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Optical phonons in Nd_2BaMO_5 ($M=Zn,Cu$)

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We report the polarized Raman spectra of Nd_2BaZnO_5 and the nonpolarized infrared-absorption spectra of Nd_2BaMO_5 ($M=Zn,Cu$). Thirteen out of a total of fifteen Raman-allowed modes ($3A_{1g}+2B_{1g}+4B_{2g}+6E_g$) were observed. The optical-phonon assignment was made using molecular-site group analysis, taking account of the fact that the ZnO_4 (CuO_4) groups are relatively isolated. In spite of the different shapes of ZnO_4 (tetrahedron) and CuO_4 (square) units resulting in different space groups of Nd_2BaZnO_5 ($I4/mcm$) and Nd_2BaCuO_5 ($P4/mbm$), a comparison between the modes in the two structures is done. We argue that the high-frequency bands in ir spectra involve mainly vibrations of Nd-plane oxygen atoms.

INTRODUCTION

Compounds with chemical formula L_2BaMO_5 (L rare earth, $M=Cu,Zn$) belong to three different structural types. One was reported by Michel and Raveau.[1,2] It is orthorhombic [space group $Pbnm$, $Z=4$ (four formula units in the unit cell)], contains isolated MO_5 square-pyramidal units, and exists for $L=Sm–Lu$ and Y. Later it became known as the "green phase"[3] in studies of Y-Ba-Cu-O superconductivity ceramics. The other two structures exist for $L=La,Nd$. They are tetragonal and have isolated MO_4 units. For $M=Cu$, the MO_4 units are squares and the space group of the structure is $P4/mbm$,[4–6] $Z=2$ [see Fig. 1(a)]. For $M=Zn$, the MO_4 units are tetrahedra, the **c** axis of the lattice is double, and the space group of the structure is $I4/mcm$ ($Z=4$)[7] [see Fig. 1(b)]. In both structures, the shape and symmetry of the L-O(1) layers between the $M[O(2)_4]$-Ba slabs are the same. The similarity between these two structures justifies their parallel study.

Nonpolarized Raman spectra of Nd_2BaCuO_5 were reported by Loo, Burns, and Xidis[8] without discussion. Both nonpolarized Raman and ir-transmission spectra of the same compound were presented by Baran *et al.*[9] and tentative assignment of the vibrations of the CuO_4 units was given on the basis of the irreducible representations of a square-planar D_{4h} molecule. In a previous paper[10] we presented the polarized Raman spectra of this compound and discussed the mode assignment in the framework of molecular-site group analysis. In this work we use the same approach to analyze the polarized Raman and ir-transmittance spectra of Nd_2BaMO_5 ($M=Zn,Cu$). The model used predicts the existence of Davydov's pairs of modes, both of which are Raman active for Nd_2BaCuO_5 and one of which is Raman active and one ir active for Nd_2BaZnO_5. The analysis allows us to determine approximately the frequencies of some of the ir-active modes of Nd_2BaMO_5 ($M=Zn,Cu$). The observation of the corresponding bands in the ir spectra of these two compounds can be consistently explained by phonon modes involving motion of the identical Nd-O(1) layers in both structures.

EXPERIMENTAL

The Nd_2BaZnO_5 samples were prepared by mixing the starting components (Nd_2O_3, $BaCO_3$, and ZnO) in the appropriate ratios and calcining in air at 900 °C for 17 h.

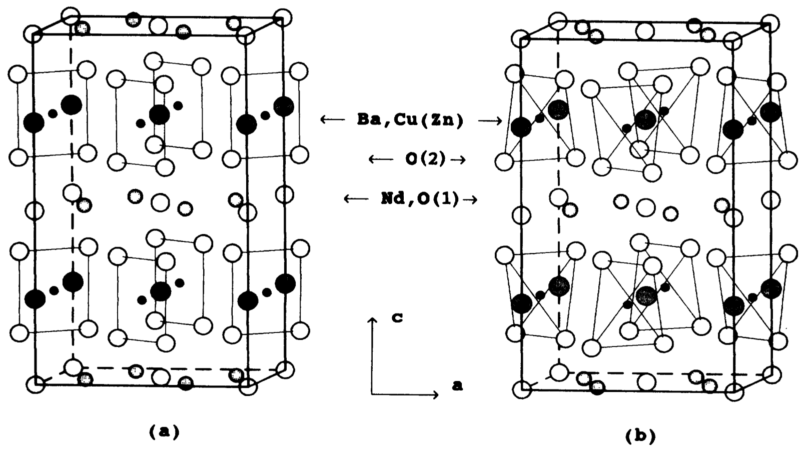

FIG. 1. Structure of (a) Nd_2BaCuO_5 and (b) Nd_2BaZnO_5. For better comparison two adjacent cells along **c** for Nd_2BaCuO_5 are given.

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The resulting materials were ground and pressed into 1-g pellets. To obtain ceramics with grains of sufficient size for micro-Raman measurements (about 5 μm), the pellets were annealed at temperatures from 1000 to 1150 °C for several days. The synthesis of Nd_2BaCuO_5 was similar, as described elsewhere.[10]

The purity of the samples was tested with a Philips SEM 515 scanning electron microscope, equipped with an EDAX 9100/72 energy-dispersive x-ray spectrometer. Measurements of the chemical content of the investigated microcrystals confirmed that the ratio Nd:Ba:Zn(Cu) is 2:1:1.

The Raman spectra were measured at room temperature using a triple multichannel spectrometer Microdil 28 (DILOR) equipped with an optical microscope. A 100× objective was used to focus the incident laser beam in a spot of about 1 μm diameter on the surface of the microcrystals and to collect the backward-scattered light. The 488.0-nm Ar^+ laser line was used for excitation. The ir transmission spectra from CsI pellets containing 1% by weight Nd_2BaMO_5 (M=Zn,Cu) powder were obtained using a Fourier transform infrared spectrometer (Bomem DA3).

RESULTS

First we present the classification of the Γ-point modes based on factor-group analysis. Nd_2BaZnO_5 crystallizes in the tetragonal $I4/mcm$ (D_{4h}^{18}) ($Z=4$) structure,[11] whereas Nd_2BaCuO_5 crystallizes in the $P4/mbm$ (D_{4h}^{5}) ($Z=2$) structure.[5] The site symmetry of the atoms, the number and symmetry of their Γ-point modes, and the symmetry-allowed directions of vibrations for both structures are given in Table I. It is seen that Nd, O(1), and O(2) atoms in both structures have identical site symmetry and types of modes. The Ba and Cu atoms in Nd_2BaCuO_5 are located at the center of symmetry and contribute only to ir-active modes, whereas the Ba and Zn atoms in Nd_2BaZnO_5 can give rise to ir- as well as Raman-active modes. In order to identify the symmetry of the Raman lines, we measured polarized Raman spectra from three differently oriented surfaces of the microcrystals, namely, zx, zx', and $xy(x'y')$ (z, x, y, x', and y' refer to the [001], [100], [010], [110], and [1$\bar{1}$0] crystallographic directions, respectively). The A_{1g} modes should appear in parallel zz, xx (yy), and $x'x'$ ($y'y'$) scattering configurations, E_g in crossed zx and zx', B_{1g} in parallel xx (yy) and crossed $x'y'$, and B_{2g} in parallel $x'x'(y'y')$ and crossed xy geometry. Note that even if one cannot distinguish the [100] from the [110] direction, the B_{1g} and B_{2g} modes can be separated into two groups, without specifying which group contains B_{1g} and B_{2g} modes. In our case, the number of B_{1g} and B_{2g} modes, however, is different ($2B_{1g}$ and $4B_{2g}$) and thus the assignment becomes unambiguous.

The polarized Raman spectra of Nd_2BaZnO_5 as obtained from the zx, zx', and xy surfaces are shown in Figs. 2 and 3. We observed all three A_{1g} and six E_g modes, but only one B_{1g} and three B_{2g} modes. In an attempt to assign the Raman lines to definite atomic vibrations we begin with those of Ba and Nd. The Ba atoms participate in only one Raman-active E_g mode (vibration in the xy plane). As the Ba atoms have the lowest charge-mass ratio in the unit cell, we tentatively assign the lowest of the Raman lines (at 79 cm^{-1}) to their vibrations. For identification of the Nd modes one can take into account the similarity between the Nd environments in Nd_2BaZnO_5 and Nd_2BaCuO_5. For R_2BaCuO_5 (R =La,Nd) all four modes of La (Nd) atoms have been observed, as follows: A_{1g} mode at 154 (152), E_g at 173, B_{1g} at 196, and B_{2g} at 231 cm^{-1}.[10] The same four Nd

TABLE I. Normal modes in Nd_2BaMO_5 (M=Cu,Zn).

Atom	Wickoff notation	Site symmetry	Normal modes	Symmetry-allowed directions of Raman and ir-active vibrations					
				A_{1g}	B_{1g}	B_{2g}	E_g	A_{2u}	E_u
			Nd_2BaCuO_5, $P4/mbm(D_{4h}^{5})$, a=6.7015 Å, c=5.8211 Å, $Z=2$[a]						
Ba	$2b$	C_{4h}	$A_{1u}+A_{2u}+2E_u$					z	xy plane
Nd	$4g$	C'_{2v}	$A_{1g}+A_{2g}+A_{2u}+B_{1g}$ $+B_{1u}+B_{2g}+E_g+2E_u$	x',y'	x',y'	x',y'	z	z	xy plane
Cu	$2c$	D'_{2h}	$A_{2u}+B_{1u}+2E_u$					z	xy plane
O(1)	$2a$	C_{4h}	$A_{1u}+A_{2u}+2E_u$					z	xy plane
O(2)	$8k$	C_s^d	$2A_{1g}+A_{1u}+A_{2g}+2A_{2u}+B_{1g}$ $+2B_{1u}+2B_{2g}+B_{2u}+3E_g+3E_u$	zx' plane	x',y'	zx' plane	all	zx' plane	all
			Nd_2BaZnO_5, $I4/mcm(D_{4h}^{18})$, a=6.747 Å, c=11.537 Å, $z=4$[b]						
Ba	$4a$	D_4	$A_{2g}+A_{2u}+E_g+E_u$				xy plane	z	xy plane
Nd	$8h$	C'_{2v}	$A_{1g}+A_{2g}+A_{2u}+B_{1g}$ $+B_{1u}+B_{2g}+E_g+2E_u$	x',y'	x',y'	x',y'	z	z	xy plane
Zn	$4b$	D'_{2d}	$A_{2u}+B_{2g}+E_g+E_u$			z	xy plane	z	xy plane
O(1)	$4c$	C_{4h}	$A_{1u}+A_{2u}+2E_u$					z	xy plane
O(2)	$16l$	C_s^d	$2A_{1g}+A_{1u}+A_{2g}+2A_{2u}+B_{1g}$ $+2B_{1u}+2B_{2g}+B_{2u}+3E_g+3E_u$	zx' plane	x',y'	zx' plane	all	zx' plane	all

[a] Reference 5.

[b] Reference 7.

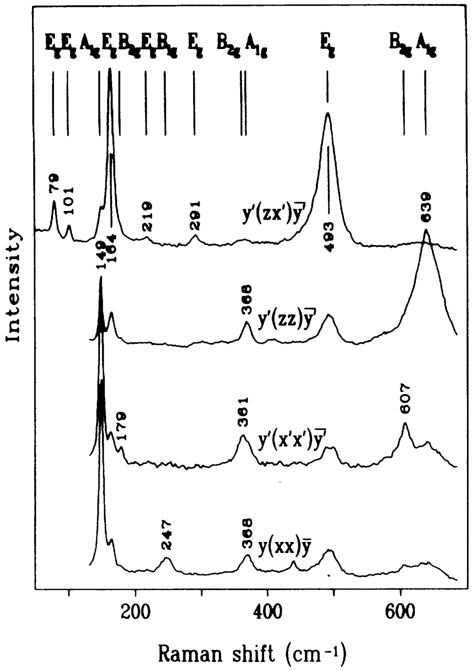

FIG. 2. Polarized Raman spectra obtained from an $x'z$ (110) surface (the top three spectra) and from an xz (010) surface (the bottom spectrum) of Nd_2BaZnO_5 microcrystals. The symmetry of the lines is indicated.

modes are allowed for Nd_2BaZnO_5, too. Thus, it is natural to assign the 149- and 164-cm^{-1} lines in the Nd_2BaZnO_5 spectra to Nd A_{1g} and E_g modes [the weak shift towards lower frequencies can be explained by the slight increase of lattice parameter **a** in the zinc compound compared to **a** in the copper compound (see Table I)]. We could not observe, however, the B_{1g} and B_{2g} modes of Nd in the Nd_2BaZnO_5 spectrum near their expected frequencies. Thus, we suppose that all remaining modes observed in these spectra originate from ZnO_4 vibrations.

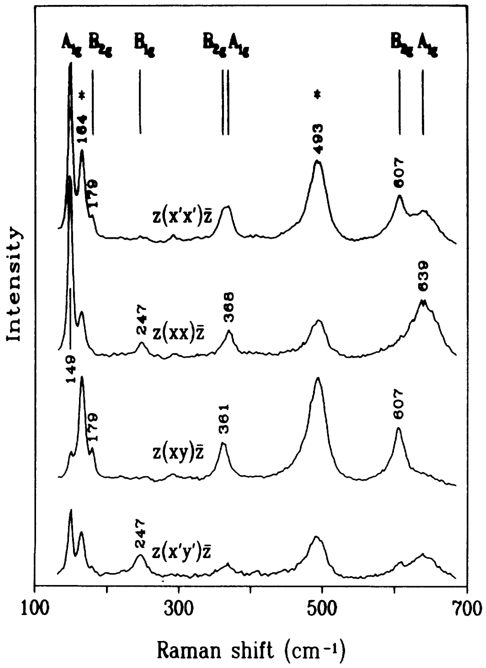

FIG. 3. Polarized Raman spectra obtained from an xy (001) surface of Nd_2BaZnO_5 microcrystals. The positions of the E_g lines forbidden for these polarizations are indicated by asterisks.

The assignment of the O(2) and Zn modes meets with definite difficulties due to their large number, possible mixing, and weaker limitations for the shape of these modes from group-theory considerations [in particular for the three E_g modes of O(2)]. In order to avoid these difficulties we used molecular-site group analysis, i.e., an approximation that regards the normal modes of O(2) and Zn in a Nd_2BaZnO_5 crystal as normal modes in a free ZnO_4 molecule. Such an approach has been used by Baran *et al.*[9] for assignment of the optical phonons in Nd_2BaCuO_5. In the latter study, however, there was a lack of information on the symmetry of the observed lines and on the correlation between the modes in a free CuO_4 molecule and modes of Cu and O(2) atoms in the crystal. This approximation has also been used by Popovic *et al.*[12] to analyze the phonons in the Y_2BaCuO_5 "green phase," considering the Y_2O_5 unit as an isolated molecule. In a recent study of vibrational properties of Bi_2CuO_4,[13] which also contains isolated CuO_4 squares like Nd_2BaCuO_5, the results for the shapes and frequencies of the normal modes were obtained using lattice-dynamical calculations (on the basis of a rigid-ion model). The results for the shapes of Cu and O modes in Bi_2CuO_4, however, many excellently be interpreted using a molecular-site group analysis alone.

The shapes of the normal vibrations of a free ZnO_4 unit with T_d symmetry and of a CuO_4 unit with D_{4h} symmetry are given in Fig. 4. The correlations between the vibrations of the free MO_4 molecule and the normal modes originating from M and O(2) atoms in both structures, as obtained using the techniques developed in Refs. 14, 15, are given in Table II. Placed at a crystal site of lower symmetry, the degenerate vibrations of the free MO_4 molecule split. This splitting (Bethe splitting) may be large, depending on the anisotropy and intensity of the crystal field at the site. One has to take into account also the directions of vibrations. As the primitive cell contains two MO_4 units, to each mode of the MO_4 molecule correspond two MO_4 modes in the crystal (Davydov partners). These modes, which are identical for each MO_4 unit if considered separately, differ in the phase of vibration in two adjacent units. The splitting of these modes is very small. It depends on the correlation between two adjacent units, placed on equivalent sites and is known as the correlation field or Davydov splitting. In the case of Nd_2BaCuO_5 the Davydov partners have been found within experimental error to have the same frequencies.[10]

The line with the highest frequency in the Raman spectrum of Nd_2BaZnO_5 is at 639 cm^{-1} and is of A_{1g} symmetry. We assign it to the Zn-O(2) fully symmetric stretching vibration (A_1 breathing mode) of ZnO_4 units. In Nd_2BaCuO_5 the corresponding line was observed at 634 cm^{-1}. In Bi_2CuO_4 the same vibration was found at 584 cm^{-1},[13] i.e., the frequency of this mode is the highest

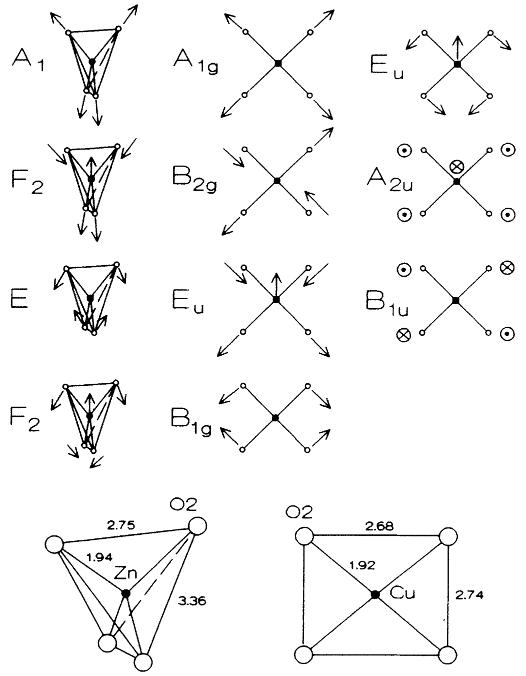

FIG. 4. Normal modes of free ZnO_4 (T_d symmetry) and free CuO_4 (D_{4h} symmetry) molecules. All distances (Å) of MO_4 (M=Zn, Cu) units in Nd_2BaMO_5 crystals are given from Refs. 7,11.

among the internal vibrations of the MO_4 unit.

In the range 291–607 cm^{-1} one observes six lines ($1A_{1g}$, $1B_{1g}$, $2B_{2g}$, and $2E_g$). According to Table II, the remaining three internal modes of the ZnO_4 molecule yield three Raman-active pairs: $A_{1g}+B_{1g}$ originating from the doubly degenerate E bending molecular mode, and $2(B_{2g}+E_g)$ from the two triply degenerate F_2 modes, one of them mainly antistretching and the other mainly bending (see Fig. 4). Using these correlations, we assign the 607-cm^{-1} (B_{2g}) and 493-cm^{-1} (E_g) modes to the internal F_2 antistretching vibration, the 361-cm^{-1} (B_{2g}) and 291-cm^{-1} (E_g) to internal F_2 bending vibration, and the 368-cm^{-1} (A_{1g}) and 247-cm^{-1} (B_{1g}) modes to the internal E scissorslike vibration of the ZuO_4 units (the same scissorslike vibration in Nd_2BaCuO_5 was found at 410 cm^{-1}). For the two ($B_{2g}+E_g$) pairs, the B_{2g} modes (involving vibrations of Zn along z) have higher frequency than the E_g counterparts (involving vibrations of Zn in the xy plane, see Table I). This can be explained by the fact that the ZnO_4 tetrahedra are elongated in the z directions (see Fig. 4). Similarly, the A_{1g} mode is harder than the B_{1g} mode (in the former mode the varying angle O-Zn-O is smaller than in the latter mode).

Modes originating from translational and rotational motions of ZnO_4 molecule are expected at lower frequencies. We assign the lines at 179 cm^{-1} (B_{2g}) and 101 cm^{-1} (E_g), to the two Raman-active modes originating from translations of F_2 symmetry, one B_{2g} (along z) and one E_g (in the xy plane). Again, as for the internal vibrations, the frequency of ZnO_4 vibrations along z is harder than of the vibration in the xy plane (the stronger atomic bonding along the z direction correlates with the fact that the crystals grow in a needlelike shape along the **c** axis). We assign the remaining Raman line at 219 cm^{-1} (E_g) to the librational mode of ZnO_4 units (arising from the rotational F_1 mode of ZnO_4 around an axis lying in the xy plane).

For analysis of the ir-transmittance spectra of Nd_2BaMO_5 (M=Zn,Cu) we note that in both structures the atoms of the Nd-O(1) layers have identical site symmetry and types of modes. Six modes ($2A_{2u}$ and $4E_u$) correspond mainly to O(1) and Nd motions. Thus, one expects that in the ir spectra of both compounds there

TABLE II. Correlation table connecting the modes of free ZnO_4 (CuO)$_4$) units and modes of Zn (Cu) and O(2) atoms in the crystals (int., rot., and tr. indicate internal, rotational, and translational modes, respectively).

	Nd_2BaZnO_5					Nd_2BaCuO_5			
Symmetry of free unit T_d	Site symmetry D'_{2d}	Crystal symmetry D_{4h}	Observed line Raman (cm $^{-1}$)	ir	Symmetry of free unit D_{4h}	Site symmetry D'_{2h}	Crystal symmetry D_{4h}	Oberved line Raman (cm^{-1})	ir
int A_1	int A_1	$A_{1g}+B_{1u}$	639		int A_{1g}	int A_g	$A_{1g}+B_{2g}$	634	
					int B_{2g}	int B_{2g}	E_g	572	
int F_2	int B_2	$A_{2u}+B_{2g}$	607	≈610	int E_u	int B_{3u}	$A_{2u}+B_{1u}$		≈564
	int E	E_g+E_u	493	?		int B_{2u}	E_u		≈514
int E	int A_1	$A_{1g}+B_{1u}$	368		int B_{1g}	int A_g	$A_{1g}+B_{2g}$	410	
	int B_1	$A_{1u}+B_{1g}$	247						
int F_2	int B_2	$A_{2u}+B_{2g}$	361	≈375	int E_u	int B_{3u}	$A_{2u}+B_{1u}$		≈350
	int E	E_g+E_u	291	?		int B_{2u}	E_u		≈350
					int A_{2u}	int B_{1u}	E_u		230
					int B_{1u}	int A_u	$A_{1u}+B_{2u}$		
rot F_1	rot A_2	$A_{2g}+B_{2u}$			rot E_g	rot B_{3g}	$A_{2g}+B_{1g}$	?	
	rot E	E_g+E_u	219	223		rot B_{2g}	E_g	?	
					rot A_{2g}	rot B_{1g}	E_g	436	
tr F_2	tr B_2	$A_{2u}+B_{2g}$	179	?	tr E_u	tr B_{3u}	$A_{2u}+B_{1u}$		?
	tr E	E_g+E_u	101	?		tr B_{2u}	E_u		167
					tr A_{2u}	tr B_{1u}	E_u		?

will exist six corresponding bands. Comparing the spectra obtained (see Fig. 5), we suggest that these corresponding bands are at 581, 404, 327, 269, 192, and 146 cm^{-1} for Nd_2BaZuO_5 and at 594, 425, 352, 287, 211, and 157 cm^{-1} for Nd_2BaCuO_5.

For identification of the ir-active modes arising from the MO_4 motions we will make use of two assumptions. First, as all ir-active modes of the ZnO_4 units are Davydov partners of Raman-active modes (see Table II), it is natural to expect that their frequencies are close. Second, although the CuO_4 and ZnO_4 molecules are of different shape, they have two similar (antistretching and bending) internal modes (see Fig. 4): two E_u for the CuO_4 and two F_2 for ZnO_4. Thus, the ir-active modes arising from these vibrations must be close in frequency.

The arrows in Fig. 5(a) shows the positions expected for the ir-active modes of ZnO_4 units (provided they have the same frequencies as their Raman counterparts). Only the 223-cm^{-1} band can definitely be assigned to the E_u librational mode. The weak bands near the 361- and 607-cm^{-1} Raman frequencies may tentatively be assigned to the A_{2u} modes (bending and antistretching) of ZnO_4. As a whole, following this scheme of assignment one can come to the conclusion that all the bands of internal ZnO_4 ir-active modes are very weak.

In the case of Na_2BaCuO_5 [Fig. 5(b)] the splitting between A_{2u} and E_u modes, arising from the internal molecular vibrations, should be weaker, as the deformation of the CuO_4 square is less strong than the deformation of the ZnO_4 tetrahedron (see Fig. 4). The two weak bands above 500 cm^{-1} could be assigned to the E_u and A_{2u} antistretching modes, whereas the E_u and A_{2u} bending ZnO_4 modes probably lie around the 352-cm Nd-O(1) band, resulting in its broadening. The two clearly pronounced bands at 230 and 167 cm^{-1} can tentatively be assigned to the E_u (internal A_{2u}) and E_u (translational E_u) modes, which do not have analogues in the Nd_2BaZnO_5 structure.

It should be noted that our assignment of the ir-active modes (in particular for these at 594, 425, and 287 cm^{-1} for Nd_2BaCuO_5 and the corresponding ones at 581, 404, and 269 cm^{-1} for Nd_2BaZnO_5) differs from that proposed in earlier reports.[9,16] In those papers a comparison between the ir-spectra of Nd_2BaCuO_5 and Nd_2CuO_4 (Ref. 17) was used and the modes were assigned to internal vibrations of the CuO_4 units. The structures of these compounds however, are rather different from each other (isolated CuO_4 units and Nd-O single layers in Nd_2BaCuO_5, and infinite CuO_2 layers and Nd-O_2-Nd CaF_2-type layers in Nd_2CuO_4) and in our opinion such a comparison is inappropriate.

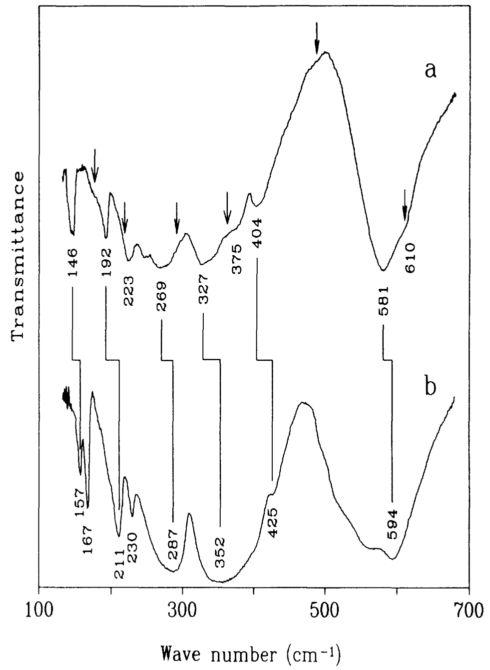

FIG. 5. ir-transmission spectra of (a) Nd_2BaZnO_5 and (b) Nd_2BaCuO_5. The bands assumed to correspond to the modes of O(1) and Nd in the two structures are connected with lines. The arrows indicate the frequencies of the Raman-active modes which have ir-active Davidov partners.

In summary, the polarized Raman spectra of Nd_2BaZnO_5 and ir-absorption spectra of Nd_2BaMO_5 (M=Zn,Cu) were measured and the symmetry of Raman-active phonons was determined. Based on molecular-site group analysis and using the similarity between the two structures, the origin of all the observed optical phonons was analyzed.

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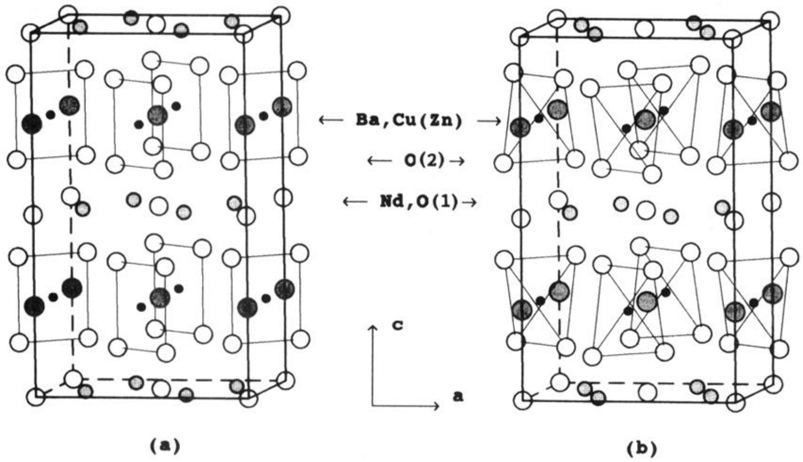

FIG. 1. Structure of (a) Nd_2BaCuO_5 and (b) Nd_2BaZnO_5. For better comparison two adjacent cells along **c** for Nd_2BaCuO_5 are given.