Structural Peculiarities of Two Layered Cuprates, $NdSrCuO_{3.5}$ and $Nd_{1.8}Sr_{1.2}Cu_2O_{6-\delta}$

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The structures of the layered copper oxides $NdSrCuO_{3.5}$ and $Nd_{1.8}Sr_{1.2}Cu_2O_{6-\delta}$ are solved from single crystal X-ray diffraction. The analysis of the results compared to those of analogous compounds $(ACuO_{3-x})_m (A'O)_n$ $(n = 1, m = 1,2)$ involving La shows several important structural features. In the rock-salt layers $[Nd_{1-x}Sr_xO]_\infty$, the $[Nd_{1-x}Sr_x]_\infty$ layers are systematically shifted out of the plane of the oxygen layer along **c**. In $NdSrCuO_{3.5}$ partial site vacancies are detected on the two oxygen sites, whereas in $Nd_{1.8}Sr_{1.2}Cu_2O_{6-\delta}$ no other oxygen vacancy is observed except the empty site located between two neighboring Cu layers. A short apical distance A–O2 between an oxygen and a metallic site (Nd, Sr) is a pecularity of the two structures and also of the similar La oxides. This distance appears as an invariant over all these intergrowths whatever the size of A, the inserted cation. Another remarkable feature deals with the influence of the size of the A cations upon the Cu–O2 apical distance of the CuO_6 octahedra in La_2CuO_4-type oxides: the replacement of cations like lanthanum or strontium by smaller ions like neodymium in the rock salt layer, leads to a significant compression of the CuO_6 octahedra along **c**. © 1991 Academic Press, Inc.

Introduction

Four years after the discovery of superconductivity at high temperature (*1*) in La_2CuO_4-type oxides doped with barium and strontium (*2–4*), the relationships between the superconducting properties of those materials and their structures still remain not well established. If it is clear that the bidimensionality of the structure is necessary for the appearance of superconductivity (*5–7*), the role of the chemical bond and of the Jahn Teller effect is still the subject of controversy. For instance, many authors have tried to establish correlations between Cu–O bonds and especially Cu–O apical distances of the CuO_5 pyramids or CuO_6 octahedra and the critical temperature of those oxides. Thus, the accurate determination of the structure of these phases, from single crystal X-ray diffraction or from neutron diffraction, is absolutely necessary for the understanding of these relationships. In this respect the knowledge of the structure of the oxides $La_{2-x}A_xCuO_4$ (*2–3*) and $La_{2-x}A_{1+x}Cu_2O_{6-y}$ (*8–9*) with A = Ca, Sr which were synthesized a long time ago is of capital importance. They indeed represent the simplest two first members of the series of intergrowth $(ACuO_{3-x})_m (A'O)_n$, built up from single rock salt layers ($n = 1$) and single ($m = 1$) or double ($m = 2$) oxygen-deficient perovskite layers, respectively. A great deal of work has been devoted to the first member of the series either by single crystal X-ray diffraction (*10–12*) or by neutron diffrac-

TABLE I

EXPERIMENTAL DATA AND STRUCTURE PARAMETERS

	$NdSrCuO_{3.5}$	$Nd_{1.8}Sr_{1.2}Cu_2O_{6-\delta}$
Formula		
Crystal size	$48 \times 48 \times 20$ μm	$42 \times 56 \times 27$ μm
Lattice parameters	$a = 3.7431$ (4) Å	$a = 3.8365$ (4) Å
($T = 294$ K)	$c = 12.839$ (1) Å	$c = 19.652$ (2) Å
	$v = 179.9$ (1) Å^3	$v = 289.2$ (1) Å^3
Space group	$I4/mmm$ (No. 139)	$I4/mmm$ (No. 139)
Dc; Z	6.49 g·cm^{-3}; 2	6.75 g·cm^{-3}; 2
Absorption coeff. (Mo$K\alpha$)	356.3 cm^{-1}	349.0 cm^{-1}
Data collection	Ω-θ scan	Ω-θ scan
	$-7 \leq h \leq 7$	$-7 \leq h \leq 7$
	$0 \leq k \leq 7$	$0 \leq k \leq 7$
	$0 \leq l \leq 25$	$0 \leq l \leq 38$
Standard reflections	3 chosen reflections	3 chosen reflections
No. of unique reflections	152 with $I > 3$ $\sigma(I)$	138 with $I > 3$ $\sigma(I)$
Structure refinement	SDP Programs	SDP Programs
Weighting scheme	Unitary	Unitary
R, Rw, S	0.030, 0.032, 1.03	0.034, 0.030, 1.71
Δ/σ	<0.02	<0.01
Residual electron density	1.08 e Å^{-3}	1.27 e Å^{-3}

tion (*13–20*), whereas for the second one, three neutron powder diffraction studies (*21–23*) have been performed. Contrary to lanthanum cuprates, neodymium cuprates have not been studied, in spite of their isostructural character. We report here on the crystal structures of the two layered cuprates $NdSrCuO_{3.5}$ and $Nd_{1.8}Sr_{1.2}Cu_2O_{6-\delta}$ determined from single crystal X-ray diffraction studies.

Experimental

The samples were prepared by solid state reaction from copper and neodymium oxides and strontium carbonate ($4CuO$, Nd_2O_3, $4SrCO_3$). The mixtures were intimately ground in an agate mortar and heated in air at 1180°C, slowly cooled at 10°C per hour down to 800°C. Single crystals providing diffraction peaks of correct width were chosen from three crystals of nominal compositions "$NdSrCuO_{3.5}$" and "$Nd_{2-x}Sr_{1+x}Cu_2O_{6-\delta}$" ($0.2 \leq x \leq 1$), respectively. The cell parameters (Table I) were obtained

by least-squares refinement of 25 centered reflections ($18.5° < \theta < 25°$). X-ray intensity data were collected with a CAD4 automatic four circle diffractometer using graphite-monochromatized Mo$K\alpha$ radiation (50 kV, 20 mA). Systematic absences of the reflections for $h + k + l = 2n + 1$ confirm the I lattice for both compounds. The data collection, extended to two octants, showed that numerous reflections were of weak intensity in spite of very long exposure times. Only 464 hkl out of 845 reflections had $I/\sigma(I) > 3$ for $NdSrCuO_{3.5}$ and 397 hkl out of 1337 for $Nd_{2-x}Sr_{1+x}Cu_2O_{6-\delta}$. The influence of absorption was estimated to be weak since $\mu R \approx 0.7$ for both crystals. Nevertheless, absorption corrections were made, taking into account an approximate morphology owing to the irregular shape of the crystals. The resulting intensities are then in good agreement with the Laue group $4/mmm$. Finally, 152 and 138 reflections were used for the refinement calculations of the two crystals, respectively.

The trial positions were those obtained

TABLE II

$NdSrCuO_{3.5}$: POSITIONAL AND THERMAL PARAMETERS WITH e.s.d's IN PARENTHESES

Site	Atom	x	y	z	B_{eq}	U_{11}	U_{22}	U_{33}
4e	Nd, Sr	0	0	0.35812 (8)	1.196 (7)	0.0163 (2)	U_{11}	0.0129 (3)
2a	Cu	0	0	0	0.81 (2)	0.0112 (5)	U_{11}	0.0086 (7)
4c	O1	0	1/2	0	2.5 (3)	0.06 (1)	0.007 (4)	0.032 (6)
4e	O2	0	0	0.172 (1)	2.9 (2)	0.037 (5)	U_{11}	0.035 (7)

Note. $B_{eq} = 4/3 \Sigma_i \Sigma_j \beta_{ij} a_i a_j$ (Å^2). $U_{ij} = 1/2 \pi^2 \beta_{ij} a_i a_j$ (Å^2). $U_{12} = U_{23} = U_{13} = 0$.

from powder data for $La_{0.8}Sr_{1.2}CuO_{3.4}$ *(3)* and $La_{2-x}Sr_{1+x}Cu_2O_{6-x/2}$ *(8)*, respectively, using $I\,4/mmm$ space group in both cases.

The resolution of the structure of $NdSrCuO_{3.5}$ was rather simple owing to the fact that only one *(4e)* site was available for Nd and Sr atoms, which were supposed to be statistically distributed over this site: the main problem was dealing with the oxygen distribution over the two anionic sites o1 and o2. Refinements of multiplier coefficients showed that both sites were oxygen deficient with occupancy factors of 0.86 (3) and 0.92 (3), respectively. Such a refinement led to the formula $NdSrCuO_{3.56}$ which is in perfect agreement with the nominal composition $NdSrCuO_{3.5}$ in the limit of the standard deviation (3.56 ± 0.08).

For $Nd_{2-x}Sr_{1+x}Cu_2O_{6-\delta}$, the first problem was to determine the molar ratio Nd/Sr and the distribution of neodymium and strontium over the two metallic sites *(2a)* with

coordinates 000 and *(4e)* with coordinates 00z. Starting from the formula "$Nd_2SrCu_2O_6$", the distribution of Sr and Nd on *(2a)* and *(4e)* sites, respectively, led to negative B_{2a} factor and to a very high B_{4e} factor. The total replacement of Sr by Nd on the *(2a)* sites led to the opposite effect (very high B_{2a} factor and $B_{4e} < 0$), suggesting a mixed occupancy of both sites by neodymium and strontium. Thus, the multipliers of those sites were refined using Nd scattering factor with SDP programs *(24)*. A preferential occupation of the *(2a)* sites by neodymium (0.75 Nd, 0.25 Sr) was observed, whereas *(4e)* sites were found to be occupied for half by neodymium (0.52) and for half by strontium (0.48). Thus significant distribution of the metallic atoms led to the formula $Nd_{1.8}Sr_{1.2}Cu_2O_{6-\delta}$ whatever the starting distribution. Contrary to $NdSrCuO_{3.5}$, the refinement of the occupancy factors of the anionic sites did not

TABLE III

$Nd_{1.8}Sr_{1.2}Cu_2O_{6-\delta}$: POSITIONAL AND THERMAL PARAMETERS WITH e.s.d's IN PARENTHESES

Site	Atom	x	y	z	B_{eq} or B	U_{11}	U_{22}	U_{33}
2a	Nd, Sr	0	0	0	0.46 (2)	0.0068 (5)	U_{11}	0.0040 (7)
4e	Nd, Sr	0	0	0.18025 (9)	1.00 (2)	0.0144 (5)	U_{11}	0.0091 (6)
4e	Cu	0	0	0.5916 (2)	0.60 (3)	0.0060 (7)	U_{11}	0.011 (1)
8g	O1	0	1/2	0.0817 (6)	1.9 (2)*			
4e	O2	0	0	0.701 (1)	2.8 (5)*			

Note. Starred atoms were refined isotropically. $B_{eq} = 4/3 \Sigma_i \Sigma_j \beta_{ij} a_i a_j$ (Å^2). $U_{ij} = 1/2 \pi^2 \beta_{ij} a_i a_j$ (Å^2). $U_{12} = U_{23} = U_{13} = 0$.

TABLE IV

QUANTITATIVE ELEMENTAL ANALYSES (%)

	NdSrCuO$_{3.5}$			Nd$_{1.8}$Sr$_{1.2}$Cu$_2$O$_{6-\delta}$				
	-1-	-2-	Average	-1-	-2-	-3-	-4-	Average
Nd	36.1	35.7	35.9	37.4	34.9	36.7	36.7	36.4
Sr	35.2	35.1	35.2	23.9	25.1	24.1	25.2	24.6
Cu	28.7	29.2	28.9	38.7	40.0	39.2	38.1	39.0

lead to a significant deviation from the "O$_6$" stoichiometry; nevertheless an oxygen deficiency, corresponding to the only presence of Cu (II), i.e., to $\delta = 0.10$, cannot be ruled out, taking into account the low scattering factor of oxygen and the too low number of observed reflections which did not allow in that case, the anisotropical thermal factors of oxygen to be refined, contrary to NdSrCuO$_{3.5}$.
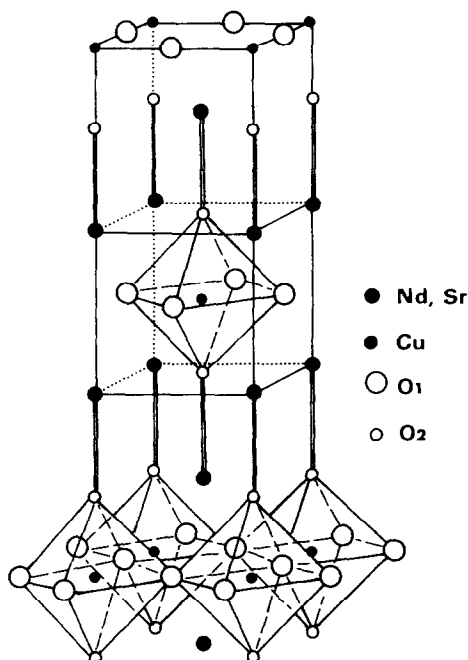
The final positional parameters for both oxides are given in Tables II and III.

Quantitative analyses of the metallic elements were performed using a Tracor dispersive X-ray analysis system on a JEOL 840 scanning electron microscope operated at 15 kV in order to check the refinements of the occupancy factors of the metallic sites. A standard ZAF correction was applied to the raw signal. A pure ceramic of composition Nd$_2$SrCu$_2$O$_6$ was used as standard. The measurements (Table IV) attest that both crystals are homogeneous and confirm entirely the results of the structure refinements.

Analysis of the Structures and Discussion

The crystal structure determination of those oxides confirms that they both belong to the same family of intergrowths of single rock salt layers [Sr$_{1-x}$Nd$_x$O]$_\infty$ with single perovskite layers and double perovskite layers for NdSrCuO$_{3.5}$ (Fig. 1) and Nd$_{1.8}$Sr$_{1.2}$Cu$_2$O$_{6-\delta}$ (Fig. 2), respectively.

The analysis of the structure of those two phases leads to the following original features:

(i) In both oxides the Nd/Sr molar ratio in the rock salt [Sr$_{1-x}$Nd$_x$O]$_\infty$ layers is close to one ($x = 0.5$ for NdSrCuO$_{3.5}$ and $x = 0.52$ for Nd$_{1.8}$Sr$_{1.2}$Cu$_2$O$_{6-\delta}$), suggesting that the presence of at least about 50% of strontium is necessary for the stabilization of such layers. This is explained by the fact that neo-
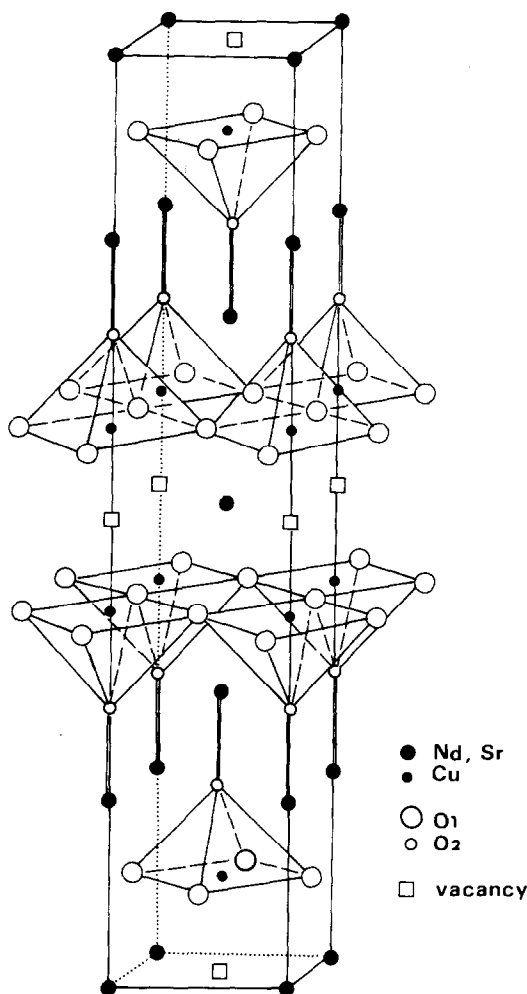

● Nd, Sr

● Cu

○ O$_1$

○ O$_2$

FIG. 1. Crystal structure of NdSrCuO$_{3.5}$.

FIG. 2. Crystal structure of $Nd_{1.8}Sr_{1.2}Cu_2O_{6-\delta}$.

TABLE V

$NdSrCuO_{3.5}$: INTERATOMIC DISTANCES (Å)

A–O (1)	($\times 4$)	2.612 (1)
A–O (2)	($\times 1$)	2.38 (2)
A–O (2)	($\times 4$)	2.676 (3)
Cu–O (1)	($\times 4$)	1.872 (1)
Cu–O (2)	($\times 2$)	2.21 (2)

This phenomenon is observed in other (La, Sr) compounds, since there is also a shifting of the $[La, Sr]_\infty$ planes with respect to the O2 oxygen layers: 0.57 Å for $La_{1.85}Sr_{0.15}CuO_4$ (*11, 12, 16, 17*) and 0.48 Å for $La_2SrCu_2O_6$ (*21*); and more generally, it appears in La_2CuO_4, in $La_{1.85}Ba_{0.15}CuO_4$, and in $La_{1.9}Ca_{1.1}Cu_2O_6$ (Tables VII and VIII).

(iii) The distribution of the anionic vacancies in the two structures is very different. In $Nd_{1.8}Sr_{1.2}Cu_2O_{6-\delta}$, one only observes the classical absence of one oxygen at the same level as the (*2a*) sites with respect to the stoichiometric perovskite leading to the formation of layers of corner-sharing CuO_5 pyramids (Fig. 2), but no other oxygen vacancies were detected in the limit of the X-ray diffraction refinements. On the other hand, the oxide $NdSrCuO_{3.5}$ exhibits oxygen vacancies on both sites, i.e., in the basal planes of the CuO_6 octahedra (o1 sites, Fig. 1) and in the rock salt layers on the apical site of the CuO_6 octahedra (o2 sites, Fig. 1). The first types of vacancies which are more numerous were already observed for $La_{0.8}Sr_{1.2}CuO_{3.4}$ (*3*). Although less numer-

dymium tends to take a pseudocubic coordination, forming fluorite-type layers. The preferential occupancy of the (*2a*) sites (75%) by neodymium in $Nd_{1.8}Sr_{1.2}Cu_2O_{6-\delta}$ (Fig. 2) supports strongly this view point.

(ii) In both oxides the rock salt layers exhibit a very similar geometry. One does not observe planar $[Nd_{1-x}Sr_xO]_\infty$ layers contrary to the ideal rock salt structure. The $[Nd_{1-x}Sr_x]_\infty$ layers are indeed shifted along c with respect to the oxygen layers, leading to a puckering of the $[Nd_{1-x}Sr_xO]_\infty$ layers.

TABLE VI

$Nd_{1.8}Sr_{1.2}Cu_2O_{6-\delta}$: INTERATOMIC DISTANCES (Å)

$A1$–O (1)	($\times 8$)	2.502 (7)
$A2$–O (1)	($\times 4$)	2.725 (7)
$A2$–O (2)	($\times 1$)	2.34 (2)
$A2$–O (2)	($\times 4$)	2.743 (3)
Cu–O (1)	($\times 4$)	1.928 (1)
Cu–O (2)	($\times 1$)	2.15 (2)

TABLE VII

STRUCTURAL FEATURES OF SOME La$_2$CuO$_4$-TYPE COMPOUNDS AT ROOM TEMPERATURE

Compound	Space Group	c(Å)	Distance A–O2 (Å)	Distance A–A (Å)	Sequence O2–A–A–O2 (Å)	Shift in the r.s. layer (Å)	Distance Cu–O2 (Å)	Ref.
La$_2$CuO$_4$	Bmab	13.15	2.37	3.635	8.375	0.579	2.397	(10)
La$_2$CuO$_4$	Bmab	13.127 (2)	2.352	3.625	8.329	0.585	2.398	(15)
La$_2$CuO$_4$	Bmab	13.1529 (9)	2.330	3.656	8.316	0.589	2.417	(19)
La$_{1.85}$Sr$_{0.15}$CuO$_4$	I4/mmm	13.186 (4)	2.354	3.667	8.375	0.573	2.406	(11)
La$_{1.85}$Sr$_{0.15}$CuO$_4$	I4/mmm	13.225 (3)	2.359	3.683	8.401	0.570	2.412	(12)
La$_{1.85}$Sr$_{0.15}$CuO$_4$	I4/mmm	13.2260 (3)	2.356	3.691	8.402	0.567	2.412	(16)
La$_{1.85}$Sr$_{0.15}$CuO$_4$	I4/mmm	13.237 (4)	2.360	3.693	8.413	0.565	2.412	(17)
La$_{1.85}$Ba$_{0.15}$CuO$_4$	Pccn	13.234 (4)	2.349	3.678	8.376	0.589	2.431	(12)
La$_{1.85}$Ba$_{0.15}$CuO$_4$	I4/mmm	13.2883 (3)	2.363	3.704	8.430	0.577	2.429	(13)
NdSrCuO$_{3.5}$	I4/mmm	12.839 (1)	2.38	3.643	8.403	0.39	2.21	This work

ous, the second sort of vacancies can be considered as significant.

(iv) Both oxides are characterized by one abnormally short (Nd, Sr)–O2 distance (Tables V, VI) corresponding to the apical bond, i.e., parallel to c, whereas the other distances are absolutely normal. One indeed observes distances of 2.38 and 2.34 Å for NdSrCuO$_{3.5}$ and Nd$_{1.8}$Sr$_{1.2}$Cu$_2$O$_{6-\delta}$, respectively. Such distances are in agreement with ionic radii of neodymium and oxygen according to Shannon (25), but should not be compatible with the size of strontium which occupies here half the sites. This viewpoint is supported by the observations made for SrCuO$_2$ (26) and Sr$_2$CuO$_3$ (27), which exhibit very closely related structures with correct Sr–O distances ranging from 2.5 to 2.6 Å. In fact such an abnormally short A–O distance appears to be a characteristic of these intergrowths. Lanthanum cuprates exhibit similar A–O distances ranging from 2.33 to 2.37 Å in La$_2$CuO$_4$ (10, 15, 19), La$_{1.85}$Sr$_{0.15}$CuO$_4$ (11, 12, 16, 17), and La$_{1.85}$Ba$_{0.15}$CuO$_4$ (12, 13) and from 2.34 to 2.36 Å in La$_{1.9}$Ca$_{1.1}$Cu$_2$O$_6$ (22) and La$_2$SrCu$_2$O$_6$ (21), in spite of the great sizes of lanthanum and strontium, which are rather similar.

(v) The apical Cu–O2 distances of the CuO$_6$ octahedra of NdSrCuO$_{3.5}$ (Table V) and of the CuO$_5$ pyramids of Nd$_{1.8}$Sr$_{1.2}$Cu$_2$O$_{6-\delta}$ (Table VI) are shorter than those observed for lanthanum cuprates. One indeed observes a Cu–O2 apical distance of 2.21 Å for NdSrCuO$_{3.5}$ against 2.40 to 2.43 Å in La$_2$CuO$_4$ (10, 15, 19), La$_{1.85}$Sr$_{0.15}$CuO$_4$ (11, 12, 16, 17), and La$_{1.85}$Ba$_{0.15}$CuO$_4$ (12, 13); in fact a similar Cu–O distance of 2.23 Å was observed for LaSrCuO$_4$ (28), which contains only Cu (III). In the same manner Nd$_{1.8}$Sr$_{1.2}$Cu$_2$O$_{6-\delta}$ has a Cu–O apical distance of 2.15 Å to be compared to 2.21 Å in La$_2$SrCu$_2$O$_6$ (21) and to 2.31 Å in La$_{1.9}$Ca$_{1.1}$Cu$_2$O$_6$ (22).

(vi) The [CuO$_2$]$_\infty$ layers are much less puckered than the rock-salt-type layers. The Cu and O1 atoms of the CuO$_6$ octahedra in NdSrCuO$_{3.5}$ are indeed at the same level along c, forming planar [CuO$_2$]$_\infty$ layers. In Nd$_{1.8}$Sr$_{1.2}$Cu$_2$O$_{6-\delta}$, the Cu atoms are displaced by 0.19 Å along c out of the basal planes inside the CuO$_5$ pyramids, to be compared to 0.15 Å in La$_2$SrCu$_2$O$_6$ (21) and to 0.06 Å in La$_{1.9}$Ca$_{1.1}$Cu$_2$O$_6$ (22).

(vii) In Nd$_{1.8}$Sr$_{1.2}$Cu$_2$O$_{6-\delta}$, the metallic atoms of the (2a) sites in pseudocubic coordination (Fig. 2) exhibit A–O1 distances of 2.50 Å (Table VI), similar to those of La$_{1.9}$Ca$_{1.1}$Cu$_2$O$_6$ (2.49 Å) and slightly smaller than those of La$_2$SrCu$_2$O$_6$ (2.56 Å), according to the smaller size of Nd^{3+} and Ca^{2+} with respect to La^{3+} and Sr^{2+}.

Thus, the first structural characteristics of the cuprates NdSrCuO$_{3.5}$ and

$Nd_{1.8}Sr_{1.2}Cu_2O_{6-\delta}$ deal with the puckering of the $[Nd_{1-x}Sr_xO]_\infty$ rock salt layers in which the A atoms are shifted of 0.39 −0.41 Å along c out of the plane of the O2 oxygen layer. The second point deals with the fact that the A–O2 apical distance of the $[AO]_\infty$ layers appears as invariant whatever the size of A = Sr, La, Nd, Ca and is abnormally short. The third remarkable feature deals with the influence of the size of the A cations upon the Cu–O2 apical distance of the CuO_6 octahedra in La_2CuO_4-type oxides (Table VII). From the comparison with the La, La–Sr, and La–Ba phases it appears clearly that the replacement of cations like lanthanum or strontium by smaller ions like neodymium in the rock salt layer leads to a significant compression of the CuO_6 octahedra along c, whereas the A–O2 distance of the rock salt layer paradoxically does not change. Consequently, the decrease of the c parameter from 13.00 Å for $LaSrCuO_{3.5}$ (3) to 12.84 Å for $NdSrCuO_{3.5}$ is mainly due to a shortening of the apical Cu–O2 bonds along c and not to a decrease of the A–O distances. Considering that the c parameter of $NdSrCuO_{3.5}$ is determined by the linear sequence "Cu–O2–A–A–O2–Cu" (Fig. 1) one indeed observes from the comparison with other K_2NiF_4-type cuprates that the sequence "O2–A–A–O2" is an invariant (Table VII). The c parameter of the second family exhibits a similar behaviour, i.e., it decreases as the size of the A cation decreases. It can also be determined by the sequence "A–A–O2–Cu–□–Cu–O2–A–A", the A–O2 distance being an invariant (Table VIII). However, in that case the A–A distance along c cannot be considered as an invariant. One indeed observes that the O1–O1 interlayer distance decreases from $La_2SrCu_2O_6$ to $La_{1.9}Ca_{1.1}Cu_2O_6$. This is explained by the size of the A cations in eightfold coordinations intercalated between the pyramidal layers. On the other hand, the Cu–Cu interlayer distance shows an abnormal behavior for $La_{1.9}Ca_{1.1}Cu_2O_6$ (3.30 Å)

TABLE VIII

STRUCTURAL FEATURES OF SOME $Ln_{2-x}A_{1+x}Cu_2O_6$-TYPE COMPOUNDS AT ROOM TEMPERATURE

Compound	Space Group	c (Å)	Distance A2–O2 (Å)	Distance A1–A2 (Å)	Shift in the r.s. layer (Å)	Distance Cu–O2 (Å)	Distance Cu–Cu (Å)	Distance O1–O1 (Å)	Shift Cu (Å)	Ref.
$La_2SrCu_2O_6$	$I4/mmm$	19.9410 (6)	2.363	3.563	0.478	2.210	3.664	3.370	0.147	(21)
$La_{1.9}Ca_{1.1}Cu_2O_6$	$I4/mmm$	19.420 (1)	2.339	3.412	0.545	2.306	3.306	3.191	0.057	(22)
$La_2CaCu_2O_{6+y}$	$I4/mmm$	19.5169 (4)	2.346	3.433	0.546	2.315	3.330	3.205	0.062	(23)
$Nd_{1.8}Sr_{1.2}Cu_2O_{6-\delta}$	$I4/mmm$	19.652 (2)	2.34	3.542	0.41	2.15	3.600	3.21	0.19	This work

compared to the other phases (3.60, 3.66 Å). This is correlated to the fact that in the Ca compound almost planar $[CuO_2]_\infty$ layers are observed whereas in the two other phases Cu is displaced by 0.15 to 0.19 Å out of the O1 plane.

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