | 0.6920(6)   | 0.016(2)                             |

\*  $U_{\text{eq}} = (\sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j) / 3$

Table S2 Anistropic displacement parameters ( $U_{ij}/\text{\AA}^2$ ) for  $\text{Sr}_3\text{Bi}_2\text{O}_6$ .

| Atom | $U_{11}$  | $U_{22}$  | $U_{33}$   | $U_{23}$     | $U_{13}$     | $U_{12}$    |
|------|-----------|-----------|------------|--------------|--------------|-------------|
| Bi1  | 0.0072(3) | 0.0066(2) | 0.0091(3)  | 0.00009(18)  | -0.00019(18) | 0.0039(2)   |
| Bi2  | 0.0074(3) | 0.0073(3) | 0.0094(3)  | 0.00029(18)  | 0.00084(18)  | 0.0036(2)   |
| Bi3  | 0.0086(3) | 0.0101(3) | 0.0100(3)  | 0.0002(2)    | -0.0004(2)   | 0.0056(2)   |
| Bi4  | 0.0099(3) | 0.0059(3) | 0.0107(3)  | -0.00060(19) | 0.0020(2)    | 0.0031(2)   |
| Bi5  | 0.0098(3) | 0.0071(3) | 0.0099(3)  | 0.00027(19)  | 0.00243(19)  | 0.0038(2)   |
| Bi6  | 0.0099(3) | 0.0099(3) | 0.0115(5)  | 0.000        | 0.000        | 0.00494(14) |
| Sr7  | 0.0068(9) | 0.0068(9) | 0.0099(15) | 0.000        | 0.000        | 0.0034(4)   |
| Sr8  | 0.0071(6) | 0.0070(6) | 0.0134(7)  | 0.0038(5)    | 0.0007(5)    | 0.0032(5)   |
| Sr9  | 0.0070(8) | 0.0064(8) | 0.0092(9)  | 0.0010(7)    | 0.0005(6)    | 0.0027(7)   |
| Sr10 | 0.0062(6) | 0.0088(6) | 0.0134(7)  | -0.0003(5)   | -0.0003(5)   | 0.0041(5)   |
| Sr11 | 0.0083(6) | 0.0059(6) | 0.0125(7)  | -0.0010(5)   | -0.0012(5)   | 0.0039(5)   |
| Sr12 | 0.0085(6) | 0.0078(6) | 0.0113(7)  | 0.0012(5)    | -0.0005(5)   | 0.0045(5)   |
| Sr13 | 0.0094(6) | 0.0075(6) | 0.0123(7)  | -0.0018(5)   | -0.0040(5)   | 0.0034(5)   |
| Sr14 | 0.0076(6) | 0.0088(6) | 0.0134(7)  | 0.0002(5)    | 0.0001(5)    | 0.0040(5)   |
| Sr15 | 0.0096(7) | 0.0096(7) | 0.0126(11) | 0.000        | 0.000        | 0.0048(3)   |
| Sr16 | 0.0099(6) | 0.0092(6) | 0.0110(7)  | -0.0016(5)   | -0.0015(5)   | 0.0065(5)   |
| O18  | 0.014(6)  | 0.020(6)  | 0.027(6)   | 0.008(5)     | 0.010(5)     | 0.011(5)    |
| O19  | 0.012(5)  | 0.019(6)  | 0.021(6)   | 0.005(4)     | 0.006(4)     | 0.011(5)    |
| O21  | 0.011(5)  | 0.012(5)  | 0.018(6)   | -0.001(4)    | -0.001(4)    | 0.007(4)    |
| O23  | 0.008(5)  | 0.016(5)  | 0.010(5)   | 0.006(4)     | 0.001(4)     | 0.005(4)    |
| O26  | 0.009(5)  | 0.010(5)  | 0.028(6)   | -0.010(4)    | -0.002(4)    | 0.004(4)    |
| O27  | 0.024(6)  | 0.015(6)  | 0.020(6)   | -0.011(5)    | -0.010(5)    | 0.005(5)    |
| O28  | 0.019(6)  | 0.015(5)  | 0.015(5)   | -0.006(4)    | -0.006(4)    | 0.012(5)    |
| O29  | 0.006(5)  | 0.010(5)  | 0.033(6)   | -0.001(4)    | -0.004(4)    | 0.006(4)    |
| O30  | 0.009(5)  | 0.014(5)  | 0.021(6)   | -0.003(4)    | -0.010(4)    | 0.005(4)    |
| O31  | 0.010(5)  | 0.014(5)  | 0.026(6)   | 0.002(5)     | 0.000(4)     | 0.004(5)    |
| O32  | 0.016(6)  | 0.010(5)  | 0.024(6)   | -0.004(4)    | 0.000(4)     | 0.007(5)    |

## Figures

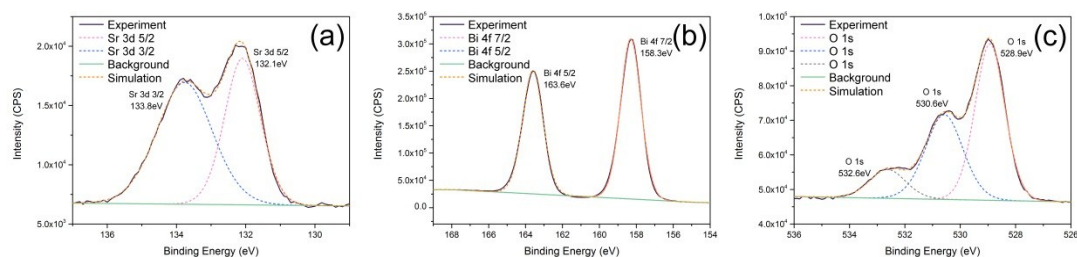


Fig. S1 XPS spectra of  $\text{Sr}_{1-x}\text{Bi}_x\text{O}_{1+0.5x}$  ( $x=0.813$ ). High-resolution XPS spectra of (a) Sr 3d core level, (b) Bi 4f core level, and (c) O 1s core level.

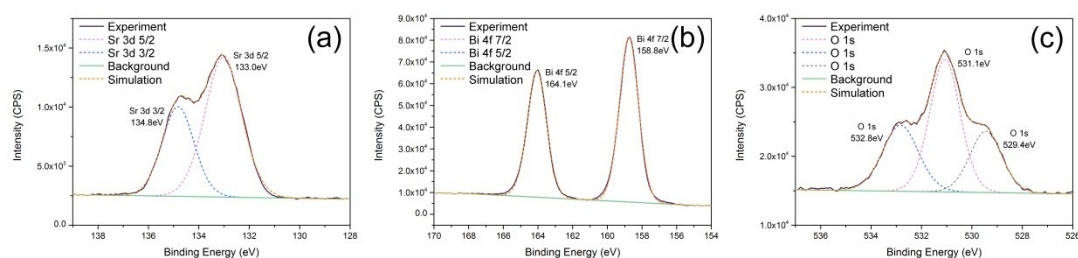


Fig. S2 XPS spectra of  $\text{Sr}_2\text{Bi}_2\text{O}_5$ . High-resolution XPS spectra of (a) Sr 3d core level, (b) Bi 4f core level, and (c) O 1s core level.

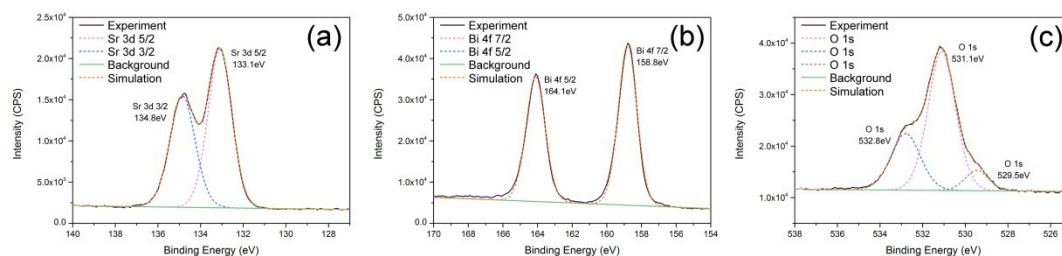


Fig. S3 XPS spectra of  $\text{Sr}_3\text{Bi}_2\text{O}_6$ . High-resolution XPS spectra of (a) Sr 3d core level, (b) Bi 4f core level, and (c) O 1s core level.