

Structural phase diagram and electron-phonon interaction in $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$

A.I. Liechtenstein,* I.I. Mazin,† C.O. Rodriguez, O. Jepsen, and O.K. Andersen
Max-Planck-Institut für Festkörperforschung, D-7000 Stuttgart 80, Federal Republic of Germany

M. Methfessel
Fritz-Haber-Institut, Faradayweg 4-6, D-1000 Berlin 33, Federal Republic of Germany
 (Received 24 June 1991)

Using the local-density approximation and the full-potential linear muffin-tin-orbital method we have calculated the total energy of $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ for $x = 0$ and 0.5 as a function of tilting and breathing distortions. For $x = 0$ we find an instability for a combination of both distortions and we correctly reproduce the monoclinic structure. For $x = 0.5$ we correctly find the cubic phase to be stable. The frequencies of the tilting and breathinglike phonons are calculated for $x = 0$ and 0.5 . In the cubic structure we calculate the strength λ_b of the electron-phonon coupling for the breathing mode as a function of x using a rigid-band approximation. For $0.37 < x < 0.5$, $\lambda_b \approx 0.3$ and follows the trend of T_c . The superconductivity is conceivably mediated by the electron-phonon coupling.

$\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ is distinct from other high-temperature superconductors.¹⁻³ Its bonding is three rather than two dimensional, CuO_2 planes are missing, and there are no indications of strong electronic correlations near $x = 0$. The mechanism for superconductivity ($T_c \approx 30$ K for $x \approx 0.4$) is presumably the electron-phonon coupling.⁴

$\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ has a complicated structural phase diagram.^{5,6} For the semiconducting compositions ($0 \leq x < 0.12$) the structure is monoclinic ($I2/m$) and may be derived from the cubic perovskite structure by *simultaneous* tilting (t) and breathing (b) distortions of the BiO_6 octahedra. For $0.12 < x < 0.37$ the structure is orthorhombic ($Ibmm$) with a t , but no b , distortion and, for the superconducting compositions ($0.37 < x < 0.53$), the structure is simple cubic (sc) ($t = 0, b = 0$).

Several *ab initio* band-structure calculations using the local density-functional approximation (LDA) have been performed for $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ with the compositions $x=0$ (Refs. 7-10) and $x = 0.5$.¹⁰ More recently the stability of sc BaBiO_3 against t or b was studied by means of LDA total-energy calculations using, respectively, the pseudopotential and the linear augmented-plane-wave methods. The former calculation¹¹ found a t instability but was unable to find the energy minimum. The latter¹² found a b instability and a minimum of -6 mRy, but the experimental equilibrium structure could not be reproduced because no attempt was made to include t . In this paper we present LDA calculations for $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ ($x = 0$ and 0.5) with simultaneous t and b distortions and we quantitatively reproduce the phase diagram. Furthermore, we calculate the frequencies of the t - and b -like phonons for $x = 0$ and 0.5 . Finally, we evaluate the strength λ_b of the electron-phonon coupling in the sc phase for the breathing mode as a function of x using, for the electrons, the LDA bands.

The full-potential linear muffin-tin-orbital (FPLMTO) method¹³ which makes no shape approximation for the

potential or the charge density was used. In order to have sufficient variational freedom in the interstitial region between the nearly touching muffin-tin (MT) spheres, we included one or two basis functions per site and angular momentum ($2 \times s, 2 \times p, 2 \times d$, and $1 \times f$ for Ba, and $2 \times s, 2 \times p$, and $1 \times d$ for Bi, K, and O. For the first radial function, $\kappa^2 = 0$ and, for the second, $\kappa^2 = -7$ eV). The MT radii were 2.9 (Ba, K), 2.0 (Bi), and 1.8 (O) Bohr radii. The semicore $\text{Ba}(5p)$, $\text{K}(3p)$, $\text{Bi}(5d)$, and $\text{O}(2s)$ states were treated as bands, while the other core states were treated as soft core. One energy panel was judged to suffice. Since the t , b , and combined tb distortions of the sc structure have $\mathbf{q} = (1, 1, 1)\pi/a = \mathbf{R}$, the total-energy and frozen-phonon calculations were performed with two $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ units per cell. The Brillouin-zone (BZ) integrations were done with the full-zone tetrahedron method with 47, 38, and 52 inequivalent \mathbf{k} points in the sc , orthorhombic, and monoclinic BZ's used for, respectively, b , t , and tb . For small b we used as many as 145 inequivalent \mathbf{k} points. The exchange-correlation potential of Ref. 14 and the scalar-relativistic Dirac equation were employed.

Energy-volume calculations for (hypothetical) sc BaBiO_3 yielded the bulk modulus: $B = 1.37$ Mbar and an equilibrium volume Ω_{sc} which is 3.6% smaller than the experimental one. Such an overbinding is expected for the LDA. The sc structure observed for $\text{Ba}_{0.5}\text{K}_{0.5}\text{BiO}_3$ has three possible simple superstructures with very similar energy bands and, choosing the structure with alternating Ba and K (111) planes, we calculated an equilibrium volume 5% smaller than the experimental one.⁵

Guided by the structural data for the orthorhombic phase,⁶ we took *tilting* to be rigid rotations of the BiO_6 octahedra around their [110] axes and with alternating sign ($\mathbf{q} = \mathbf{R}$). This means, that the orthorhombic lattice constants perpendicular to [110] vary with t according to $c(t) = 2l \cos t$ and $b'(t) = 2\sqrt{2}l \cos t$, whereas, along

[110], $a' = 2\sqrt{2}l = \sqrt{2}a$ is fixed. Here, l is the Bi-O distance and a the lattice constant in the sc phase ($t = 0$, $b = 0$). The double-cell volume therefore decreases with tilt: $\Omega(t) = 2\Omega_{sc} \cos^2 t$. If we now add *breathing*, the double-cell volume remains $\Omega(t)$ but alternate octahedra breathe out and in: $l_{\pm} \approx l \pm b$, $t_{\pm} \approx t(1 \mp b/l)$, and the structure becomes monoclinic. In order to obtain the phase diagram, we calculated the total energies for t , b , and tb distortions, starting from ($t = 0$, $b = 0$) and letting l be the value obtained from the *calculated* volume [$8l^3 = \Omega_{sc}$]. The results for $x = 0$ and $x = 0.5$ are shown in Fig. 1 and we now first discuss the case $x = 0$.

The breathing mode has caught attention because, for $x = 0$ and in the tight-binding nearest-neighbor $sp\sigma$ model with Bi $6s$ orbitals (Cu $3d_{x^2-y^2}$ orbitals for the CuO_2 compounds) and O $2p$ orbitals, this mode opens a gap at the Fermi level throughout the BZ due to perfect nesting of the Fermi surface. In realistic calculations (Fig. 2), however, the nesting is far from perfect: O-O hopping increases the energy near $\mathbf{k} = \mathbf{W}$ ($\frac{1}{2}\text{XM}$ in the sc BZ), and $pp\sigma$ hopping between the O $2p$ and Bi $6p$ (Cu $3d_{3z^2-1}$) orbitals lowers the energy near \mathbf{L} ($\frac{1}{2}\Gamma\text{X}$). To create a gap throughout the BZ requires

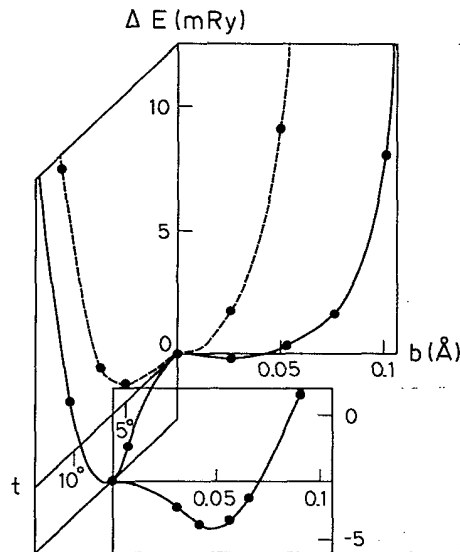


FIG. 1. Calculated total energy for $2\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ as a function of the breathing b of the BiO_6 octahedra and the angle t of their tilt around the [110] axis. Solid line: $x = 0$. Broken line: $x = 0.5$. As explained in the text the cell volume depends on tilt according to $\Omega(t, x) = 2\Omega_{sc}(x) \cos^2 t$, where $\Omega_{sc}(x)$ is the volume calculated for the sc structure. For simultaneous t and b , we displaced the O atom, which in the sc structure has its nearest-neighbor Bi atoms at $(0, 0, \pm l)$, by $d\mathbf{R} = l(\sin t/\sqrt{2}, -\sin t/\sqrt{2}, v)$. Hereby, the BiO_6 octahedra which breathe out (in) attain a Bi-O distance given by $l_{\pm} = l\sqrt{(\cos t \pm v)^2 + \sin^2 t} \approx l \pm b$, where $b \equiv vl \cos t$, and a tilt angle given by $\tan t_{\pm} = \sin t / (\cos t \pm v) \approx (1 \mp b/l) \tan t$. The octahedra stay cubic. For $x = 0$ the total energy (in Ry per 2BaBiO_3) is fitted by $E(u \equiv \sin t, v) = -0.358^2 u^2 - 1.463^2 v^2 - 2.043^4 u^4 - 3.294^4 u^2 v^2 + 7.155^4 v^4 + 3.024^6 u^6 + 3.428^6 u^4 v^2 + 5.164^6 u^2 v^4 - 7.130^6 v^6$.

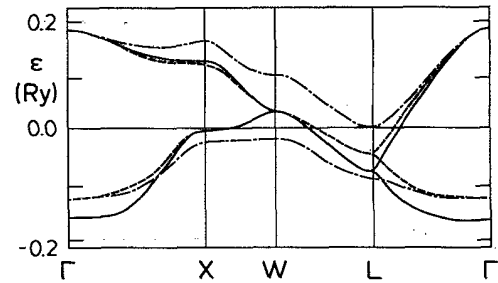


FIG. 2. The FPLMTO energy bands near the Fermi level for 2BaBiO_3 . Other bands are omitted from the figure. Solid line: $t = 0$, $b = 0$. Dashed line: $t = 10^\circ$, $b = 0$. Dot-dashed line: $t = 10^\circ$, $b = 0.09 \text{ \AA}$. The folding of the sc BZ is as follows: $\text{R} \rightarrow \Gamma$, $\text{M} \rightarrow \text{X}$, $\frac{1}{2}\text{XM} \rightarrow \text{W}$, and $\frac{1}{2}\Gamma\text{R} \rightarrow \text{L}$ (see Ref. 7).

$b > 0.08 \text{ \AA}$ (when $t = 0$). Breathing always lowers the sum of the one-electron energies, but this gain is nearly compensated by an increase of electrostatic energy and, as a result, there is only a tiny instability of the *pure* b type as seen from the full line in Fig. 1; the total-energy minimum is $\Delta E = -0.1 \text{ mRy}/2\text{BaBiO}_3$ and occurs for $b = 0.03 \text{ \AA}$. The shape of the curve at small b is mostly determined by the imperfectness of the nesting. It may be noted that, although the Bi $6s$ -charge transfer amounts to $\pm 0.15 e$ (between the Bi MT spheres for $b = 0.09 \text{ \AA}$), this charge is screened by the tails of O $2p$ orbitals to the extent that the total Bi MT-charge transfer is only $\pm 0.01 e$.

We find that sc BaBiO_3 is unstable against *pure* tilting too (Fig. 1); the total-energy minimum is $\Delta E = -3.5 \text{ mRy}/2\text{BaBiO}_3$ and occurs for $t = 8^\circ$. This tilt instability seems to be driven by the Madelung energy.

Now, in the tilted structure, the nesting becomes more perfect because the O $2p$ to Bi $6p$ hopping is reduced due to misalignment of the orbitals and, hence, the band is raised near \mathbf{L} (Fig. 2, dashed line). Consequently, *tilting helps breathing*. In order to find the equilibrium structure we performed total-energy calculations for about 20 (t, b) points and fitted to a sixth-order polynomial (Fig. 1). The resulting calculated equilibrium has $\Delta E = -4.6 \text{ mRy}/2\text{BaBiO}_3$, $t = 8.5^\circ$, and $b = 0.055 \text{ \AA}$, which is in quite good agreement with the experimental^{5,6} values: $t = 10.3^\circ$ and $b = 0.085 \text{ \AA}$. We finally checked the assumption of constant l by varying the cell volume away from $\Omega(t)$ at the (t, b) minimum.

Diagonalization of the dynamical matrix obtained from the second derivatives of the total energy at the global minimum, gave the normal-mode frequencies: 235 cm^{-1} (t -like) and 370 cm^{-1} (b -like). Taking the second derivatives under the constraint of constant volume, rather than constant pressure ($\approx \text{const } l$), made the phonon frequencies increase to 307 cm^{-1} (t -like) and 373 cm^{-1} (b -like). The total energy profile is extremely anharmonic, and this causes renormalization of the phonon frequencies. This we estimated perturbatively¹⁵ from the third and the fourth derivatives (neglecting interactions with all other phonons) and, for zero temperature and constant pressure, we found $\delta\omega/\omega = (\delta_3\omega/\omega) + (\delta_4\omega/\omega) =$

$-9\%+8\% = -1\%$ for the t -like, and $-23\%+9\% = -14\%$ for the b -like mode. The experimental phonon frequencies are controversial, which is hardly surprising in view of the strong anharmonicity and the line broadening due to strong electron-phonon interaction.

Considering now $x = 0.5$, we find that BaKBi_2O_6 is stable with respect to both t and b displacements (Fig. 1). The calculated phonon frequencies are, respectively, 105 and 530 cm^{-1} . (In this case, where the total-energy minimum is at $t = 0$, there is no difference between constant-volume and constant-pressure frequencies.) Since for $x = 0.5$ merely the lower quarter of the $sp\sigma$ band is full, the nesting effect which favors breathing is absent. Also, substitution of half the Ba by K weakens the tilt-favoring Madelung energy.

In the last part of this paper we evaluate the strength $\lambda_{\nu\mathbf{q}}$ of the electron-phonon (e -ph) coupling for the $\mathbf{q} = \mathbf{R}$ breathing mode in the sc structure (for tilting it vanishes by symmetry). This structure is the one which superconducts below a T_c which is shown in Fig. 3 as a function of x . We first describe the technique for calculating λ .

The linewidth of the $\nu\mathbf{q}$ phonon due to the e -ph coupling is given by Fermi's golden rule:¹⁶

$$\gamma_{\nu\mathbf{q}} = 2\pi \sum_{n,m,\mathbf{k}} [\theta(\epsilon_m(\mathbf{k}+\mathbf{q})) - \theta(\epsilon_{n\mathbf{k}})] \times \delta(\epsilon_m(\mathbf{k}+\mathbf{q}) - \epsilon_{n\mathbf{k}} - \omega_{\nu\mathbf{q}}) |g_{\nu,n\mathbf{k},m(\mathbf{k}+\mathbf{q})}|^2. \quad (1)$$

Here, $|n\mathbf{k}\rangle$ are the electronic states in the undistorted crystal and $\epsilon_{n\mathbf{k}}$ are their energies relative to the Fermi

level. n and m run over the bands, the factor 2 is from the spin degeneracy, and the sum over \mathbf{k} is the average over the BZ [i.e., $\Sigma_{\mathbf{k}} \equiv (2\pi)^{-3} \Omega_{sc} \int d^3k$]. For the energy bands we shall use the LDA eigenvalues and, for sc $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ in the virtual-crystal approximation, there is only one band ($n = m = 1$). In (1) the phonon energy is $\omega_{\nu\mathbf{q}}$ and the e -ph matrix element is

$$g_{\nu,n\mathbf{k},m(\mathbf{k}+\mathbf{q})} = \langle n\mathbf{k} | dV(\mathbf{r}) | m(\mathbf{k}+\mathbf{q}) \rangle / dQ_{\nu\mathbf{q}}. \quad (2)$$

Here, the perturbation of the self-consistent electronic potential due to the phonon is $dV(\mathbf{r}) = \Sigma_{ij} [\partial V(\mathbf{r}) / \partial R_{ij}] dR_{ij}$ with the displacement in the i direction of the j th atom given by $dR_{ij} = e_{ij,\nu\mathbf{q}} (2M_j \omega_{\nu\mathbf{q}})^{-1/2} dQ_{\nu\mathbf{q}}$. Here, $e_{\nu\mathbf{q}}$ is the phonon eigenvector normalized to unity in the primitive cell and M_j is the mass of the j th atom. For the b mode, only the three O atoms are involved and $e_{ij} = \delta_{ij} / \sqrt{3}$. Now, the Eliashberg function $\alpha^2 F(\omega)$ is essentially the phononic density of states weighted by the relative linewidth γ/ω . The strength λ of the e -ph coupling may therefore be expressed as¹⁶

$$\lambda \equiv 2 \int_0^\infty \frac{\alpha^2 F(\omega)}{\omega} d\omega = \frac{1}{\pi N_{\uparrow}(0)} \sum_{\nu,\mathbf{q}} \frac{\gamma_{\nu\mathbf{q}}}{\omega_{\nu\mathbf{q}}^2} \equiv \sum_{\nu,\mathbf{q}} \lambda_{\nu\mathbf{q}}, \quad (3)$$

where $N_{\uparrow}(0) \equiv \sum_{n,\mathbf{k}} \delta(\epsilon_{n\mathbf{k}})$ is the electronic density of states per spin at the Fermi level.

If the energy bands are linear functions of \mathbf{k} within the energy range $\omega_{\nu\mathbf{q}}$ around the Fermi level and if $q \gg \omega_{\nu\mathbf{q}}/v_{n\mathbf{k}}$, where $v_{n\mathbf{k}} \equiv \partial \epsilon_{n\mathbf{k}} / \partial \mathbf{k}$ is the Fermi velocity, then (1) may be written as a line integral along the cut between the n th sheet of the Fermi surface, $\epsilon_{n\mathbf{k}} = 0$, and the m th sheet of the \mathbf{q} -displaced Fermi surface, $\epsilon_m(\mathbf{k}+\mathbf{q}) = 0$:

$$\begin{aligned} \gamma_{\nu\mathbf{q}} / \omega_{\nu\mathbf{q}} &= 2\pi \sum_{n,m,\mathbf{k}} \delta(\epsilon_m(\mathbf{k}+\mathbf{q})) \delta(\epsilon_{n\mathbf{k}}) |g|^2 \\ &= 2\pi \sum_{n,m} \int \frac{(2\pi)^{-3} \Omega_{sc} d\mathbf{k}}{|v_{n\mathbf{k}} \times v_{m(\mathbf{k}+\mathbf{q})}|} |g|^2. \end{aligned} \quad (4)$$

For simplicity we have dropped the subscripts on g .

With muffin-tin orbitals and a frozen-phonon supercell technique, it is inconvenient to evaluate integrals like $\langle n\mathbf{k} | dV(\mathbf{r}) | m(\mathbf{k}+\mathbf{q}) \rangle$ which involve orbitals at the equilibrium positions and the potential for the displaced atoms. Instead, we obtain the e -ph matrix elements from the self-consistent energy bands with ($\tilde{\epsilon}$) and without (ϵ) the displacement, using that, for a point on the cut: $\epsilon_{n\mathbf{k}} = \epsilon_m(\mathbf{k}+\mathbf{q}) = 0$, the degeneracy is split by $\Delta\tilde{\epsilon}_k = 2|\langle n\mathbf{k} | dV(\mathbf{r}) | m(\mathbf{k}+\mathbf{q}) \rangle|$. In practice, the nm cut is found by calculating the ϵ bands on a fine mesh in the sc BZ (145 irreducible points) and interpolating them linearly inside each tetrahedron. Using the supercell, where $\mathbf{k} + \mathbf{q}$ falls onto \mathbf{k} , the ϵ bands are then recalculated along the cut and, since this cut is merely interpolated, the n and m bands (those near the Fermi level) are split slightly, by $\Delta\epsilon_k$. A self-consistent supercell calculation is now performed *with* the frozen phonon and, for the re-

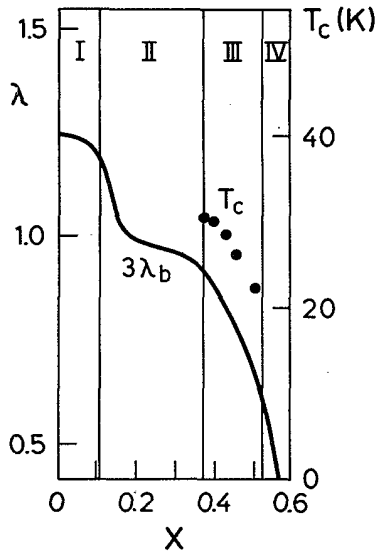


FIG. 3. Electron-phonon coupling constant for the oxygen breathing mode calculated for sc $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$. We used the phonon frequency calculated for $x = 0.5$ ($\omega_b = 530 \text{ cm}^{-1}$), the self-consistent frozen-phonon potentials calculated for $x = 0$, and the rigid-band approximation for x values other than 0. Indicated by dots are the T_c values measured in Ref. 5. The vertical lines indicate the regions of stability of the monoclinic (I), orthorhombic (II), and sc (III) structures.

sulting potential, the energy bands are traced along the interpolated cut. The splitting $\Delta\tilde{\epsilon}_k$ of the near-zero energies finally yields the e -ph matrix element according to $|\langle nk|dV(\mathbf{r})|m(\mathbf{k}+\mathbf{q})\rangle|^2 \approx [(\Delta\tilde{\epsilon}_k)^2 - (\Delta\epsilon_k)^2]/4$.

Using (4) we calculated the e -ph coupling strength $\lambda_b(x)$ for the breathing mode in the sc structure ($0.37 < x < 0.53$) using the phonon frequency ($\omega_b = 530 \text{ cm}^{-1}$) calculated for $x = 0.5$ plus the rigid-band approximation for the electrons. Specifically, we performed the self-consistent calculations with and without breathing ($b = 0.03 \text{ \AA}$ and 0) for sc BaBiO_3 and then moved the Fermi level within the resulting ϵ and $\tilde{\epsilon}$ bands according to the hole count x . Although this means that the screening of the frozen phonon corresponds to $x = 0$, rather than to $x \approx 0.5$, we believe that this procedure, which was dictated by its practicality, leads to a reasonable approximation.

The resulting $\lambda_b(x)$ is shown in Fig. 3, even for x outside the range of stability of the sc structure. The b mode presumably has the largest λ because this mode strongly modulates the $sp\sigma$ -hopping integral so that $|g|^2$ is large. Moreover, at least for small x , the phase space is large due to near Fermi-surface nesting [the Fermi velocities in (6) are nearly antiparallel]. From Fig. 3 two features are noticeable. Firstly, the sharp increase of λ_b as x decreases below 0.15. This is the nesting effect and, had we included the proper x dependence of the phonon frequency, λ_b would even have diverged for $x \approx 0.1$ because, here, the b phonon becomes unstable. Secondly, for the superconducting compositions, where the x dependence of ω_b is presumably negligible, $\lambda_b(x)$

follows the same trend as the experimental $T_c(x)$. This suggests that the pairing agents are, indeed, the breathinglike phonons. If we estimate the total λ to be about three times λ_b (roughly speaking, because of the 9 O modes 3 are stretching) we find $\lambda \approx 0.9$ at $x = 0.4$. This is close to the estimate found from model tight-binding calculations by Shirai, Suzuki, and Motzuki.⁴ By solving the Eliashberg equations using $\mu^* = 0.12$, these authors furthermore estimated that $T_c \approx 30 \text{ K}$, which is close to the experimental value. The McMillan formula¹⁷ yields about the same value. Hence, the superconductivity in sc $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ seems to be conventional and mediated by the e -ph coupling.

In summary, we have presented LDA calculations of the structural phase diagram of $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ for $x = 0$ and $x = 0.5$. We found equilibrium crystal structures in good agreement with experiments, namely, for $x = 0$ a simultaneous tilting and breathing distortion amounting to $t = 8.5^\circ$ and $b = 0.055 \text{ \AA}$ of the cubic structure and, for $x = 0.5$ the absence of both instabilities. The frequencies of the tilting and breathinglike phonons were calculated and for $x = 0$, the effect of anharmonicity was discussed. We calculated the e -ph coupling constant λ_b for the breathing mode as a function of x in the cubic structure. The result is in accord with the experimental values of $T_c(x)$ and this supports the view that the superconductivity is conventional.

Three of us (A.I.L., C.O.R., and I.I.M.) thank the Alexander von Humboldt Foundation for financial support.

*On leave from Institute of Chemistry, Sverdlovsk, U.S.S.R.

†On leave from Lebedev Physical Institute, Moscow, U.S.S.R.

¹L.F. Mattheiss, E.M. Gyorgy, and D.W. Johnson Jr., *Phys. Rev. B* **3**, 3745 (1988).

²R.J. Cava, B. Batlogg, J.J. Krajewski, R. Farrow, L.W. Rupp Jr., A.E. White, K. Short, W.F. Peck, and T.Y. Komemati, *Nature (London)* **332**, 814 (1988).

³D.G. Hinks, B. Dabrowski, B.D. Jorgensen, A.W. Mitchell, D.R. Richards, S. Pei, and D. Shi, *Nature (London)* **333**, 836 (1988).

⁴M. Shirai, N. Suzuki, and K. Motzuki, *J. Phys. Condens. Matter* **2**, 3553 (1990).

⁵S. Pei, J.D. Jorgensen, B. Dabrowski, D.G. Hinks, D.R. Richards, A.W. Mitchell, J.M. Newsam, S.K. Sinha, D. Vaknin, and A.J. Jacobson, *Phys. Rev. B* **41**, 4126 (1990).

⁶D.E. Cox and A.W. Sleight, *Solid State Commun.* **19**, 969 (1976); *Acta Crystallogr. Sect. B* **35**, 1 (1979).

⁷L.F. Mattheiss and D.R. Hamann, *Phys. Rev. B* **28**, 4227 (1983).

⁸K. Takegahara and T. Kasuya, *J. Phys. Soc. Jpn.* **56**, 1478 (1987).

⁹N. Hamada, S. Massidda, A.J. Freeman, and J. Redinger, *Phys. Rev. B* **40**, 4442 (1989).

¹⁰L.F. Mattheiss and D.R. Hamann, *Phys. Rev. Lett.* **60**, 2681 (1988).

¹¹R. Zeyher and K. Kunc, *Solid State Commun.* **74**, 805 (1990).

¹²P. Blaha, K. Schwarz, G. Vielsack, and W. Weber, in *Electronic Properties of High- T_c Superconductors and Related Compounds*, edited by H. Kuzmany, M. Mehring, and J. Fink (Springer, Berlin, 1990).

¹³M. Methfessel, C.O. Rodriguez, and O.K. Andersen, *Phys. Rev. B* **40**, 2009 (1989).

¹⁴U. von Barth and L. Hedin, *J. Phys. C* **5**, 1629 (1972).

¹⁵A.A. Maradudin and A.E. Fein, *Phys. Rev. B* **128**, 2589 (1962).

¹⁶P.B. Allen, *Phys. Rev. B* **6**, 2577 (1972).

¹⁷W.L. McMillan, *Phys. Rev.* **167**, 331 (1968).