Acta Cryst. (1981). A**37**, 843–847

Homometric Structures in MX_2-Type Compounds

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(*Received* 20 *November* 1980; *accepted* 21 *April* 1981)

Abstract

Representation of close-packed structures by Zhdanov symbols is compact and quite informative, but sometimes quite misleading also. Similar-looking symbols may or may not represent the same structure. Some structures look different but can always be brought to coincide by some symmetry operation like translation, rotation or inversion. Therefore, these are various manifestations of the same structure and will give rise to the same intensities on calculation. But there are certain pairs of structures which although giving rise to the same X-ray diffraction intensities on calculation cannot be brought to coincide by any of these symmetric operations. In the MX_2 type of compound it has been shown theoretically that two homometric structures are those in which X atoms are at the same position but M atoms shift their position in such a way that they occupy the voids of the first structure. Under what conditions the intensities of two structures remain the same (homometric structures) is examined in this paper.

Introduction

The MX_2 structures form a major contribution to the phenomenon of polytypism which has been studied extensively (Trigunayat & Verma, 1976). Cadmium iodide, lead iodide and cadmium bromide are some of the substances in this class. The major study in polytypic substances is finding the position of atoms in the unit cell. With this information, theories of polytypism and growth of polytypes can be understood. During the structure determination of any substance in general and a polytypic one in particular, the problem of representation arises. The various types of substances are generally represented either by an ABC sequence or by the Zhdanov symbols (Trigunayat & Chadha, 1971). Representing close-packed structures by the Zhdanov symbols is compact and informative but sometimes misleading. Similar-looking symbols may or may not represent the same structure. Some structures look different but can be made to coincide by some symmetry operation like translation, rotation or inversion. These are congruent structures and are various manifestations of the same structure and give rise to the same intensities on calculation. There are certain other pairs of structures which although giving rise to the same X-ray diffraction intensities cannot be brought to coincide by any of these symmetric operations. These pairs are called homometric pairs of structures. This nonunique determination of crystal structure by X-ray methods was first observed by Pauling & Shappell (1930) during the structure determination of the mineral bixbyite. Patterson (1944) has cited many theoretical examples of one-dimensional homometric sets and has extended them to two and three dimensions. Dornberger-Schiff & Farkas-Jahnke (1970) have shown the existence of homometric structures in MX-type polytypes. Recently, Jain & Trigunayat (1977) have given certain semi-empirical rules for finding an infinite number of such pairs without giving any condition or reason for these types of structures. Here we shall see why certain MX_2-type pairs which are non-congruent still give the same X-ray intensities.

Conditions for homometric structures

The positions of atoms in a polytype, arranged in different sequences of close-packed layers, can be represented by various notations. The Zhdanov sequence is one of these ways. Different Zhdanov sequences may represent the same structure if these sequences are related to each other by some symmetry. For example, Zhdanov symbols 222211 and 221122 are the structures for the same 10H since they represent the same set of atoms with a different origin. Various rules and ambiguities in Zhdanov symbols have been discussed recently (Jain & Trigunayat, 1977) and will be used for further discussion. Here we are interested in those structures which cannot be made coincident by any operation like the odd shift in Zhdanov symbols (11211112221122 and 12111122211221) and reverse sequence (424226 and 622424) but give rise to the same calculated X-ray intensities.

0567-7394/81/060843-05$01.00

The structure factor for any hkl reflection may in general be written as

$$F_{hkl} = \sum_{p=1}^{n} f_p \exp 2\pi i(hx_p + ky_p + lz_p).$$

Intensities for $10.l$ reflections which are sufficient from the structure determination of any polytype MX_2 can be written from the above expression. The summation is taken over all atoms in the unit cell lying on the vertical A, B, C axes, passing through (0,0,0), $(\frac{2}{3},\frac{1}{3},0)$ and $(\frac{1}{3},\frac{2}{3},0)$, respectively. Writing the summation for M and X atoms separately for an nH polytype having n X atoms and $n/2$ M atoms lying symmetrically between two alternate X atoms, we get

$$F_{10.l} = f_X \sum_{z_j=0,2,\ldots}^{2n-2} \exp 2\pi i\left(x_j + \frac{lz_j}{2n}\right) + f_M \sum_{z_{j'}=1,5,\ldots}^{2n-3} \exp 2\pi i\left(x_{j'} + \frac{lz_{j'}}{2n}\right),$$

where f_X and f_M are the atomic structure factors for X and M atoms, respectively, and the summation over the atoms has been replaced by the summation over the z coordinates of all the atoms with the x coordinate of the atoms taken as a function of z. Therefore, x_j and $x_{j'}$ are functions of z_j and $z_{j'}$, respectively. x_j and $x_{j'}$, which are the x coordinates of the atoms, will be 0, $-\frac{1}{3}$ or $\frac{1}{3}$ depending upon whether the atom is at A(or α), B(or β) or C(or γ) orientation for a certain value of z_j or $z_{j'}$. Let us take a structure MX_2 and write in ABC notation the value of z_j and $z_{j'}$

	$A\gamma B$	$C\beta A$	$B\gamma A$	$C\beta A$	$B\ldots$
$z_j =$	0 2 4	6 8	10 12	14 16	$\ldots$
$z_{j'} =$	1	5	9	13	....

In this example the value of $x_j = -\frac{1}{3}$ for $z_j = 8$ and $x_{j'} = \frac{1}{3}$ for $z_{j'} = 9$. From this notation the intensities for $10.l$ reflections can be calculated easily. The intensities will be

$$I_{10.l} = |F|^2 = FF^*.$$

This can be written as

$$I_{10.l} = f_X^2 \sum_{z_{j_1}=0,2,\ldots}^{2n-2} \sum_{z_{j_2}=0,2,\ldots}^{2n-2} \exp 2\pi i\left[x_{j_1} - x_{j_2} + \frac{l(z_{j_1} - z_{j_2})}{2n}\right] + f_M^2 \sum_{z_{j'}=1,5,\ldots}^{2n-3} \sum_{z_{j'}=1,5,\ldots}^{2n-3} \exp 2\pi i\left[x_{j'_1} - x_{j'_2} + \frac{l(z_{j'_1} - z_{j'_2})}{2n}\right]$$

$$+ 2f_X f_M \sum_{z_j=0,2,\ldots}^{2n-2} \sum_{z_{j'}=1,5,\ldots}^{2n-3} \cos 2\pi\left[x_j - x_j + \frac{l(z_j - z_{j'})}{2n}\right]. \quad (1)$$

For each value of z, *i.e.* 0, 2, 4, ... for X atoms and 1, 5, 9, ... for M atoms, the orientation of the atom ($A\alpha$, $B\beta$ or $C\gamma$) is checked and the corresponding value of x is used in the summation. Let

$$I_{10.l} = f_X^2 A_1 + f_M^2 B_1 + 2f_X f_M C_1. \quad (2)$$

The intensities obtained are multiplied by the Lorentz–polarization factor and absorption factor to get the observed X-ray intensities.

The structures of MX_2 polytypic substances are asymmetric. Two adjacent X atoms contain either an M atom or a void and this occurs alternately. Therefore, if we shift the position of M atoms in a structure to its voids we will get another structure. The new structure cannot be made congruent to the first by any of the symmetry operations unless it has some symmetric Zhdanov symbols. Therefore, in general the intensities obtained from this new configuration should be different from the first. We will show that there are certain arrangements of X atoms which give the same intensities for both structures defined above although they are non-congruent structures.

For the same set of X atoms let us choose the origin at the second A atom so that the M atoms are in a different sandwich from before. The ABC sequence will be

	$A\ \gamma\ B$		$C\ \beta\ A$		$B\ \gamma\ A$		$C\ \beta\ A$		B	$\cdots$	structure I
z_j	0	2	4	6	8	10	12	14	16	$\cdots$	
			$A\ \gamma\ B$		$A\ \beta\ C$		$A\ \gamma\ B$		$\cdots$	structure II	
z'_j			0	2	4	6	8	10			
$z'_{j'}$				1		5		9		.	

The structure factor for the new arrangement of atoms can be written by replacing x_j, $x_{j'}$, z_j and $z_{j'}$ by x'_j, $x'_{j'}$, z'_j and $z'_{j'}$, respectively:

$$F'_{10.l} = \sum_{z'_j=0,2,\ldots}^{2n-2} f_X \exp 2\pi i\left(x'_j + \frac{lz'_j}{2n}\right) + \sum_{z'_{j'}=1,5,\ldots}^{2n-3} f_M \exp 2\pi i\left(x'_{j'} + \frac{lz'_{j'}}{2n}\right),$$

where x'_j and $x'_{j'}$ are functions of z'_j and $z'_{j'}$, respectively. Since the new structure contains the same arrangement of X atoms as before and the value of n is also the same the summation over the X atoms can be written in terms of the first structure, *i.e.* z_j and x_j. Substitute

$$z_j = z'_j + 6, \quad (3)$$

then

$$F'_{10.l}=f_X\sum_{z_j=6,8,\ldots}^{2n+4}\exp 2\pi i\left[x_j+\frac{l(z_j-6)}{2n}\right]+f_M\sum_{z'_{j'}=1,5,\ldots}^{2n-3}\exp 2\pi i\left(x'_{j'}+\frac{lz'_{j'}}{2n}\right).$$

Here x'_j is a function of (z_j-6) and x_j a function of z_j. Since now the summation is over z_j, x'_j has been replaced by x_j. The structure factor can be written as

$$F'_{10.l}=\exp\left(-\frac{2\pi i6l}{2n}\right)f_X\sum_{z_j=0,2,\ldots}^{2n-2}\exp 2\pi i\left(x_j+\frac{lz_j}{2n}\right)+f_M\sum_{z'_{j'}=1,5,\ldots}^{2n-3}\exp 2\pi i\left(x'_{j'}+\frac{lz'_{j'}}{2n}\right).$$

Therefore

$$I'_{10.l}=|F'_{10.l}|^2=F'F'^*$$

$$=f_X^2\sum_{z_{j_1}=0,2,\ldots}^{2n-2}\sum_{z_{j_2}=0,2,\ldots}^{2n-2}\exp 2\pi i\left[x_{j_1}-x_{j_2}+\frac{l(z_{j_1}-z_{j_2})}{2n}\right]+f_M^2\sum_{z'_{j'_1}=1,5,\ldots}^{2n-3}\sum_{z'_{j'_1}=1,5,\ldots}^{2n-3}\exp 2\pi i\left[x'_{j'_1}-x'_{j'_2}+\frac{l(z'_{j'_1}-z'_{j'_2})}{2n}\right]+2f_Xf_M\sum_{z_j=0,2,\ldots}^{2n-2}\sum_{z'_{j'}=1,5,\ldots}^{2n-3}\times\cos 2\pi\left[x_j-x'_{j'}+\frac{l(z_j-z'_{j'})-6l}{2n}\right]. \quad (4)$$

Let

$$I'_{10.l}=f_X^2A_2+f_M^2B_2+2f_Xf_MC_2. \quad (5)$$

In order that the two structures give the same intensity sequences, A_1, B_1 and C_1 should be equal to A_2, B_2 and C_2, respectively, since each has a different multiplying atomic structure factor. Since we have taken the same sequence of X atoms in both structures, the first summation is the same ($A_1=A_2$). B_1 and B_2 represent the summations due to M atoms alone in both the structures, and in order for the intensities to be same, B_1 must be equal to B_2 independently. Let us see how these summations can be made equal. B_1 is the contribution of M atoms in the first structure when the summation is taken over all values of $z_{j'}$, with corresponding values of $x_{j'}$, with respect to the first origin. B_2 is also the contribution of M atoms in the second structure for different values of $z'_{j'}$, with corresponding values of $x'_{j'}$ but with respect to the new origin. The values which $z_{j'}$ and $z'_{j'}$ take in the two summations are exactly the same, *i.e.* 1, 5, 9, ... These two summations can be made equal term by term if we assume that the x coordinates for the M atoms also match like the z coordinates for both structures. This is only possible if the same squence of M atoms is there in the two structures. For example, if for $z_{j'}=1, 5, 9, \ldots$ there are the sequences $\gamma,\beta,\gamma,\ldots$ ($x_{j'}=\frac{1}{3},-\frac{1}{3},\frac{1}{3},\ldots$), respectively, then there should be $\gamma,\beta,\gamma,\ldots$ ($x'_{j'}=\frac{1}{3},-\frac{1}{3},\frac{1}{3},\ldots$) for $z'_{j'}=1, 5, 9,\ldots$ also. This is possible only under special circumstances which are determined by the special sequence of X atoms. Under the assumption that $B_1=B_2$, $z'_{j'}$ and $x'_{j'}$ can be replaced by $z_{j'}$ and $x_{j'}$ respectively. With the constraint just mentioned, to make A_1, B_1 equal to A_2, B_2 if C_1 also becomes equal to C_2, then the intensities will be same, otherwise not. The summations over C_2 are from different origins and to remove such an ambiguity they can be brought to the same point with (3). The condition for the equality of the structures would be

$$\sum_{z_j=0,2,\ldots}^{2n-2}\sum_{z_{j'}=1,5,\ldots}^{2n-3}\cos 2\pi\left[x_j-x_{j'}+\frac{l(z_j-z_{j'})}{2n}\right]=\sum_{z'_j=0,2,\ldots}^{2n-2}\sum_{z_{j'}=1,5,\ldots}^{2n-3}\cos 2\pi\left[x'_j-x_{j'}+\frac{l(z'_j-z_{j'})}{2n}\right]. \quad (6)$$

Condition for the equality of cross terms

Equation (6) relates the summations of X and M atoms in one structure with similar summations for a second structure from their respective origins. In order to prove this equality we have to find the relation between the X and M atoms in one structure and compare it with the atoms in the other structure. It would be easier to deal with (6) if we could convert it to only one type of atom rather than two. The summation of X atoms can be written in terms of the summation of M atoms in clockwise and anticlockwise orientations as shown recently by the author (Chadha, 1980). The structure factor in this form is given by

$$F_{10.l}=\left[2f_X\cos 2\pi\left(\tfrac{1}{3}+\frac{l}{2n}\right)+f_M\right]\times\sum_{z_c=\text{clockwise}}\exp 2\pi i\left(x_c+\frac{lz_c}{2n}\right)+\left[2f_X\cos 2\pi\left(-\tfrac{1}{3}+\frac{l}{2n}\right)+f_M\right]\times\sum_{z_a=\text{anticlockwise}}\exp 2\pi i\left(x_a+\frac{lz_a}{2n}\right),$$

where the first summation is over z_c, for all M atoms lying in clockwise-type sandwiches, *i.e.* γ in $A\gamma B$, α in $B\alpha C$ and β in $C\beta A$. Similarly, the second summation is over z_a, for all M atoms in anticlockwise sandwiches,

i.e. γ in $B\gamma A$, α *in* $C\alpha B$ and β in $A\beta C$. Although both structures have the same set of M atoms, their being in different orientations will give rise to different values to the two summations. The term C_1 or C_2 can be obtained from the intensity expression with the above structure factor by multiplying it by its complex conjugate. C_1 or C_2, or either side of (6) will be the coefficient of the cross term $2f_X f_M$ and can be shown to be

$$\left\langle \left[\cos 2\pi\left(\tfrac{1}{3}+\frac{l}{2n}\right)+\cos 2\pi\left(-\tfrac{1}{3}+\frac{l}{2n}\right)\right]\right.$$
$$\times\left\{\left[\sum_{z_c}\cos 2\pi\left(x_c+\frac{lz_c}{2n}\right)+\sum_{z_a}\cos 2\pi\left(x_a+\frac{lz_a}{2n}\right)\right]^2\right.$$
$$\left.\left.+\left[\sum_{z_c}\sin 2\pi\left(x_c+\frac{lz_c}{2n}\right)+\sum_{z_a}\sin 2\pi\left(x_a+\frac{lz_a}{2n}\right)\right]^2\right\}\right\rangle$$
$$+\left\langle\left[\cos 2\pi\left(\tfrac{1}{3}+\frac{l}{2n}\right)-\cos 2\pi\left(-\tfrac{1}{3}+\frac{l}{2n}\right)\right]\right.$$
$$\times\left\{\left[\sum_{z_c}\cos 2\pi\left(x_c+\frac{lz_c}{2n}\right)\right]^2+\left[\sum_{z_c}\sin 2\pi\left(x_c+\frac{lz_c}{2n}\right)\right]^2\right.$$
$$-\left[\sum_{z_a}\cos 2\pi\left(x_a+\frac{lz_a}{2n}\right)\right]^2$$
$$\left.\left.-\left[\sum_{z_a}\sin 2\pi\left(x_a+\frac{lz_a}{2n}\right)\right]^2\right\}\right\rangle.$$

The two summations over z_c and z_a in the first part of the expression when considered together are just the summation over all the M atoms, irrespective of their orientation clockwise or anticlockwise. The value of this summation is the same for both structures for the type of atoms we are considering. Therefore, in order to have the same intensity sequence from the two structures,

$$\left[\cos 2\pi\left(\tfrac{1}{3}+\frac{l}{2n}\right)-\cos 2\pi\left(-\tfrac{1}{3}+\frac{l}{2n}\right)\right]$$
$$\times\left\{\left[\sum_{z_c}\cos 2\pi\left(x_c+\frac{lz_c}{2n}\right)\right]^2+\left[\sum_{z_c}\sin 2\pi\left(x_c+\frac{lz_c}{2n}\right)\right]^2\right.$$
$$\left.-\left[\sum_{z_a}\cos 2\pi\left(x_a+\frac{lz_a}{2n}\right)\right]^2-\left[\sum_{z_a}\sin 2\pi\left(x_a+\frac{lz_a}{2n}\right)\right]^2\right\} \tag{7}$$

should be same for both of them. In general, this expression should give different values for different orientations of M atoms unless there is some correlation between clockwise and anticlockwise atoms in the two cases. Therefore, we have to look for the conditions under which the two structures have similar X atoms which give rise to the same orientation of M atoms at two different places and secondly compare (7) for each to see if they are homometric or not.

Examples of homometric structures

Case I

Any polytype based on the basic structures $2H$ or $4H$ will contain sandwiches of the type $A\gamma B$ and $A\gamma B\ C\alpha B$ or various other combinations of these sandwiches. In these types of structure, each sandwich will have a B atom in the second place and a C or an A atom in the first place of a sandwich. In a complete structure each atom in the A orientation as well as in the C orientation will be surrounded by atoms in the B orientation. Therefore, on both sides of these X atoms an M atom of the same kind can be fitted. Atoms in the C orientation can have only an M atom in the α orientation on either side, while an atom in the A orientation can have an atom in the γ orientation only. These structures will look like

$$A\gamma B\ \ A\gamma B\ \ C\alpha B\ \ C\alpha B\ \ A\gamma B\ldots$$
$$B\gamma A\ \ B\gamma A\ \ B\alpha C\ \ B\alpha C\ \ B\gamma A\ldots.$$

The Zhdanov symbols for these types of structures with a B atom in the second place of all the sandwiches will contain the symbol 2 and pairs of 1 only. Some examples are 2211, 211222 and $22(11)_3$ $(2112)_2$. The two structures formed by placing M atoms at different positions can be made congruent if the Zhdanov symbol is symmetric like 2211 or 211222. But the nonsymmetric structures like $22(11)_3(2112)_2$ or 22112111122211 cannot coincide with the structure represented either by a truly reverse symbol or even a shift in the origin, which of course represent the same structure. Therefore, we have two structures like 22112111122211 $(20H_a)$ and 11222111121122 $(20H_b)$ which have the same set of X atoms and also the same orientation of M atoms but at different places. For these structures A_1, B_1 are equal to A_2, B_2 respectively.

Let us see if the two structures give the same value for (7). All γ atoms are in a clockwise orientation and all α atoms are in an anticlockwise orientation in the first structure. The situation is reversed in the other structure, *i.e.* all γ atoms are in an anticlockwise position while α atoms are in a clockwise position. Therefore, the two summations over clockwise and anticlockwise atoms will be reversed for the two structures and (7) will be the same but with a negative sign for this type of structure. Therefore, in general, the structures are not homometric. But the negative sign can be absorbed in $[\cos 2\pi(\frac{1}{3}+l/2n)-\cos 2\pi(-\frac{1}{3}+l/2n)]$ in the following way. With the same origin, writing the structure in the backward direction will change each z coordinate of M atoms in 20 H_b to $-z$. Now if we compute $10.\bar{l}$ instead of $10.l$ for $20H_b$, the product $l\times z$ will be invariant and the two summations will also be the same but $\cos 2\pi(\frac{1}{3}+\bar{l}/2n)-\cos 2\pi(-\frac{1}{3}+\bar{l}/2n)$ will give a negative sign which will cancel with

the other negative sign already existing to make (7) the same for $20H_a$ and $20H_b$. It can also be seen very easily that the other factors in (6) as well as A_2 and B_2 remain invariant under this change. Therefore $10.l$ of the structure $20H_a$ will give rise to the same sequence of intensities as $10.\bar{l}$ of $20H_b$. Since the orientation of layers, *i.e.* *A*, *B* and *C*, and the *c* axis are arbitrarily defined it is not possible to define uniquely $10.l$ or $10.\bar{l}$ for MX_2 types of structures. Hence, pairs of structures of a similar nature are homometric in this category.

Case II

The conditions under which the equivalent *M* atoms can be located in the second void rather than the adjacent void, as above, can be determined. Starting with the first sandwich $A\gamma B$, we can write the other *X* atoms in such a way that if an *M* atom is placed in the second void it must be in the γ orientation. By extending this process to other sandwiches also we can see that this condition will be satisfied only if the Zhdanov number of the structure has only even digits. One example under this category is a $20H_c$ with Zhdanov symbols 424226. The *ABC* sequence will be

1	2	3	4	5	6	7	8	9	10		
$A\gamma B$	$C\beta A$	$B\gamma A$	$C\beta A$	$B\alpha C$	$A\beta C$	$B\alpha C$	$A\beta C$	$B\gamma A$	$C\alpha B$	$A\gamma B$	C
	$A\gamma B$	$A\beta C$	$A\gamma B$	$C\beta A$	$C\alpha B$	$C\beta A$	$C\alpha B$	$A\beta C$	$B\gamma A$	$B\alpha C$	
	1	2	3	4	5	6	7	8	9	10	.

The Zhdanov symbol for the derived structure is $1242263(20H_d)$. This structure is reversibly congruent to $622424(20H_d)$.

Let us examine (7) under this class. Since all Zhdanov numbers are even and any of these numbers contribute from the second atom of the sandwich when the first has already been defined by the previous Zhdanov number, any sandwich and its next void will always be in the same state clockwise or anticlockwise, *i.e.* $C\beta A$ *B* or $A\beta C$ *B* (β being at number 4 or 6 respectively). Therefore, for any clockwise atom (or anticlockwise) in the first structure there will be a corresponding clockwise (or anticlockwise) atom in the second structure. The clockwise *M* atoms in the first structure in α, β and γ orientations will have clockwise *M* atoms in the second structure in β, γ, and α orientations, respectively, at a distance $(z_c - 4)/2n$ with respect to the first structure. Therefore, each term for the summation over z_c atoms can be replaced by $[\frac{2}{3} + (z_c - 4)/2n]$ and under these conditions the total positive term in (7) will remain the same. Similarly, for anticlockwise terms α, β and γ in the first structure have γ, α and β respectively in the second structures, z_a will be replaced by $[-\frac{2}{3} + (z_a - 4)/2n]$ and the negative terms in the summation will also be the same. Hence the two will give the same intensities although they are different structures. Therefore we can generalize that structures represented by Zhdanov symbols consisting of only even digits and their reverse sequences if not related by symmetry will be homometric.

Conclusions

We can obtain other combinations of atoms in which the same set of *M* atoms separated by three or four or more sandwiches fit into a set of *X* atoms. For these structures A_1, B_1 are equal to A_2, B_2 but C_1 may or may not be equal to C_2. Therefore, these structures will be homometric only if C_1 is equal to C_2. One such example in which C_1 is not equal to C_2 since there is no correlation between the clockwise and anticlockwise sandwiches is $41412211(16H)$ whose *ABC* sequence is

1	2	3	4	5	6	7	8		
$A\gamma B$	$C\beta A$	$B\gamma A$	$B\alpha C$	$A\gamma B$	$A\gamma B$	$C\alpha B$	$A\gamma B$	$A\gamma B$	$C\beta A$	B
	$A\gamma B$	$C\beta A$	$B\gamma A$	$B\alpha C$	$B\gamma A$	$B\gamma A$	$B\alpha C$	$A\gamma B$		
	1	2	3	4	5	6	7	8		.

In this case (7) is not the same for both the structures, hence they are not homometric.

Therefore, in order to have homometric pairs the same *X* atoms must contain the same set of *M* atoms at two different places although shifted from each other but must satisfy (7) also.

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