Classification of octahedral tilting phases in the perovskitelike A_2BX_4 structure

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The possible lower symmetries (subgroups) of the A_2BX_4 structure (space-group symmetry D_{4h}^{17}) due to rigid octahedral tiltings at phase transitions are investigated. The method for obtaining subgroups determined by reducible representations (i.e., coupled order parameters) is described. This method depends upon subgroup information for irreducible representations (i.e., single uncoupled order parameters). All subgroup symmetries which are allowed by the coupling of two simple octahedral tiltings are listed for this structure.

I. INTRODUCTION

During the last fifteen years a great interest has developed in perovskites and perovskite-related structures. Of particular interest has been the description and the classification of their various phases with the ultimate aim of clarifying the mechanism for the phase transitions. The perovskites have the general structure formula ABX_3, space-group symmetry O_h^1, and were shown to undergo transitions (e.g., $SrTiO_3$, $NaNbO_3$) arising from the condensation of soft phonon modes from the R and M Brillouin zone points of symmetry.[1–3] The dominant mechanism for the transitions was isolated, and the transitions were described in terms of the tilting of the rigid BX_6 octahedra.[4,2] As the octahedra tilt and distort the original structure, the symmetry of the structure is changed. Similarly the mechanism for selected sequences of transitions in the antifluorites [(A_2BX_6) (Refs. 5 and 6)] as well in the perovskitelike ABX_4 structures[7,8] was identified as the tilting of rigid octahedral units.

Complex sequences of transitions in the ABX_3 structures can be described by coupling the rigid octahedral tiltings of more simple (component) distortions. Glazer,[9] emphasizing this mechanism for transitions in the ABX_3 structures, classified the possible displacive distortions which could arise from the octahedral tiltings and listed 23 lower symmetry space groups. For the ABX_3 structures [Fig. 1(a)] a three-dimensional network of corner-linked octahedra is defined. Any tilting (and its accompanying corner displacements) will demand neighboring octahedral corner displacements which in many cases involve more than one x-y layer of octahedra. For example tilting around the y axis automatically doubles the periodicity the z direction [Fig. 2(a)].

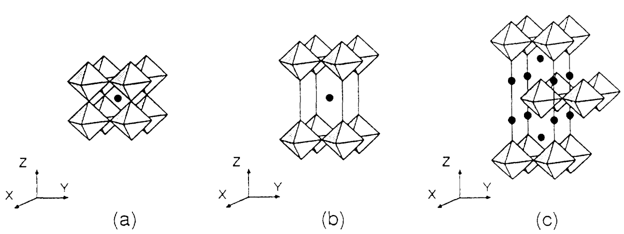

FIG. 1. Structures of (a) ABX_3 type, (b) ABX_4 type, and (c) A_2BX_4 type. The BX_6 octahedra are the hatched units. The B atom is assumed to be at the center of the octahedron and an X atom at each vertex. The solid circles are the A cations.

Recently a similar approach was used to classify the sequences of transitions[10–12] which are allowed in the ABX_4 structures of space group symmetry D_{4h}^1 (e.g., $RbAlF_4$, $TlAlF_4$). The ABX_4 structures [Fig. 1(b)] have BX_6 octahedra corner linked only in the x-y plane. Successive layers along the z axis are positioned directly above one another. In contrast to the ABX_3 structures the tilting around the y axis does not necessarily double

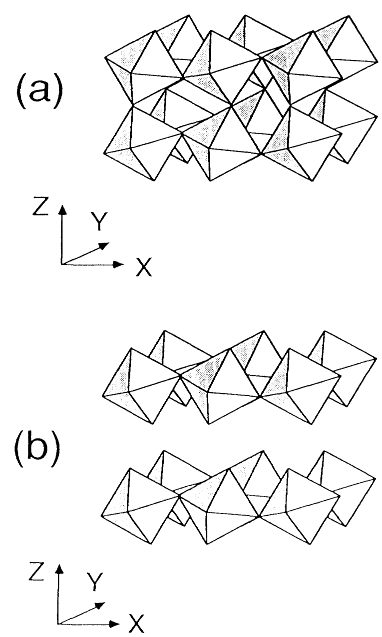

FIG. 2. (a) Titling of octahedra (around y in axis) in ABX_3 structure. The lattice spacing (along z) of Fig. 1(a) is no longer the repeat distance. The smallest cell change would result in a doubling of the periodicity of the structure along z. (b) Titling of the octahedra (around y axis) in ABX_4 structure which does not double the periodicity along z since the octahedra are not top-bottom linked between layers.

the periodicity along the z axis [Fig. 2(b)], because the ochtahedral are not top-bottom linked between two layers. A very thorough analysis of the subgroups of D^1_{4h} due to coupled octahedral tiltings was performed by Deblieck *et al.*[10] but they made no connection to the mode symmetry (i.e., to the space-group representations) which determine the new space group. Aleksandrov *et al.*[11] also studied transitions in D^1_{4h} due to coupled tiltings and they did make the association to irreducible representations of D^1_{4h}. However they did not consider the complete variety of couplings, as was easily seen by comparing their listing of subgroups with those of Deblieck *et al.*[10] In order that the complete list be given of the possible subgroup symmetries for D^1_{4h} together with their associated symmetry labeling, we also analyzed the subgroup phases determined by coupled octahedral tiltings in D^1_{4h}.[12]

TABLE I. Irreducible representations allowing octahedral tiltings in the A_2BX_4 structure are listed. The subgroups resulting from the tilting are shown along with the conventional "basis" vectors and origins (in terms of the original conventional vectors of D^{17}_{4h}). The order parameter orbit is also indicated for each subgroup.

Irrep	Subgroup	Orbit	Basis vectors	Origin
X_3^+	$D^{18}_{2h}(64)$	$P3$	(1,1,0),(0,0,1),(1,−1,0)	(0,0,0)
	$D^{16}_{4h}(138)$	$P1$	(1,1,0),(−1,1,0),(0,0,1)	$(0,-1,-\frac{1}{2})$
	$D^{10}_{2h}(56)$	$C1$	(1,1,0),(−1,1,0),(0,0,1)	(0,0,0)
X_4^+	$D^{20}_{2h}(66)$	$P3$	(0,0,1),(1,1,0),(−1,1,0)	$(\frac{1}{4},\frac{1}{4},-\frac{1}{4})$
	$D^{12}_{4h}(134)$	$P1$	(1,1,0),(−1,1,0),(0,0,1)	$(-\frac{1}{2},-\frac{1}{2},-\frac{1}{2})$
	$D^{2}_{2h}(48)$	$C1$	(1,1,0),(−1,1,0),(0,0,1)	$(\frac{1}{2},-\frac{1}{2},0)$
N_1^+	$C^{3}_{2h}(12)$	$P5$	(0,1,−1),(−1,0,0),(0,1,1)	(0,0,0)
	$D^{19}_{2h}(65)$	$P1$	(0,0,2),(0,−2,0),(1,0,0)	$(\frac{1}{2},\frac{1}{2},-\frac{1}{2})$
	$C^{3}_{2h}(13)$	$P11$	$(0,0,-4)(2,2,0),\frac{1}{4},-\frac{1}{4},\frac{1}{2})$	(0,0,0)
	$C^{1}_{2h}(10)$	$C3$	(0,−1,−1),(1,0,0),(0,−1,1)	(0,0,0)
	$C^{i}_{1}(2)$	$C12$	$(-1,1,1),(\frac{1}{2},-\frac{1}{2},\frac{1}{2}),(1,1,-1)$	(0,0,0)
	$D^{19}_{4h}(141)$	$P4$	(2,0,0),(0,2,0),(0,0,2)	(0,0,−1)
	$D^{17}_{4h}(139)$	$P3$	(2,0,0),(0,2,0),(0,0,2)	$(-\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	$D^{28}_{2h}(74)$	$C2$	(2,0,0),(0,2,0),(0,0,2)	(0,0,0)
	$D^{25}_{2h}(71)$	$C1$	(2,0,0),(0,2,0),(0,0,2)	$(-\frac{1}{2},\frac{1}{2},\frac{1}{2})$
	$C^{6}_{2h}(15)$	$C10$	$(0,0,4),(-2,-2,0),(\frac{1}{2},-\frac{1}{2},-1)$	$(\frac{1}{2},\frac{1}{2},-\frac{1}{2})$
	$C^{3}_{2h}(12)$	$C8$	$(0,0,4),(-2,-2,0),(\frac{1}{2},-\frac{1}{2},-1)$	(0,0,0)
	$C^{3}_{2h}(12)$	$S1$	(2,0,2),(0,−2,0),(0,0,−2)	$(\frac{1}{2},-\frac{1}{2},\frac{1}{2})$
	$C^{1}_{i}(2)$	$4D1$	(−1,1,1),(1,−1,1),(1,1,−1)	(0,0,0)
$P5$	$D^{12}_{2d}(122)$	$P1$	(1,−1,0),(1,1,0),(0,0,2)	$(0,\frac{1}{2},\frac{3}{4})$
	$D^{11}_{2d}(121)$	$P4$	(1,−1,0),(1,1,0),(0,0,2)	$(0,\frac{1}{2},\frac{3}{4})$
	$D^{28}_{2h}(74)$	$P5$	(0,0,2),(1,−1,0),(1,1,0)	$(1,-\frac{1}{2},\frac{1}{2})$
	$D^{26}_{2h}(72)$	$P12$	(0,0,2),(1,−1,0),(1,1,0)	$(\frac{1}{4},\frac{1}{4},\frac{3}{4})$
	$D^{24}_{2h}(70)$	$P3$	(0,0,2),(2,0,0),(0,2,0)	$(-\frac{7}{4},-\frac{5}{4},-\frac{5}{4})$
	$D^{23}_{2h}(69)$	$P11$	(2,0,0),(0,2,0),(0,0,2)	$(1,-\frac{1}{2},\frac{1}{2})$
	$S^{2}_{4}(82)$	$C2$	(1,−1,0),(1,1,0),(0,0,2)	$(\frac{1}{2},0,\frac{1}{4})$
	$C^{22}_{2v}(46)$	$C13$	(1,−1,0),(1,1,0),(0,0,2)	$(0,\frac{1}{2},0)$
	$C^{19}_{2v}(43)$	$C1$	(2,0,0),(0,2,0),(0,0,2)	$(0,\frac{1}{2},0)$
	$C^{18}_{2v}(42)$	$C10$	(2,0,0),(0,2,0),(0,0,2)	$(0,\frac{1}{2},0)$
	$D^{2}_{9}(24)$	$C2$	(1,1,0),(−1,1,0),(0,0,2)	$(\frac{1}{4},\frac{1}{4},0)$
	$D^{2}_{8}(23)$	$C11$	(1,1,0),(−1,1,0),(0,0,2)	$(\frac{1}{2},0,\frac{3}{4})$
	$D^{2}_{7}(22)$	$C8$	(0,−2,0),(2,0,0),(0,0,2)	$(\frac{1}{2},0,0)$
	$C^{6}_{2h}(15)$	$C9$	(2,0,0),(0,0,−2),(−1,1,0)	$(\frac{1}{4},\frac{1}{4},\frac{1}{4})$
	$C^{3}_{2h}(12)$	$C12$	(2,0,0),(0,0,−2),(−1,1,0)	$(1,-\frac{1}{2},\frac{1}{2})$
	$C^{2}_{3}(5)$	$4D1$	(2,0,0),(0,0,−2),(−1,1,0)	$(0,\frac{1}{2},0)$

A_2BX_4 structures (e.g., K_2MgF_4, Rb_2CdCl_4) with space-group symmetry D_{4h}^{17} [Fig. 1(c)] are similar to the ABX_4 structures in that they consist of layers of octahedral units separated by the A cation. However the successive layers of the octahedra are shifted by one half the conventional cell diagonal.

In spite of detailed studies of these structures[13,15] no observed transitions connected with the octahedral tiltings had been observed until recently. From EPR data a transition in Rb_2CdCl_4 near 133 K has been found which is attributed to the coupled octahedral tiltings arising from X-point distortions.[16]

With the expectation that other tilting modes may be found in the A_2BX_4 structures, in this paper we classify the possible subgroups of D_{4h}^{17} which arise from octahedral tiltings. The procedure outlined in Ref. 12 will be used. This approach relies heavily upon the detailed results of subgroup listings for irreducible representations of D_{4h}^{17}. Thus in Sec. II we briefly discuss our method of obtaining all subgroup symmetries for the irreducible representations (irreps). The results for the specific case of D_{4h}^{17} are presented in Table I. In addition we show an example of a simple octahedral tilting for each irrep. In Sec. III we outline the method for obtaining subgroups due to coupled tiltings. In Table II we then list all subgroups which may be obtained by distortions of D_{4h}^{17} for bicoupled (two irrep) octahedral tiltings.

II. ISOTROPY SUBGROUPS DETERMINED BY IRREDUCIBLE REPRESENTATIONS

The group-subgroup classification of continuous phase transitions was initiated by Landau many years ago.[17] Since that time his approach has been used to study transitions in a wide variety of physical systems. The method of selection of subgroups proposed by Landau was by minimization of the lowest-order expansion of the free energy (up to quartic order) in terms of the order parameter. The order parameter represents the physical property of the system that changes as the system goes through the transition. Thus it denotes the "distortion" of the crystal taking place at the transition. For a system with a multicomponent order parameter and multiple independent quartic invariants, the minimization process becomes extremely difficult and numerical computer methods must be used.[18]

Emphasis on group-theoretical ideas have allowed a more systematic approach to the classification of possible space-group changes. The order parameter $\boldsymbol{\eta}$ is taken as a vector in the carrier space of the representation of G_0. Stability of the system with respect to homogeneous and inhomogeneous fluctuations can be implemented in terms of symmetrized (Landau condition[17,19]) and antisymmetrized (Lifshitz condition[19,20]) products of the irrep. Rather than selecting subgroups through minimization, the subgroups are selected by seeking the subgroup of G_0 which leaves $\boldsymbol{\eta}$ invariant. The free-energy expansion is not needed and the possible subgroups are dependent only upon the choice of irrep. To obtain the maximal subgroup of G_0 leaving a given $\boldsymbol{\eta}$ invariant (an isotropy subgroup), the subduction[21] and chain subduction criteria[22] are imposed. As $\boldsymbol{\eta}$ varies throughout the representation space all possible isotropy subgroups of G_0 are obtained corresponding to the given irrep. We have used essentially this group theoretical procedure to obtain isotropy subgroups (ISG's) of all 230 space groups[23] for all irreps arising from $\mathbf{k}$ points of symmetry.[24]

The details of the method have been discussed recently,[25,26] and we refer the reader to those discussions. However we do want to point out that, for an irrep $D^{(*\mathbf{k},\gamma)}$ of the space group G_0, the representation determines a set of distinct matrices (this set is called the image). The representation is a map from G_0 onto the image, and each matrix is an operator in the carrier space E of the representation. For a given $\boldsymbol{\eta}$ in E the complete set of matrices leaving $\boldsymbol{\eta}$ fixed (the image isotropy subgroup) then defines the ISG of G_0 by the inverse map. The same image, up to equivalence, may occur for different representations and for different space groups. The *image* isotropy subgroups will be the same wherever that image occurs even though the ISG's of the space groups will differ due to the variety of representations being considered.

For example the C_{4v} image is a set of eight matrices which act in a two-dimensional carrier space E. For a particular choice of axes (see Fig. 3) the eight matrices are generated by the matrices $\sigma_{da}=\left(\begin{smallmatrix}0&-1\\-1&0\end{smallmatrix}\right)$ and $C_{4z}^{+}=\left(\begin{smallmatrix}0&-1\\1&0\end{smallmatrix}\right)$. This image appears often in the listing of representations of the 230 space groups and in particular is an image of interest for D_{4h}^{17}. For this image the subgroup $m(\sigma_d)$, consisting of the identity matrix and σ_{da}, leaves the vector $\boldsymbol{\eta}^{(1)}$ in Fig. 3 fixed. The action of the image group on $\boldsymbol{\eta}^{(1)}$ yields three additional vectors obtained by 90° rotations of $\boldsymbol{\eta}^{(1)}$. This family of vectors (points in the vector space of Fig. 3) is called the orbit of $\boldsymbol{\eta}^{(1)}$ and each vector is left fixed by a subgroup of the image group conjugate to $m(\sigma_d)$. This particular orbit is $P3$ in our notation and the points of the orbit are numbered one through four.

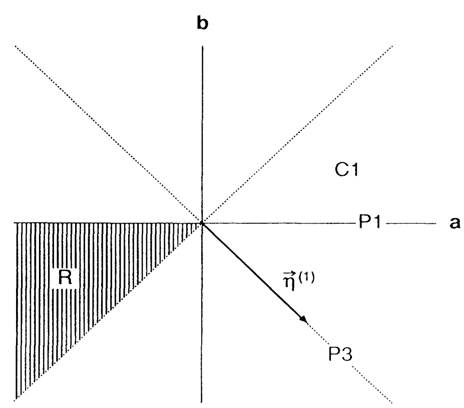

FIG. 3. Carrier space E for the C_{4v} image. The vector $\boldsymbol{\eta}^{(1)}$ is invariant under the image subgroup $m(\sigma_d)$. The orbit of $\boldsymbol{\eta}^{(1)}$ is obtained by 90° rotations and is denoted $P3$. A $P1$ orbit is obtained by 90° rotations of a vector along the $\mathbf{a}$ axis. A $C1$ orbit is obtained from a general vector and is left invariant under the image subgroup consisting of the identity. Every vector in the region R has the same image symmetry group.

TABLE II. The subgroups obtained from reducible representations of D_{4h}^{17} are listed. The irreps being coupled are shown as well as the order parameter orbits and stratum subspaces. The subgroup conventional basis vectors and origin are expressed in terms of the original conventional basis vectors of D_{4h}^{17}.

Irreps	Subgroup	Orbit	Subspace	Basis	Origin
$X_3^+ \oplus X_4^+$	D_{2h}^{21}	$P1,P1$	1,1	$(0,-2,0),(2,0,0),(0,0,1)$	$(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$
	C_{4h}^{4}	$P1,P1$	1,2	$(-1,-1,0),(-1,1,0),(0,0,-1)$	$(\frac{15}{8},\frac{3}{8},\frac{9}{8})$
	C_{2h}^{6}	$P3,P3$	1,1	$(1,1,0),(0,0,1),(0,-1,0)$	$(\frac{1}{4},\frac{1}{4},-\frac{1}{4})$
	D_{2h}^{7}	$P3,P3$	1,2	$(-1,-1,0),(0,0,-1),(1,-1,0)$	$(0,0,0)$
	C_{2h}^{4}	$C1,C1$	1,1	$(-1,1,0),(0,0,-1),(0,-2,0)$	$(0,0,0)$
$X_3^+ \oplus N_1^+$	D_{2h}^{26}	$P1,P1$	1,3	$(0,-2,0),(0,0,2),(-2,0,0)$	$(0,0,0)$
	C_{4h}^{6}	$P1,P4$	1,2	$(-2,0,0),(0,2,0),(0,0,-2)$	$(-\frac{1}{4},-1,\frac{17}{8})$
	D_{2h}^{28}	$P1,C2$	1,1	$(0,-2,0),(2,0,0),(0,0,2)$	$(\frac{1}{4},\frac{1}{4},\frac{1}{4})$
	C_{2h}^{3}	$P1,S1$	1,1	$(-2,0,2),(0,-2,0),(0,0,2)$	$(\frac{1}{4},\frac{1}{4},-\frac{1}{4})$
	C_{2h}^{3}	$P3,C8$	1,1	$(0,0,-4),(-2,-2,0),(-\frac{1}{2},\frac{1}{2},1)$	$(0,0,0)$
	C_{2h}^{6}	$C1,C2$	1,1	$(-2,2,0),(0,0,-2),(0,-2,0)$	$(0,0,0)$
	C_i^{1}	$C1,4D1$	1,1	$(-1,-1,1),(-1,1,-1),(1,-1,-1)$	$(0,0,0)$
$X_3^+ \oplus P_5$	D_{2h}^{21}	$P1,P11$	1,1	$(0,-2,0),(2,0,0),(0,0,2)$	$(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$
	D_{2h}^{22}	$P1,P11$	1,2	$(0,-2,0),(2,0,0),(0,0,2)$	$(\frac{1}{8},\frac{1}{8},-\frac{3}{8})$
	D_{2d}^{3}	$P1,P4$	1,1	$(-1,-1,0),(1,-1,0),(0,0,2)$	$(\frac{11}{16},\frac{3}{16},\frac{1}{16})$
	D_{2d}^{4}	$P1,P4$	1,3	$(-1,-1,0),(1,-1,0),(0,0,2)$	$(\frac{11}{16},\frac{3}{16},\frac{1}{16})$
	S_4^{1}	$P1,C2$	1,1	$(-1,-1,0),(-1,1,0),(0,0,-2)$	$(\frac{5}{16},\frac{5}{16},\frac{7}{16})$
	C_{2v}^{11}	$P1,C10$	1,1	$(0,-2,0),(2,0,0),(0,0,2)$	$(0,0,\frac{3}{4})$
	C_{2v}^{13}	$P1,C10$	1,3	$(0,-2,0),(2,0,0),(0,0,2)$	$(0,0,\frac{3}{4})$
	D_2^{6}	$P1,C8$	1,1	$(0,-2,0),(2,0,0),(0,0,2)$	$(\frac{1}{4},-\frac{1}{4},\frac{1}{2})$
	D_{2h}^{6}	$P3,P5$	1,1	$(0,0,-2),(1,-1,0),(-1,-1,0)$	$(0,0,0)$
	D_{2h}^{7}	$P3,P5$	1,2	$(-1,-1,0),(0,0,-2),(1,-1,0)$	$(0,0,0)$
	D_2^{2}	$P3,C3$	1,1	$(-1,-1,0),(0,0,-2),(1,-1,0)$	$(0,0,\frac{3}{4})$
	D_{2h}^{11}	$P3,P12$	1,1	$(0,0,-2),(1,-1,0),(-1,-1,0)$	$(\frac{1}{16},\frac{11}{16},-\frac{1}{16})$
	D_{2h}^{14}	$P3,P12$	1,2	$(-1,-1,0),(0,0,-2),(1,-1,0)$	$(-\frac{1}{16},\frac{1}{16},\frac{11}{16})$
	C_{2v}^{6}	$P3,C13$	1,1	$(1,-1,0),(-1,-1,0),(0,0,-2)$	$(0,0,\frac{3}{4})$
	C_{2v}^{4}	$P3,C13$	1,2	$(-1,-1,0),(-1,1,0),(0,0,-2)$	$(0,0,\frac{3}{4})$
	C_{2h}^{4}	$P3,C9$	1,1	$(0,-2,0),(0,0,-2),(1,-1,0)$	$(\frac{5}{16},\frac{5}{16},\frac{7}{16})$
	C_{2h}^{4}	$C1,C12$	1,1	$(-1,1,0),(0,0,-2),(0,-2,0)$	$(0,0,0)$
	D_2^{3}	$C1,C11$	1,1	$(-1,-1,0),(-1,1,0),(0,0,-2)$	$(\frac{5}{16},\frac{5}{16},\frac{7}{16})$
	C_2^{1}	$C1,4D1$	1,1	$(-1,1,0),(0,0,-2),(0,-2,0)$	$(-\frac{3}{8},\frac{3}{8},\frac{3}{8})$
$X_4^+ \oplus N_1^+$	D_{2h}^{26}	$P1,P1$	1,3	$(0,-2,0),(0,0,2),(-2,0,0)$	$(0,0,0)$
	D_{4h}^{19}	$P1,P4$	1,1	$(0,-2,0),(-2,0,0),(0,0,-2)$	$(\frac{3}{4},0,\frac{17}{8})$
	D_{2h}^{28}	$P1,C2$	1,1	$(0,-2,0),(2,0,0),(0,0,2)$	$(\frac{1}{4},\frac{1}{4},\frac{1}{4})$
	C_{2h}^{3}	$P1,S1$	1,1	$(-2,0,2),(0,-2,0),(0,0,2)$	$(\frac{1}{4},\frac{1}{4},-\frac{1}{4})$
	C_{2h}^{3}	$P3,P11$	1,3	$(0,0,4),(-2,2,0),(-\frac{1}{4},-\frac{1}{4},\frac{1}{2})$	$(0,0,0)$
	C_{2h}^{3}	$P3,C8$	1,3	$(0,0,4),(-2,2,0),(-\frac{1}{2},-\frac{1}{2},1)$	$(0,0,0)$
	D_{2h}^{24}	$C1,P4$	1,1	$(-2,-2,0),(2,-2,0),(0,0,2)$	$(\frac{5}{16},\frac{61}{16},-\frac{23}{16})$
	C_{2h}^{6}	$C1,C2$	1,1	$(-2,2,0),(0,0,-2),(0,-2,0)$	$(0,0,0)$
	C_{2h}^{6}	$C1,C10$	1,1	$(0,0,-4),(-2,-2,0),(-\frac{1}{2},\frac{1}{2},1)$	$(\frac{1}{4},\frac{1}{4},-\frac{1}{4})$
	C_i^{1}	$C1,4D1$	1,1	$(-1,-1,1),(-1,1,-1),(1,-1,-1)$	$(0,0,0)$

TABLE II. (*Continued*).

Irreps	Subgroup	Orbit	Subspace	Basis	Origin
$X_4^+ \oplus P_5$	D_{2h}^{21}	$P1,P11$	1,1	(0, −2,0),(2,0,0),(0,0,2)	$(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$
	D_{2h}^{22}	$P1,P11$	1,2	(0, −2,0),(2,0,0),(0,0,2)	$(\frac{1}{8},\frac{1}{8},-\frac{3}{8})$
	D_{2d}^{1}	$P1,P4$	1,1	(−1, −1,0),(1, −1,0),(0,0,2)	$(\frac{5}{16},\frac{5}{16},\frac{7}{16})$
	D_{2d}^{2}	$P1,P4$	1,3	(−1, −1,0),(1, −1,0),(0,0,2)	$(\frac{5}{16},\frac{5}{16},\frac{7}{16})$
	S_4^1	$P1,C2$	1,1	(−1, −1,0),(−1,1,0),(0,0, −2)	$(\frac{3}{16},\frac{11}{16},\frac{1}{16})$
	C_{2v}^{11}	$P1,C10$	1,1	(0, −2,0),(2,0,0),(0,0,2)	$(0,0,\frac{3}{4})$
	C_{2v}^{13}	$P1,C10$	1,3	(0, −2,0),(2,0,0),(0,0,2)	$(0,0,\frac{3}{4})$
	D_2^6	$P1,C8$	1,1	(0, −2,0),(2,0,0),(0,0,2)	$(\frac{1}{4},-\frac{1}{4},\frac{1}{2})$
	D_{2h}^{7}	$P3,P5$	1,1	(−1,1,0),(0,0, −2),(−1, −1,0)	(0,0,0)
	D_{2h}^{6}	$P3,P5$	1,2	(0,0, −2),(−1, −1,0),(−1,1,0)	(0,0,0)
	D_2^2	$P3,C3$	1,1	(−1,1,0),(0,0, −2),(−1, −1,0)	$(-\frac{3}{8},\frac{3}{8},\frac{3}{8})$
	D_{2h}^{4}	$P3,P12$	1,1	(0,0, −2),(1, −1,0),(−1, −1,0)	$(\frac{1}{16},\frac{11}{16},\frac{15}{16})$
	D_{2h}^{3}	$P3,P12$	1,2	(0,0, −2),(−1, −1,0),(−1,1,0)	$(\frac{1}{16},-\frac{1}{16},\frac{11}{16})$
	C_{2v}^{4}	$P3,C13$	1,1	(1, −1,0),(−1, −1,0),(0,0, −2)	$(0,0,\frac{3}{4})$
	C_{2v}^{6}	$P3,C13$	1,2	(−1, −1,0),(−1,1,0),(0,0, −2)	$(0,0,\frac{3}{4})$
	C_{2h}^{4}	$P3,C9$	1,1	(0, −2,0),(0,0, −2),(1, −1,0)	$(\frac{5}{16},\frac{5}{16},\frac{7}{16})$
	C_{2h}^{4}	$C1,C12$	1,1	(−1,1,0),(0,0, −2),(0, −2,0)	(0,0,0)
	D_2^1	$C1,C11$	1,1	(0,0, −2),(1, −1,0),(−1, −1,0)	$(\frac{5}{16},\frac{7}{16},\frac{7}{16})$
	C_2^1	$C1,4D1$	1,1	(−1,1,0),(0,0, −2),(0, −2,0)	$(-\frac{3}{8},\frac{3}{8},\frac{3}{8})$
$N_1^+ \oplus P_5$	D_{2h}^{19}	$P1,P11$	1,1	(0,0, −2),(0, −2,0),(−2,0,0)	$(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$
	D_{2h}^{20}	$P1,P11$	1,3	(0,0, −2),(0, −2,0),(−2,0,0)	$(\frac{5}{8},\frac{1}{8},-\frac{1}{8})$
	C_{2h}^{3}	$P1,C12$	1,1	(0, −2,0),(0,0, −2),(2, −2,0)	$(\frac{1}{4},\frac{1}{4},-\frac{1}{4})$
	C_{2h}^{6}	$P1,C12$	1,9	(0, −2,0),(0,0, −2),(2, −2,0)	$(\frac{1}{8},\frac{5}{8},\frac{1}{8})$
	C_{2v}^{14}	$P1,C10$	1,1	(−2,0,0),(0, −2,0),(0,0,2)	$(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$
	D_2^6	$P1,C8$	1,1	(0,0, −2),(0, −2,0),(−2,0,0)	$(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$
	C_2^3	$P1,4D1$	1,1	(0, −2,0),(0,0, −2),(2, −2,0)	$(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$
	D_{2h}^{17}	$P3,P5$	1,1	(2, −2,0),(−2, −2,0),(0,0, −2)	$(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$
	D_{2h}^{18}	$P3,P5$	1,5	(2, −2,0),(−2, −2,0),(0,0, −2)	$(\frac{3}{8},\frac{3}{8},\frac{3}{8})$
	D_2^5	$P3,C3$	1,1	(−2, −2,0),(−2,2,0),(0,0, −2)	$(\frac{1}{8},\frac{5}{8},-\frac{1}{8})$
	C_{2v}^{12}	$P3,C13$	1,1	(2, −2,0),(−2, −2,0),(0,0, −2)	$(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$
	D_{2h}^{13}	$C1,P11$	1,1	(0, −2,0),(0,0,2),(−2,0,0)	$(0,\frac{1}{2},\frac{1}{4})$
	D_{2h}^{12}	$C1,P11$	1,3	(0, −2,0),(0,0,2),(−2,0,0)	$(\frac{3}{8},\frac{3}{8},\frac{3}{8})$
	C_{2h}^{2}	$C1,C12$	1,1	(−2,2,0),(0,0, −2),(0, −2,0)	(0,0,0)
	C_{2h}^{5}	$C1,C12$	1,9	(0, −2,0),(0,0, −2),(2, −2,0)	$(0,\frac{3}{4},0)$
	C_{2v}^{7}	$C1,C10$	1,1	(0, −2,0),(−2,0,0),(0,0, −2)	$(-\frac{3}{8},\frac{3}{8},\frac{3}{8})$
	D_2^3	$C1,C8$	1,1	(0,0, −2),(0, −2,0),(−2,0,0)	$(0,0,\frac{3}{4})$
	C_2^2	$C1,4D1$	1,1	(−2,2,0),(0,0, −2),(0, −2,0)	(0,0,0)
	C_{2h}^{4}	$P5,P3$	1,1	(0, −1, −1),(−2,0,0),(0,1, −1)	$(\frac{1}{16},\frac{13}{16},-\frac{1}{16})$
	C_{2h}^{5}	$P5,P3$	1,2	(0, −1, −1),(−2,0,0),(0,1, −1)	$(\frac{1}{16},\frac{13}{16},-\frac{1}{16})$
	C_s^2	$P5,C1$	1,1	(0, −1, −1),(−2,0,0),(0,1, −1)	$(\frac{7}{16},\frac{7}{16},-\frac{7}{16})$
	C_s^2	$P5,C1$	3,1	(2,0, −4),(0,2,0),(−1,0,3)	$(\frac{5}{16},\frac{5}{16},-\frac{5}{16})$
	C_i^1	$P5,C9$	1,1	(0, −1, −1),(0,1, −1),(2, −2,0)	$(\frac{5}{16},\frac{5}{16},\frac{9}{16})$
	D_{2d}^{5}	$P4,P4$	1,1	(2,0,0),(0, −2,0),(0,0, −2)	$(\frac{9}{16},\frac{5}{16},\frac{3}{16})$
	D_{2d}^{8}	$P4,P4$	1,3	(2,0,0),(0, −2,0),(0,0, −2)	$(\frac{9}{16},\frac{5}{16},\frac{3}{16})$

TABLE II. (*Continued*).

Irreps	Subgroup	Orbit	Subspace	Basis	Origin
	S_4^1	$P4,C2$	1,1	$(0,-2,0),(-2,0,0),(0,0,-2)$	$(\frac{5}{16},\frac{9}{16},-\frac{5}{16})$
	D_2^6	$P4,C11$	1,1	$(-2,-2,0),(-2,2,0),(0,0,-2)$	$(\frac{5}{16},\frac{9}{16},-\frac{5}{16})$
	C_{2h}^1	$C3,P11$	1,1	$(0,-1,1),(-2,0,0),(0,-1,-1)$	(0,0,0)
	C_{2h}^2	$C3,P11$	1,2	$(0,-1,1),(-2,0,0),(0,-1,-1)$	(0,0,0)
	C_i^1	$C3,C12$	1,1	$(0,-1,-1),(0,1,-1),(2,-2,0)$	(0,0,0)
	C_s^1	$C3,C10$	1,1	$(0,-1,1),(-2,0,0),(0,-1,-1)$	(0,0,0)
	C_2^1	$C3,C8$	1,1	$(0,-1,1),(-2,0,0),(0,-1,-1)$	(0,0,0)
	C_2^2	$C3,C8$	1,3	$(0,-1,1),(-2,0,0),(0,-1,-1)$	(0,0,0)
	C_1^1	$C3,4D1$	1,1	$(0,-1,-1),(0,1,-1),(2,-2,0)$	(0,0,0)
	C_{2h}^3	$P11,P12$	1,1	$(2,-2,0),(-2,-2,0),(0,0,-2)$	$(\frac{1}{16},\frac{13}{16},\frac{1}{16})$
	C_{2h}^6	$P11,P11$	1,2	$(2,-2,0),(-2,-2,0),(0,0,-2)$	$(-\frac{3}{16},\frac{9}{16},\frac{5}{16})$
	D_{2h}^5	$C2,P11$	1,1	$(0,-2,0),(-2,0,0),(0,0,-2)$	(0,0,0)
	D_{2h}^6	$C2,P11$	1,2	$(0,-2,0),(-2,0,0),(0,0,-2)$	(0,0,0)
	C_{2h}^4	$C2,C12$	1,1	$(-2,2,0),(0,0,-2),(0,-2,0)$	(0,0,0)
	C_{2v}^1	$C2,C10$	1,1	$(-2,0,0),(0,-2,0),(0,0,2)$	$(\frac{3}{8},-\frac{3}{8},\frac{3}{8})$
	C_{2v}^{10}	$C2,C10$	1,3	$(-2,0,0),(0,-2,0),(0,0,2)$	$(\frac{3}{8},-\frac{3}{8},\frac{3}{8})$
	D_2^2	$C2,C8$	1,1	$(0,0,2),(-2,0,0),(0,-2,0)$	$(\frac{3}{8},\frac{3}{8},-\frac{3}{8})$
	C_2^1	$C2,4D1$	1,1	$(-2,2,0),(0,0,-2),(0,-2,0)$	$(-\frac{3}{8},\frac{3}{8},\frac{3}{8})$
	C_i^1	$C12,C9$	1,1	$(0,-2,0),(0,0,-2),(2,-2,0)$	$(\frac{3}{4},-\frac{1}{8},\frac{1}{8})$
	C_2^3	$C10,C11$	1,1	$(2,-2,0),(-2,-2,0),(0,0,-2)$	$(-\frac{5}{16},\frac{5}{16},\frac{9}{16})$
	C_{2h}^6	$C8,P5$	1,1	$(2,-2,0),(-2,-2,0),(0,0,-2)$	$(\frac{1}{4},\frac{1}{4},-\frac{1}{4})$
	C_{2h}^3	$C8,P5$	1,2	$(2,-2,0),(-2,-2,0),(0,0,-2)$	(0,0,0)
	C_2^3	$C8,C3$	1,1	$(2,-2,0),(-2,-2,0),(0,0,-2)$	$(-\frac{1}{8},\frac{1}{8},\frac{5}{8})$
	C_s^4	$C8,C13$	1,1	$(2,-2,0),(-2,-2,0),(0,0,-2)$	$(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$
	C_s^3	$C8,C13$	1,2	$(2,-2,0),(-2,-2,0),(0,0,-2)$	(0,0,0)
	C_{2h}^2	$S1,P11$	1,1	$(0,0,-2),(0,-2,0),(-2,0,0)$	(0,0,0)
	C_{2h}^4	$S1,P11$	1,2	$(0,0,-2),(0,-2,0),(-2,0,-2)$	(0,0,0)
	C_{2h}^5	$S1,P11$	1,3	$(0,0,-2),(0,-2,0),(-2,0,-2)$	$(0,\frac{3}{4},0)$
	C_{2h}^1	$S1,P11$	1,4	$(0,0,-2),(0,-2,0),(-2,0,0)$	$(\frac{3}{8},\frac{3}{8},\frac{3}{8})$
	C_s^1	$S1,C10$	1,1	$(0,0,-2),(0,-2,0),(-2,0,0)$	$(\frac{3}{8},\frac{3}{8},-\frac{3}{8})$
	C_s^2	$S1,C10$	1,3	$(0,0,-2),(0,-2,0),(-2,0,-2)$	(0,0,0)
	C_2^2	$S1,C8$	1,1	$(0,0,-2),(0,-2,0),(-2,0,0)$	(0,0,0)
	C_2^1	$S1,C8$	1,3	$(0,0,-2),(0,-2,0),(-2,0,0)$	$(0,0,\frac{3}{4})$
	C_i^1	$4D1,C12$	1,1	$(0,-2,0),(0,0,-2),(2,-2,0)$	(0,0,0)
	C_1^1	$4D1,4D1$	1,1	$(0,-2,0),(0,0,-2),(2,-2,0)$	(0,0,0)

Notice that a vector of arbitrary length in the same direction as $\eta^{(1)}$ will have the same image isotropy subgroup. The same class of conjugate image subgroups is then defined for any orbit point of this subspace. This subspace together with the three subspaces obtained by the group action make up a stratum. In a similar fashion other sets of invariant subspaces can be connected by conjugacy and they correspond to classes of conjugate image subgroups. Each stratum defines a class of image isotropy subgroups and, by the inverse map of the representation, a conjugacy class of ISG's of the space group G_0.

There are three distinct orbit types (strata) for C_{4v} (besides the stratum consisting of the point at the origin). One stratum corresponds to the $P3$ orbit structure. An orbit corresponding to the image subgroup $m(\sigma_x)$ we denote $P1$ (see Fig. 3), and gives another stratum of E. An orbit for the subgroup consisting just of the identity is denoted $C1$ and gives the third stratum of E. Since any vector in a stratum subspace has the same image isotropy subgroup, any vector in region R of Fig. 3 (a stratum subspace of $C1$) will have the image isotropy subgroup consisting of the identity.

The above separation into strata has physical relevance to the possible symmetry changes which are possible at phase transitions for a solid of space group symmetry G_0. At the transition the order parameter η will appear linearly in some physical quantity (e.g., particle density, or charge density, or dipole moment, etc.) and the new symmetry is the isotropy subgroup of G_0 which leaves η invariant. As the parameters of the system are varied (pressure, temperature, etc.) the value of the order parameter may vary. When it remains within a specific stratum subspace no symmetry change takes place and correspondingly no phase transition takes place. Only when the order parameter passes from one stratum subspace to another (for example in going from the stratum containing the origin to a nonzero value of η) will there be a symmetry change and a phase transition. At a phase transition it often happens that local inhomogeneities or fluctuations will determine which member of the orbit is selected. Different members of the same orbit will correspond to different domains of the same lower symmetry phase, i.e., to different orientations of the order parameter and to the corresponding conjugate symmetries. The entire conjugacy class characterizes a single phase transition. Each image is analyzed in a similar manner, the set of all orbits being broken down into its component strata. Each orbit corresponds to a single transition and the members of each orbit denote the subspace orientations or domains of the lower symmetry phase.

In Table I, we list the ISG's of D_{4h}^{17} for each irrep which allows octahedral tilting distortions. By octahedral tilting, we mean that the angles and distances between atoms in the octahedron do not change to first order in the displacements. We obtained the atomic displacements of the possible distortions allowed by each irrep of D_{4h}^{17} using projection operator techniques and retained only those compatible with octahedral tilting. In Fig. 4 we show an example of the octahedral tilting distortions for each irrep. Each figure represents four conventional unit cells in the x-y plane. Each dot represents the center of mass of an octahedral unit. The dots labeled $\frac{1}{2}$ lie a distance $\frac{1}{2}c$ above the plane shown. The distortions determined by the X_3^+ and X_4^+ irreps do not cause cell doubling in the z direction. Those determined by N_1^+ and P_5 do, however, and thus x-y planes at both $z=0$ and $z=\frac{1}{2}c$ are shown.

The arrows represent a tilted octahedral unit. For example, an arrow in the $+x$ direction means that the atom at $(0,0,z)$ moves in the $+x$ direction, the atom at $(0,0,\bar{z})$ moves in the $-x$ direction, the atom at $(\frac{1}{2},0,0)$ moves in the $-z$ direction, the atom at $(\frac{\bar{1}}{2},0,0)$ moves in the $+z$ direction, and the atoms at $(0,\frac{1}{2},0)$ and $(0,\frac{\bar{1}}{2},0)$ do not move at all. This particular example is a rotation of the octahedral unit about the y axis.

Not all independent modes for each irrep are shown in the figure, but the other modes can be obtained by symmetry. Note that we only found modes where the octahedral units rotate about the x or y axis. We found no modes where the octahedral units rotate about the z axis, in contrast to the ABX_3 and ABX_4 structures. The irrep labels in Table I follow the convention of Miller and Love.[27] We use the space-group settings of Hahn.[28] The basis vectors and origin of each subgroup is given in terms of the basis vectors of D_{4h}^{17}. (Note that conventional basis vectors are used and they are therefore nonprimitive for the case of D_{4h}^{17} and other centered lattices.)

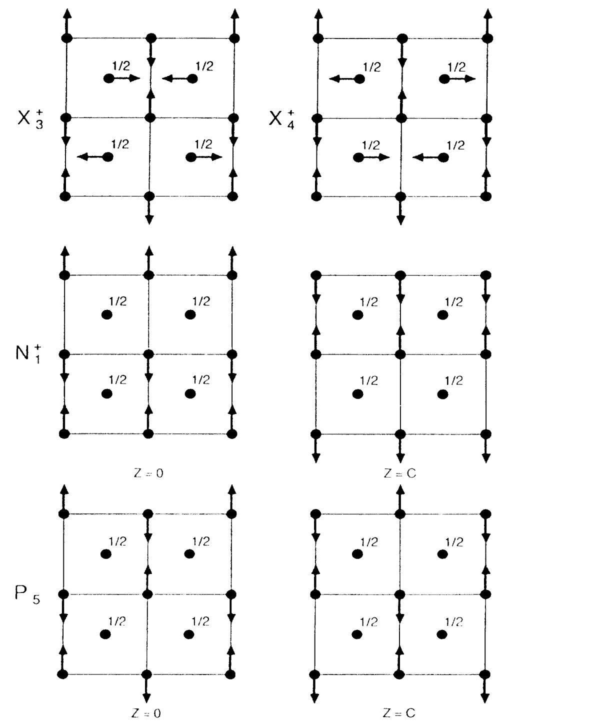

FIG. 4. Examples of octahedral tilting allowed by irreducible representations of interest. Arrows indicate the displacement directions of the top vertex of the rigid octahedral units. Each dot represents the center of mass of the octahedral unit. The dots labeled $\frac{1}{2}$ lie a distance $\frac{1}{2}c$ above the plane shown. Not all independent modes for each irrep are shown but other modes can be obtained by symmetry. See text for more details.

III. ISOTROPY SUBGROUPS OF REDUCIBLE REPRESENTATIONS

To obtain ISG's for a reducible representation we select a vector from the reducible carrier space with nonzero components in each of the irreducible subspaces. Thus if $\eta^{(\alpha)}$ is a vector from the irreducible carrier space $E^{(\alpha)}$ (with subgroup symmetry G^{α}) and $\xi^{(\beta)}$ is a vector from the irreducible carrier $E^{(\beta)}$ (with subgroup symmetry G^{β}) then the subgroup corresponding to $\eta^{(\alpha)}\oplus\xi^{(\beta)}$ in the reducible carrier space $E^{(\alpha)}\oplus E^{(\beta)}$ will be the elements of G_0 which simultaneously leave $\eta^{(\alpha)}$ and $\xi^{(\beta)}$ fixed, i.e., the intersection of the groups $G^{(\alpha)}$ and $G^{(\beta)}$. Every vector of the same stratum subspace determines the same isotropy subgroup. However, distinct subspaces of the same stratum yield conjugate subgroups of G_0 and therefore may give distinct intersections for $G^{(\alpha)}$ and $G^{(\beta)}$. Thus to obtain all isotropy subgroups for reducible representations (RISG's), vectors from all strata as well as all stratum subspaces must be considered for both η and ξ. This intersection process is most simply performed by computer methods using the results obtained earlier for each irrep.

In Table II we list all RISG's due to the direct sum of any two of the irreps listed in Table I. As mentioned above the complete variety of stratum subspaces is to be considered in the intersection process. As a specific example, the intersection of D_{2h}^{18} (an ISG of X_3^+) with D_{2h}^{20} (an ISG of X_4^+) yields the isotropy subgroup C_{2h}^{6} for the reducible representation $X_3^+ \oplus X_4^+$ (see Table II). The intersection of D_{2h}^{18} with $\{C_{2x}\,|\,000\}D_{2h}^{20}\{C_{2x}\,|\,000\}^{-1}$ yields D_{2h}^{7}, an isotropy subgroup distinct from C_{2h}^{6}. $\{C_{2x}\,|\,000\}D_{2h}^{20}\{C_{2x}\,|\,000\}^{-1}$ is an ISG conjugate to D_{2h}^{20} and arises from a different subspace of the same stratum. The column labeled "Subspaces" in Table II indicates which ISG's are used in the intersection. Subspace 1 always refers to the ISG given in Table I. The numbering of the other subspaces are our own arbitrary numbering and simply refers to some ISG conjugate to the one given in Table I.

The labeling of the orbit ($P1$, $P3$, $C1$, etc.) follows a convention first introduced in Ref. (18). Note that the irreps X_3^+ and X_4^+ both yield the C_{4v} image discussed above. As we can see in Table I, there are three isotropy subgroups (labeled $P1$, $P3$, $C1$) for each of these two irreps. They correspond to the three strata shown in Fig. 3. The directions of η for orbits of N_1^+ and P_5 can be obtained in a manner similar to those for C_{4v}.

We have also imposed a subduction criterion in the listing of Table II. This criterion selects the maximum stratum dimension yielding a given RISG. For example consider the subgroup obtained from $\eta \oplus \xi$ where η is a vector of irrep X_3^+, orbit $P3$, and subspace 1 and ξ is a vector of irrep X_4^+, orbit $P1$, and subspace 1. We will use the notation $(X_3^+, P3,1) \oplus (X_4^+, P1,1)$, for example, for such a selection. The subgroup which results is C_{2h}^{4}. The same subgroup is obtained from coupling the higher dimensional stratum $(X_3^+, C1,1)$ with the higher dimensional stratum of $(X_4^+, C1,1)$. Thus the $\eta \oplus \xi$ order parameter of $(X_3^+, P3,1) \oplus (X_4^+, P1,1)$ is simply a special case of the more general sum $(X_3^+, C1,1) \oplus (X_4^+, C1,1)$, i.e., the parameters of $P3$ and $P1$ are special directions of the larger subspaces of $C1$ and $C1$, respectively, in the reducible carrier space. Thus only the more general sum result is given in Table II.

IV. CONCLUSION

Based upon experience with perovskite-related structures, it is to be expected that additional transitions in the A_2BX_4 structure will be found which result from octahedral tilting. In many real systems the description of the phase transitions must be given in terms of coupled order parameters (reducible representations). The present work classifies all transitions obtainable by bicoupled octahedra tilting parameters and is intended to be a practical and useful guide to those investigating the D_{4h}^{17} lower symmetry phases.

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