crystals

MDPI

Supplementary Materials

Floating Zone Growth of Pure and Pb-Doped Bi-2201 Crystals

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Supplementary Information

Table S1. Crystal data and structure refinement for OD23K.

Refined composition	**$Bi_{1.902}Sr_2CuO_{5.885}$**
M_r	730.48
Crystal system, space group	Orthorhombic, *Ccc*2 (37)
Temperature (K)	298
a, *b*, *c* (Å)	5.3947(6), 24.605(3), 5.2786(6)
V (Å^3)	700.68(15)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	65.708
Crystal size (mm)	0.04×0.03×0.01
Data collection	
Diffractometer	Bruker D8 VENTURE
Absorption correction	Multi-scan
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6333, 984, 808
R_{int}	0.077
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.693
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.0478, 0.1119, 1.089
No. of reflections	984
No. of parameters	37
No. of restraints	1
	$w = 1/[\sigma^2(F_o^2) + (0.0257P)^2 + 125.5544P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\varrho_{max}$, $\Delta\varrho_{min}$ (e Å^{-3})	3.262, -2.687
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.47(6)

Table S2. Fractional Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for OD23K. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	**x/*a***	**y/*b***	**z/*c***	**U_{eq}**	**Occ.**
Bi1	0.2676(1)	0.43697(4)	0.27412(2)	17.8(3)	0.951(11)
Sr1	0.2466(4)	0.67736(11)	0.2540(8)	19.4(9)	1

Cu1	1/4	3/4	0.757(1)	16.2(11)	1
O1	-0.003(8)	0.7517(8)	0.513(6)	20(4)	1
O2	0.231(3)	0.3544(7)	0.247(5)	20	0.94(5)
O3	0.650(4)	0.4322(9)	0.374(4)	20	1

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for OD23K. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Bi1	15.2(5)	22.7(5)	15.5(5)	4.4(6)	-4.1(12)	0.5(4)
Sr1	12.1(11)	29.3(13)	16.7(19)	-0.4(16)	-5(2)	-2.3(8)
Cu1	9.2(18)	28(2)	11(3)	0	0	0.5(15)

Table S4. Crystal data and structure refinement for OD3K.

Refined composition	**$Bi_{1.88}CuO_{5.73}Sr_2$**
M_r	722.82
Crystal system, space group	Orthorhombic, *Ccc*2 (37)
Temperature (K)	298
a, *b*, *c* (Å)	5.3878(4), 24.553(2), 5.2646(4)
V ($Å^3$)	696.43(9)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	65.477
Crystal size (mm)	0.05×0.03×0.01
Data collection	
Diffractometer	Bruker D8 VENTURE
Absorption correction	Multi-scan
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12508, 1070, 855
R_{int}	0.1170
$(\sin\theta/\lambda)_{max}$ ($Å^{-1}$)	0.693
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.0852, 0.1731, 1.162
No. of reflections	1070
No. of parameters	41
No. of restraints	1
	$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 201.8843P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	6.58, -2.57
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.40(11)

Table S5. Fractional Atomic Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for OD3K. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x/*a*	y/*b*	z/*c*	U_{eq}	Occ.
Bi1A	0.2672(2)	0.43701(7)	0.2747.5(2)	25.4(5)	0.904(1)
Bi1B	0.2630(70)	0.4070(20)	0.2600(200)	25(4)	0.034(1)
Sr1	0.2473(6)	0.6772.5(18)	0.2570(20)	39.3(17)	1
Cu1	1/4	3/4	0.7590(50)	40(2)	1
O1	0.0030(80)	0.7521(11)	0.4930(70)	25(6)	0.87(2)
O2	0.2270(50)	0.3539(11)	0.2480(90)	25	1
O3	0.6480(60)	0.4321(13)	0.3850(60)	25	1

Table S6. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for OD3K. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi1A	18.2(7)	21.4(9)	36.5(8)	5.8(13)	-8.1(14)	0.8(6)
Bi1B	18(11)	21.4(7)	36.5(9)	5.8(8)	-8.1(13)	0.8(14)
Sr1	14.8(16)	34.6(19)	69(5)	-4(4)	-17(4)	-3.4(13)
Cu1	13(3)	35(3)	71(7)	0	0	-1(2)