JOURNAL OF SOLID STATE CHEMISTRY **84**, 144–152 (1990)

Crystal Structure of Nonsuperconducting $Pb_2(Sr_{0.94}Nd_{0.06})_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$

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Received June 5, 1989; in revised form September 18, 1989

The crystal structure of $Pb_2(Sr_{0.94}Nd_{0.06})_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$ was determined by single crystal X-ray diffraction. The compound was found to be orthorhombic (*Cmmm*) with $a = 5.437(3)$, $b = 5.472(2)$, $c = 15.797(7)$ Å and $Z = 2$. In the structure double layers of CuO square pyramids are separated by (Nd, Sr) oxygen deficient layers which are stacked between (PbO)–Cu–(PbO) slabs. The oxygen in the Pb planes is shifted toward a pair of Pb atoms resulting in an orthorhombic distortion of the tetragonal unit cell. The possibilities for modulations and superlattices are discussed as is the role of the PbO planes in superconductivity. © 1990 Academic Press, Inc.

Introduction

The family of high-T_c copper oxide materials has expanded rapidly in the last several years from $Ln_{2-x}M_xCuO_4$ ($x \sim 0.15$) (*1*), $LnBa_2Cu_3O_7$ (*2*), $Bi_2Sr_2Ca_{n-1}Cu_nO_{2n+4}$ (*3*), $Tl_m(Ba, Sr)_2Ca_{n-1}Cu_nO_{2n+2+m}$ ($m = 1$, 2; $n = 1$–5) (*4*) and recently to $Pb_2Sr_2Ln_{1-x}(Sr, Ca)_xCu_3O_8$ (Ln = Y, rare earth) (*5, 6*). The structure of the new lead containing superconductors are similar to the previously known high-T_c materials consisting of slabs of two planes of square pyramidal CuO separated by rare earth ions. Each slab is separated by slabs of (PbO)–Cu–(PbO). For $x = 0$, the samples are nonsuperconducting while T_c reaches a maximum of 70 K for $x \sim 0.5$. The minimum value of x and the exact doping scheme necessary for superconductivity have not been well established for this compound. The presence of anomalous thermal parameters and structural modulations in several high-T_c materials calls into question the role of the metal oxide superstructure or "electron sink." In this paper we report the structure of $Pb_2(Sr_{0.94}Nd_{0.06})_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$, a nonsuperconducting analog of $Pb_2Sr_2Ln_{1-x}(Sr, Ca)_xCu_3O_8$, and discuss the above questions.

Experimental

Single crystals were grown by flux melting using a method similar to that described in Ref. (*5*). PbO, $SrCO_3$, Nd_2O_3, and CuO were used as starting materials. A composition of $Pb_{3.5}Sr_{3.25}Nd_{0.75}Cu_4O_x$ was heated to 1050°C in an atmosphere of 1% O_2 in N_2, equilibrated for 1 hr, slowly cooled to 700°C at a rate of ~2°C/min, and furnace cooled to room temperature. Black, plate-like crystals of average size ~1 × 1 × 0.1 mm were mechanically separated from the matrix.

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0022-4596/90 $3.00

TABLE I

SINGLE CRYSTAL X-RAY DIFFRACTION DATA COLLECTION INFORMATION

Formula	$Pb_2(Sr_{0.94}Nd_{0.06})_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$
Dimensions	0.21 × 0.26 × 0.043 mm
Crystal system	Orthorhombic
a	5.437(3) Å
b	5.472(2) Å
c	15.797(7) Å
V	470.0(4) Å^3
Space group	*Cmmm*
Z	2
Formula weight	1045.67
Calculated density	7.15 g/cm^3
Diffractometer	Enraf-Nonius CAD4
Radiation	Mo$K\alpha$ (0.7107 Å)
Monochromator	Graphite
Temperature	298 K
ω scan range	$\Delta\omega = 1.2 + 0.347 \tan\theta$
θ range	0–50°
Octants	$-h, +k, \pm l$
Function minimized	$\Sigma w(\lvert F_o\rvert - \lvert F_c\rvert)^2$
$R_{av} = (\Sigma w(\lvert F_o\rvert^2 - \lvert F_{av}\rvert^2)^2/\Sigma w\lvert F_o\rvert^2)^{1/2}$	0.073
Transmission factor range	0.01124–0.1672
μ	594.3 cm^{-1}
Absorption correction	Analytical (*9*, *10*)
Data/parameters	18.2
Unique reflections	1384
Reflections in refinement	673
$R = \Sigma(\lvert F_c\rvert - \lvert F_o\rvert)/\Sigma\lvert F_c\rvert$	0.067
$R_w = \Sigma w(\lvert F_c\rvert - \lvert F_o\rvert)^2/\Sigma wF_c^2$	0.092
S	1.699

Information on the single crystal X-ray data collection and refinement is shown in Table I. Intensities were measured for 2768 reflections. The space group was orthorhombic *Cmmm* and the Friedel pairs were averaged resulting in a data set of 1384 reflections, of which 673 had $I_{obs} > 3\sigma$ and were used in the final refinement. The starting parameters were those given in the single crystal X-ray study by Cava *et al.* (*5*). The structure refinement was carried out using the full-matrix least-squares program UPALS (*7*). $R(F)$ was calculated for reflections with $0 < \sin\theta/\lambda < 1.1$. R_w was calculated for reflections with the additional constraint $0.75 < I_{obs}/I_{calc} < 1.5$ with the weighting factor $w = 2|F_o|/[\sigma^2(F_o^2) + (0.04|F_o^2|)^2]$. Scattering factors and anomalous scattering factors were taken from the *International Tables for X-ray Crystallography*, Vol. IV (*8*). The data were corrected for Lorentz, polarization, and absorption effects. The absorption correction was performed using the analytical method of de Meulenaer and Tompa (*9*, *10*). A total of 37 parameters including one scale factor, positional parameters, anisotropic thermal parameters, and occupancies were refined. Systematic absences indicated that the orthorhombic lattice of the crystal is C centered. The final refinement was done in space group *Cmmm* for direct comparison

TABLE II

POSITIONAL AND THERMAL PARAMETERS FOR $Pb_2(Sr_{0.94}Nd_{0.06})_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$

Atom	Symbol	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}
Pb	$4l$	0.5	0.0	0.38859(5)	0.0172(5)	0.0136(4)	0.0107(2)	0
Sr, Nd[a]	$4k$	0.0	0.0	0.2217(2)	0.017(1)	0.0106(9)	0.0215(9)	0
Nd, Sr[a]	$2a$	0.0	0.0	0.0	0.0067(9)	0.0068(8)	0.0196(7)	0
Cu1	$2d$	0.0	0.0	0.5	0.018(2)	0.015(2)	0.010(1)	0
Cu2	$4l$	0.5	0.0	0.1103(2)	0.009(1)	0.0056(9)	0.020(1)	0
O1	$4l$	0.5	0.0	0.257(1)	0.03(1)	0.03(1)	0.013(6)	0
O2	$16r$	0.075(8)	−0.075(8)	0.389(2)	0.03(2)	0.02(2)	0.02(1)	0
O3	$8m$	0.25	0.25	0.0985(8)	0.008(4)	0.009(4)	0.033(5)	0.001(4)

Note. Standard deviations are given in parentheses. The form of the anisotropic thermal parameters is $\exp[-2\pi^2(U_{11}a^{*2}h^2 + U_{22}b^{*2}k^2 + U_{33}c^{*2}l^2 + 2U_{12}a^*b^*hk)]$. $U_{13} = U_{23} = 0$.

[a] Occupancies are $g_{Sr} = 0.94$, $g_{Nd} = 0.06$ for Sr, Nd and $g_{Nd} = 0.76$, $g_{Sr} = 0.24$ for Nd, Sr. Occupancies and thermal parameters for these atoms were held constant in the final refinement. ESD's are taken from an earlier refinement.

to $Pb_2Sr_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$ (*5*). Observed and calculated structure factors are included as supplemental material.[1]

Results

The structure of $Pb_2(Sr_{0.94}Nd_{0.06})_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$ is shown in the ORTEP diagram in Fig. 1. It can be described as slabs of (CuO)–(Nd, Sr)–(CuO) alternating with slabs of (PbO)–Cu–(PbO) separated by rock salt layers of (Sr, Nd)O. The CuO slabs are oxygen deficient perovskite layers nearly identical to those found in $LnBa_2Cu_3O_{7-\delta}$ $(0 < \delta < 1)$, $YBa_2Cu_4O_8$, $Y_2Ba_4Cu_7O_{15}$, $Tl_m(Ba, Sr)_2CaCu_2O_{6+m}$ $(m = 1, 2)$, $Bi_2Sr_2CaCu_2O_8$, and $La_2SrCu_2O_6$. The PbO slabs are oxygen deficient rock salt layers which coordinate to the CuO slabs through an apical oxygen that bridges five coordinate copper and lead polyhedra in the same way that TlO and BiO polyhedra are bonded to the CuO planes in the $(Tl, Bi)_m(Ba, Sr)_2Ca_{n-1}Cu_nO_{2+2n+m}$ superconductors. Table II gives positional and thermal parameters for $Pb_2(Sr_{0.94}Nd_{0.06})_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$.

Cu2 is coordinated to five oxygens in a square pyramidal configuration with four short (1.937(1) Å) and one long (2.31(2) Å) bond, again very similar to the seven compounds mentioned above. The (Nd, Sr) atoms between the two CuO planes are coordinated to eight oxygen atoms, four in each plane. The (Sr, Nd) atoms have a ninefold coordination to four nearly coplanar O1 atoms, four O3 atoms in the CuO plane, and one O2 atom. Cu1 is coordinated to two O2 atoms in a linear arrangement if the O2 atoms sit on their ideal sites $(0, 0, z)$. This type of coordination is typical for Cu^{1+} and is found in many complexes including the superconductor $Y_{1-x}Ca_xBa_2Cu_3O_6$ (*11*). The Pb atoms are also in a square pyramidal configuration of oxygens similar to that

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[1] See NAPS document No. 04738 for six pages of supplementary material. Order from ASIS/NAPS. Microfiche Publications, P.O. Box 3513, Grand Central Station, New York, N.Y. 10163. Remit in advance \$4.00 for microfiche copy or for photocopy, \$7.75 up to 20 pages plus \$.30 for each additional page. All orders must be prepaid. Institutions and Organizations may order by purchase order. However, there is a billing and handling charge for this service of \$15. Foreign orders add \$4.50 for postage and handling, for the first 20 pages, and \$1.00 for additional 10 pages of material, \$1.50 for postage of any microfiche orders.

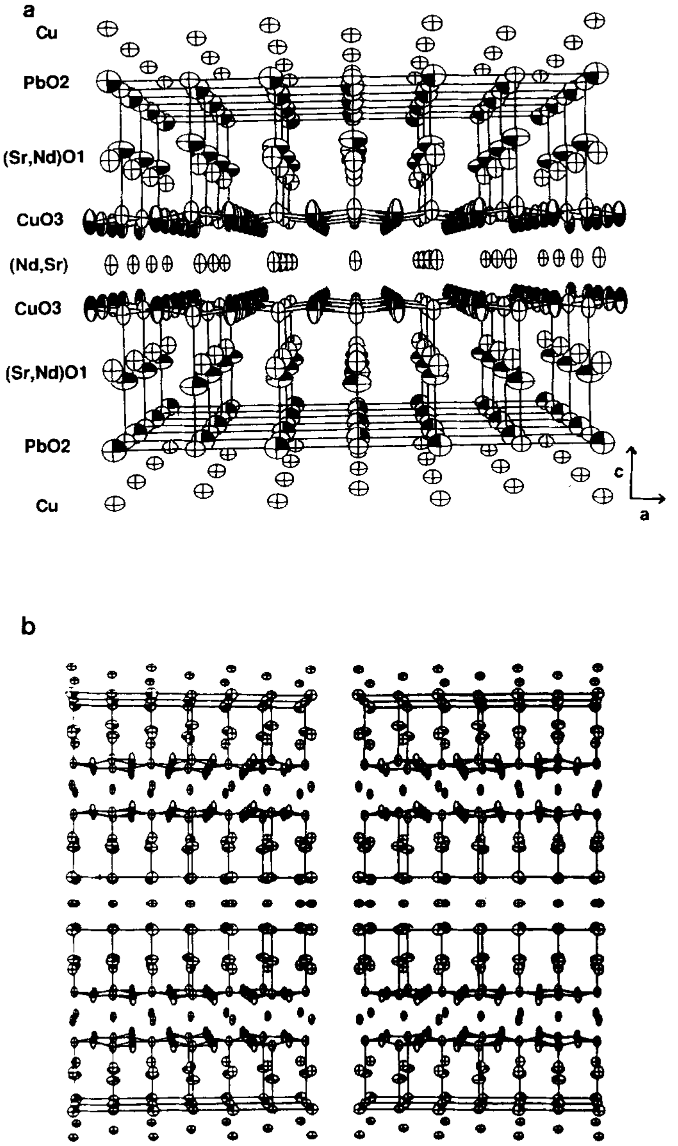

FIG. 1. (a) ORTEP diagram of the structure of $Pb_2(Sr_{0.94}Nd_{0.06})_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$. (b) Stereodiagram of the structure of $Pb_2(Sr_{0.94}Nd_{0.06})_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$. The probability ellipsoids are drawn at the 50% level with the oxygen atoms shaded. Both figures are drawn with the *a–c* plane in the plane of the paper.

of Cu2. Ideally, this would result in one short and four long Pb–O bonds. However, O2 is shifted from its ideal position by 0.075*x* and 0.075*y* and results in two short and two long coplanar bonds. Therefore, the net environment around the Pb atom is two long bonds (3.15(4) and 3.17(4) Å (Pb–O2)) and three short bonds (2.36(4), 2.35(4) Å (Pb–O2) and 2.08(2) Å (Pb–O1)). At the completion of this study we became aware

TABLE III

SELECTED BOND DISTANCES FOR $Pb_2(Sr_{0.94}Nd_{0.06})_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$

Bond	Distance (Å)	Multiplicity
Pb–O1	2.08(2)	1
Pb–O2	2.35(4)	1
Pb–O2	2.36(4)	1
Pb–O2	3.15(4)	1
Pb–O2	3.17(4)	1
(Sr, Nd)–O1	2.774(4)	2
(Sr, Nd)–O1	2.791(4)	2
(Sr, Nd)–O2	2.71(4)	1
(Sr, Nd)–O3	2.74(2)	4
(Nd, Sr)–O3	2.478(8)	8
Cu1–O2	1.84(3)	2
Cu2–O1	2.31(2)	1
Cu2–O3	1.937(1)	4

of similar compounds where this oxygen shift was also observed by single crystal X-ray diffraction and neutron powder diffraction (*6, 12*). Table III gives a summary of important bond distances.

The shift of O2 by 0.075 unit cell lengths results in a displacement of 0.408 Å along *a* and 0.410 Å along *b*. This is the source of the orthorhombic distortion in an otherwise tetragonal unit cell. The small relative scattering of O in a background matrix of Pb, Nd, and Sr gives rise to standard deviations which render the *a* and *b* displacements essentially equal. Neutron powder diffraction data on a related compound $Pb_2Sr_2YCu_3O_8$ have confirmed the unequal displacement of O2 along *a* and *b* (*12*).

Initially, the structure was assumed to be $Pb_2Sr_2NdCu_3O_8$. The occupancy of each metal atom was refined individually. Pb, Cu1, and Cu2 refined to full occupancy within 3σ. Nd calculated to less than full occupancy indicating some substitution by a lighter element. Since the structure of $Pb_2Sr_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$ has been reported (*5*), partial substitution of Nd by Sr is not surprising. Sr refined to greater than full occupancy, indicating some substitution by a heavier element. Pb^{2+} has a slightly larger ionic radius than Sr^{2+} while Nd^{3+} is smaller. Since we observe a contraction of the *c* axis relative to $Pb_2Sr_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$, we assume that Sr is partially substituted by Nd. This is also no surprise since Nd ions occupy the same positions in $Nd_3Ba_3Cu_6O_{14}$ (*13, 14*) and $Nd_2SrCu_2O_6$ (*15, 16*; $Nd_2SrCu_2O_6$ is of the $La_2SrCu_2O_6$ structure). Each pair of occupancies was refined separately as was each pair of anisotropic thermal parameters. The thermal displacement parameters of both atoms on the same site were arbitrarily set equal. These parameters were held constant in the final refinement as they were found to be highly correlated. The final formula was determined to be $Pb_2(Sr_{0.94}Nd_{0.06})_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$.

Difference Fourier maps reveal the presence of residual electron density above and below each cation in the form of lobes along the *c* direction. The effect is most prominent for Pb. This could be the result of a modulation similar to that observed in $Bi_2Sr_2CaCu_2O_8$ (*17*) and is consistent with the fact that both Pb^{2+} and Bi^{3+} have lone pairs of electrons. Small but observable regions of residual electron density along the *a* axis has also been observed. Average displacements of 0.47 Å along *c* and 0.22 Å along *a* are comparable to the 0.3 and 0.4 Å displacements reported along *c* and *a*, respectively, in $Bi_2Sr_2CaCu_2O_8$. A search along the crystallographic axes and other nonaxial directions failed to yield evidence for satellite peaks. Zero layer precession photographs taken with Mo*Kα* radiation confirm this result. Although this observation could be caused by a noncorrelated type of modulation it may also be the result of the absorption correction as this compound contains many heavy atoms.

Discussion

All known high-T_c superconductors contain a half filled valence band which is

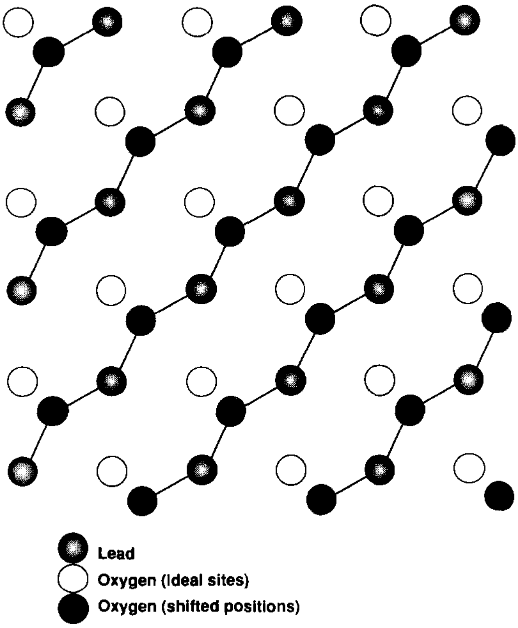

FIG. 2. (a, b) Projection of the Pb–O2 plane.

doped to slightly greater or less than half filling. This doping takes place via one of three mechanisms: (a) cation substitution such as $La_{2-x}Sr_xCuO_4$ or $Nd_{2-x}Ce_xCuO_4$, (b) anion substitution or insertion as in $Nd_2CuO_{4-y}F_y$ (*18*) or $La_2CuO_{4+\delta}$ (*19*), or (c) by an electron sink such as in $YBa_2Cu_3O_7$ (CuO chains), $Bi_2Sr_2Ca_{n-1}Cu_nO_{2n+4}$ (BiO planes), or $Tl_m(Ba, Sr)_2Ca_{n-1}Cu_nO_{2n+2+m}$ (TlO planes). In $Pb_2Sr_2Ln_{1-x}M_xCu_3O_8$ all possibilities can occur; (1) oxygen insertion into the oxygen deficient Cu^{1+} layers, (2) substitution of M^{2+} for Ln^{3+}, or (3) by an electron sink mechanism involving the PbO planes.

One of the interesting features observed in this structure involves the PbO layers where the O2 atoms are shifted off their ideal positions (see Fig. 2). If they remained on the ideal positions, two pairs of Pb–O2 bonds with lengths 2.72 and 2.74 Å would result. In their observed positions, there is a pair of short (2.35(4), 2.36(4) Å) and a pair of long (3.15(4), 3.17(4) Å) Pb–O2 bonds. The long bonds are clearly longer than any of the Pb–O distances in PbO, Pb_3O_4, or Pb_2O_3 ($Pb–O_{max}$ = 3.00 Å) (*20*). This gives rise to the possibility of ordering of the short Pb–O2 bonds. If all of the O2 atoms in the fourfold site were shifted in the same direction, chains of Pb–O bonds would result like those shown in Fig. 2. Long range ordering of this type is not likely given the absence of superlattice reflections. However, short range ordering of these chains cannot be ruled out.

Shifted oxygen positions in high-T_c superconductors are not unique to this compound. Oxygen atoms in the Tl layers as well as shifted Tl atoms have been found in several compounds (*21*). Pulsed neutron diffraction studies have provided good evidence for the presence of the short range ordering of chain structures (*22*). While shifted Pb or Bi positions have not been observed in these superconductors, modulations are clearly present in the *a–b* plane of the $Bi_2Sr_2CaCu_2O_8$ and possibly in $Pb_2Sr_2Ln_{1-x}(Sr, Ca)_xCu_3O_8$ (this work). It may be that a chain or a chain-like structure is a general feature common to all high-T_c superconductors which are doped via an electron sink mechanism.

The single crystal used in this study was placed in a Quantum Design SQUID magnetometer. No trace of superconductivity was observed. As the sample was rather small, many crystals grown in the same batch were run together to confirm this result. Why is this sample not superconducting? The most likely answer is that the doping level is not in the appropriate range since it is becoming increasingly apparent that the doping levels of many high-T_c superconductors fall in an extremely narrow range, for example, $Ln_{2-x}M_xCuO_4$ (Ln = Nd, Pr, Sm, Eu; M = Ce, Th), where $0.14 < x < 0.17$. The doping in the compound in this study can change via all three mechanisms mentioned above and all should be addressed.

(1) Anion doping can occur through oxygen deficiency or surplus. No evidence exists for oxygen deficiency below eight O atoms per formula unit. Cava *et al.* (*5*) have shown that low temperature annealing in oxygen can increase the oxygen content to as high as 9.8. Our crystal was not annealed at low temperature and no electron density in the vacant positions in the Cu^{1+} plane was observed in the difference Fourier maps. Furthermore, leakage of air into the stream of flowing 1% O_2 during synthesis would not be likely to increase the oxygen content as $Pb_2Sr_2Y_{0.75}Ca_{0.25}Cu_3O_8$ was prepared under oxygen pressure much higher than 1% by the decomposition of peroxides (Subramanian *et al.*) (*6*).

(2) In our crystal two types of cation doping are present: Nd for Sr and Sr for Nd. Doping of the type $Pb_2Sr_2(Ln_{1-x}M_x)Cu_3O_8$ results in a maximum T_c for $x \sim 0.5$ (M = Ca). Superconductivity was reported for $Pb_2Sr_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$ but no T_c was mentioned (*5*). Superconducting but multiphase, powder samples can be made for M = Sr. We prepared $Pb_2Sr_2(Nd_{0.75}Ca_{0.25})Cu_3O_8$ which showed a $T_c \sim 55$ K. This corresponds to an average Cu oxidation state (excluding Cu^{1+}) of 2.13 where as $Pb_2(Sr_{0.94}Nd_{0.06})_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$ has an average Cu oxidation state of 2.06. A powder sample of $Pb_2Sr_2(Nd_{0.875}Ca_{0.125})Cu_3O_8$, which also has an average Cu oxidation state of 2.06, has been shown to be nonsuperconducting down to 4.2 K. We note that the intermixing of Nd on Sr sites could be the source of the poor powder samples reported in Ref. (*5*) when samples are prepared to be stoichiometric to the formula $Pb_2Sr_2(Ln_{1-x}Sr_x)Cu_3O_8$. Intermixing is consistent with the fact that positional interchange is observed in $Pb_2Sr_2NdCu_3O_8$ and $Nd_2SrCu_2O_6$.

(3) The third doping scheme in this compound is achieved through the PbO layers acting as a charge sink. The layers may absorb electrons as the BiO layers are assumed to do in $Bi_2Sr_2CaCu_2O_8$ or donate electrons thus oxidizing Pb^{2+}. Band structure calculations of $Pb_2Sr_2YCu_3O_8$ show that the Pb bands do not cross the Fermi level and that the doping mechanism therefore is strictly by cation substitution (*23*). However, the analysis of the positional parameters and the unit cell lengths used in these calculations yield a long Pb–O1 length (2.43 Å) and a very short Cu2–O1 length (2.07 Å) in disagreement with the experimental results of Cava *et al.* (*12*) and Subramanian *et al.* (*6*), suggesting that these calculations may not be relevant. Table IV shows Pb–O1 and Cu2–O1 bond distances for three references as well as our results. It is clear that the overlap effect of the PbO layers was underestimated as Pb–O1 is actually ~0.2 Å shorter than assumed. With Sr partially substituted by Nd this effect becomes even more pronounced as these ions occupy the space between the PbO and CuO sheets. By decreasing the average radii of the Sr site ion, Pb–O1 is decreased to 2.08 Å. Therefore, it is possible that the apparent oxidation state of Cu is significantly different from 2.06 due to the doping effect of the PbO layers and that this is the source of the lack of observed superconductivity.

As a result of these doping effects, the absence of superconductivity may be the result of either inappropriate cation doping or the interaction of the Pb–O layers with the Cu–O layers. The effect of the Pb–O2

TABLE IV

COMPARISON OF Pb–O1 AND Cu2–O1 BOND DISTANCES

Pb–O1 (Å)	Cu2–O1 (Å)	Compound
2.43	2.07	$Pb_2Sr_2YCu_3O_8$ (*23*)
2.153(5)	2.285(5)	$Pb_2Sr_2YCu_3O_8$ (*12*)
2.19(4)	2.23(4)	$Pb_2Sr_2Y_{0.75}Ca_{0.25}Cu_3O_8$ (*6*)
2.08(2)	2.31(2)	$Pb_2(Sr_{0.94}Nd_{0.06})_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$ (this work)

TABLE V

IMPORTANT BOND ANGLES IN $Pb_2(Sr_{0.94}Nd_{0.06})_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$

Atom 1	Atom 2	Atom 3	Angle (deg)
O1	Pb	O2	90.2(7)
O2	Pb	O2	180(1)
O2	Pb	O2	160(2)
O2	Pb	O2	110(2)
O2	Pb	O2	70(2)
O2	Pb	O2	90(1)
O1	Sr, Nd	O1	157.1(7)
O1	Sr, Nd	O1	87.8(1)
O1	Sr, Nd	O2	87(1)
O1	Sr, Nd	O2	70(1)
O1	Sr, Nd	O3	128.9(3)
O1	Sr, Nd	O3	69.8(3)
O2	Sr, Nd	O3	134(1)
O2	Sr, Nd	O3	148(1)
O2	Sr, Nd	O3	123(1)
O3	Sr, Nd	O3	89.5(4)
O3	Sr, Nd	O3	59.5(2)
O3	Sr, Nd	O3	59.9(2)
O3	Nd, Sr	O3	102.2(5)
O3	Nd, Sr	O3	113.5(2)
O3	Nd, Sr	O3	113.0(3)
O3	Nd, Sr	O3	180
O3	Nd, Sr	O3	77.8(5)
O3	Nd, Sr	O3	66.5(2)
O3	Nd, Sr	O3	67.0(3)
O1	Cu2	O3	95.5(4)
O3	Cu2	O3	169.0(8)
O3	Cu2	O3	89.11(8)
O3	Cu2	O3	89.84(8)

Note. Atom 2 is the central atom of the angle.

planes on the Cu–O planes and their role in superconductivity requires further examination.

Conclusion

In this paper we have reported the crystal structure of $Pb_2(Sr_{0.94}Nd_{0.06})_2(Nd_{0.76}Sr_{0.24})Cu_3O_8$ and discussed some of its details as well as the relationship to its superconducting analogs. Oxygen atoms in the Pb planes are shifted from their ideal positions giving rise to the possibility of short range ordering. No evidence for ordered superlattices could be found but residual electron density along the *a* and *c* axes indicates that modulations similar to those found in $Bi_2Sr_2CaCu_2O_8$ may be present. The lack of superconductivity points to the interaction of the PbO planes with the superconducting CuO planes. A comparison of bond distances shows that this becomes increasingly likely as Nd is substituted for Sr.

Acknowledgments

We thank W. Kunnmann, R. K. McMullan, K. Barkigia, and J. Larese for helpful discussions. This work was carried out at Brookhaven National Laboratory under Contract DE-AC02-76CH00016 with the U.S. Department of Energy and supported by its Division of Chemical Sciences, Office of BES.

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