Since again no reference is given by HL, the reader might assume that no previous work has been done on the subject. On the contrary, several references must be quoted: the problem of the influence of the space-group symmetry in the quartet relationships was first treated in paper G3 from both the algebraic and the probabilistic points of view and the implementation of the theory in a procedure for phase solution was described by Busetta, Giacovazzo, Burla, Nunzi, Polidori & Viterbo (1980).

(*d*) An effective implementation in the *MULTAN* package of the results previously quoted for triplets has been described by Main (1985). The correct space-group weight for a triplet relationship is given by

$$w_{\mathbf{h},\mathbf{k}} = \varepsilon_{-\mathbf{h}}\varepsilon_{\mathbf{k}}\varepsilon_{\mathbf{h}-\mathbf{k}} \sum_{p,q} \delta_{p,q} \exp\left[2\pi i(-\mathbf{h}\mathbf{T}_p + \mathbf{k}\mathbf{T}_q)\right]$$

where

$$\delta_{p,q} = 1 \text{ when } \mathbf{h}(\mathbf{I}-\mathbf{R}_p) = \mathbf{k}(\mathbf{I}-\mathbf{R}_q)$$
$$= 0 \text{ otherwise.}$$

The summations are over all the space-group symmetry operations. Main's algorithm is clearly able to single out symmetry-consistent and -inconsistent triplets and to provide relative weights for their use in the phasing process. The last consideration introduces a final remark. Tables 1-3 in HL's paper are of limited use in direct-methods practice because:

(1) the method used by HL to derive the list of equivalent or inconsistent triplets can fail to recognize some special combinations of indices producing multiple solutions for (2). The supplementary rules derivable by means of the algorithm described in the present paper and those concerning triplets with restricted phase values are only two examples, but others could exist in principle.

(2) the use of large tables in routine programs is not advisable. Main's algorithm is an effective example of how relatively simple in practice the use of symmetry in such types of problems may be.

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# Space Groups of Quasicrystallographic Tilings

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### Abstract

A method is described for producing tilings with various quasicrystallographic space groups, paying particular attention to the two-dimensional space groups *pnm*1 and *pn*1*m* that can exist as distinct possibilities when the order of rotational symmetry *n* is a power of an odd prime number.

## I. Introduction

Rokhsar, Wright and Mermin have discussed the definition and classification of lattices and space groups with crystallographically forbidden point-group symmetries, taking the view that such quasi-crystallographic concepts are best formulated in Fourier space. For any material whose diffraction

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pattern consists of sharp Bragg-like peaks they define the lattice (Rokhsar, Mermin & Wright, 1987; Mermin, Rokhsar & Wright, 1987) to be the set of all integral linear combinations of wave vectors in the diffraction pattern, and they define space groups in terms of phase relations between density Fourier coefficients at lattice vectors related by point-group symmetries (see Bienenstock & Ewald, 1962; Rokhsar, Wright & Mermin, 1988*a*, *b*).

When the lattice is thus defined in terms of the diffraction pattern, there is no need to insist upon a minimum distance between its points, and therefore no basis remains for the proof that a lattice can have only two-, three-, four- or sixfold symmetry axes. Only when its point group is crystallographic, however, is a $k$-space lattice dual to a direct lattice of real-space translations that can serve as a template to specify the atomic positions of a physical structure. When the point group is quasicrystallographic, the role of the cells of the direct lattice can be played by the tiles of an aperiodic tiling, and a set of well separated point particles with a quasicrystallographic space group can be constructed by placing them at the vertices of such a tiling.

It is not always obvious how to produce a tiling with a given quasicrystallographic space group. We have recently described (Rabson, Ho & Mermin, 1988) a construction that gives tilings with quasicrystallographic space groups $p2^kgm$ (the generalization of crystallographic $p4gm$), the only *non-symmorphic* two-dimensional quasicrystallographic space groups with 'standard' lattices (defined below). The other interesting class of two-dimensional quasicrystallographic space groups with standard lattices are the pairs of symmorphic space groups $pnm1$ and $pn1m$ (the generalizations of crystallographic $p3m1$ and $p31m$) which are distinct if and only if the rotational order $n$ is a power of an odd prime number. In this paper we describe how to produce quasicrystallographic tilings with these space groups. In order to prove that our constructions do indeed have the space groups we claim, we develop methods that are more generally useful for producing quasicrystallographic tilings with a given space group or determining the space group of a given tiling.

In § II we review the pertinent quasicrystallographic generalizations of basic crystallographic concepts. In § III we prove a theorem that is useful in making a precise connection between the construction of a tiling and its space group. In § IV we apply this theorem to determining the space groups of the symmorphic tilings of interest. Finally, in § V we display tilings produced by the method developed in § IV. Readers interested only in making a real-space comparison between the quasicrystallographic analogs of the crystallographic space groups $p3m1$ and $p31m$ are invited to go directly to § V.

Although our discussion is in the context of two-dimensional lattices and tilings, many of our general points are clearly independent of dimension. Some of these points have been made in a different two-dimensional context by Niizeki (1988). Our work differs in that Niizeki focuses on point groups of tilings in real space without considering the relation between point group and lattice embodied in the Fourier-space concept of space group; we must also use a broader class of tilings than is usually considered [as was also necessary for the $p2^kgm$ tilings of Rabson *et al.* (1988)] in order to produce tilings with the space group $pn1m$ (or $pn$).

## II. Background

We summarize in this section the features of space groups and tilings pertinent to what follows. Details and derivations can be found in Rokhsar *et al.* (1988*b*) for subsection *A* and in Rabson *et al.* (1988) for subsection *B*.

### *A. Lattices and space groups*

We consider only the simplest two-dimensional lattice with $n$-fold symmetry: the set of all integral linear combinations of $n$ vectors of equal length uniformly separated by angles of $2\pi/n$. If $\mathbf{k}$ is in a lattice so is $-\mathbf{k}$, so it suffices to consider even $n$. Mermin *et al.* (1987) showed that such lattices, which they call 'standard', are the only lattices (up to scaling and rotation) when $n$ is less than 46, but for larger $n$ the lattice counting problem can be surprisingly complicated. The point group of the standard lattice $L_n$ with $n$-fold symmetry is $nmm$.

A material has lattice $L_n$ if its density Fourier coefficients are non-vanishing only on a denumerable set of wave vectors, all integral linear combinations of which yield $L_n$. In the two-dimensional case, such a material is a quasicrystal if its macroscopic point group $G$ is $nmm$ or $n$ (when $\frac{1}{2}n$ is even) or $nmm$, $n$, $\frac{1}{2}nm$ or $\frac{1}{2}n$ (when $\frac{1}{2}n$ is odd).* If $n$ is less than or equal to six, the quasicrystal is a crystal.

The manifestation of point-group symmetry in Fourier space follows from the fact that two densities $\rho$ and $\rho'$ are macroscopically indistinguishable in all their translationally invariant properties if they are related by

$$\rho'(\mathbf{k}) = \exp[2\pi i\chi(\mathbf{k})]\rho(\mathbf{k}), \qquad (2.1)$$

where $\chi$ is linear (mod 1) on the latttice. Rokhsar *et al.* (1988*b*) characterize such densities as related by a 'gauge transformation' and refer to $\chi$ as a 'gauge

* As in the crystallographic case, one does not consider point groups with lower rotational symmetry than these when the lattice is $L_n$ because there are no physical grounds for the rotational symmetry of the lattice to be higher than the minimum compatible with that of the point group.

Table 1. *The two-dimensional quasicrystallographic space groups with standard lattices*

From Rokhsar *et al.* (1988*b*).

| *Point group rotation order* | *Lattice rotation order* | *Space groups* | *Symmorphic?* | *Crystallographic case* |
|---|---|---|---|---|
| $n$ even but not $2^k$ | $n$ | *pn*, *pnmm* | yes | $n = 6$ |
| $n = 2^k$ ($k > 1$) | $n$ | *pn*, *pnmm*<br>*pngm* | yes<br>no | $n = 4$ |
| $n = p^k$ $p$ odd prime | $2n$ | *pn*, *pnm*1<br>*pn*1*m* | yes | $n = 3$ |
| $n$ odd but not $p^k$ | $2n$ | *pn*, *pnm* | yes | none |

function'.* If $g$ is in the point group $G$ of a material then $\rho(\mathbf{k})$ is macroscopically indistinguishable from $\rho(g\mathbf{k})$. Thus the point group $G$ can be characterized in Fourier space as the set of all $g$ for which $\rho(\mathbf{k})$ is gauge equivalent to $\rho(g\mathbf{k})$:

$$\rho(g\mathbf{k}) = \exp\left[2\pi i \Phi_g(\mathbf{k})\right]\rho(\mathbf{k}). \tag{2.2}$$

The particular gauge functions $\Phi_g$ associated in this way with the operations $g$ of the point group $G$ are called 'phase functions'. The classification of quasicrystals by space groups is based on their phase functions, in a manner specified in Rokhsar *et al.* (1988*a*, *b*). A space group is *symmorphic* if there is a single gauge transformation that simultaneously reduces all the phase functions to zero. The complete list of two-dimensional quasicrystallographic space groups with standard lattices is shown in Table 1.

### *B. Grids and tilings*

In the grid method for producing tilings (see, for example, de Bruijn, 1981; Gähler & Rhyner, 1986), we are given $D$ wave vectors $\mathbf{k}^{(i)} = 2\pi\mathbf{n}^{(i)}/L_i$, tiling vectors $\mathbf{a}^{(i)}$, and grid shifts $0 \le f_i < 1$. Each wave vector determines a family of lines normal to the unit vector $\mathbf{n}^{(i)}$, separated by $L_i$, and displaced from the origin (in the direction $-\mathbf{k}^{(i)}$) by the amount $f_i L_i$. Each intersection in the grid of $D$ families determines a tile whose edges are just the tiling vectors $\mathbf{a}^{(i)}$ associated with the families of the lines meeting at that intersection (Fig. 1).

* If the densities are sums of $\delta$ functions at the vertices of a tiling, then gauge equivalence of the densities is the same as membership in the same 'local isomorphism class' for the tilings. See Gähler (1986).

We follow Ho's version of the grid method (Ho, 1986; Rabson *et al.*, 1988) in which the grid wave vectors and tiling vectors are constrained only by the condition

$$\sum_{i=0}^{D-1} a_\mu^{(i)} k_\nu^{(i)} = 2\pi\delta_{\mu\nu}. \tag{2.3}$$

With this condition one can extend the $D$ grid and tiling vectors to two sets of $D$-dimensional vectors $(\mathbf{a}^{(i)}, \mathbf{b}^{(i)})$ and $(\mathbf{k}^{(i)}, \mathbf{q}^{(i)})$ that satisfy the condition of mutual orthonormality,*

$$\mathbf{a}^{(i)} \cdot \mathbf{k}^{(j)} + \mathbf{b}^{(i)} \cdot \mathbf{q}^{(j)} = 2\pi\delta^{ij}. \tag{2.4}$$

If the density $\rho(\mathbf{r})$ is a sum of delta functions at the vertices of the tiling, then its Fourier transform $\rho(\mathbf{k})$ is non-vanishing only on the lattice of integral linear combinations of the $\mathbf{k}^{(i)}$. The Fourier coefficients are given by

$$\rho(\mathbf{k}) = \sum \exp(i\mathbf{q} \cdot \mathbf{f})\varphi(\mathbf{q}) \tag{2.5}$$

where the sum is over all $\mathbf{q} = \sum n_i \mathbf{q}^{(i)}$ such that $\sum n_i \mathbf{k}^{(i)} = \mathbf{k}$, the 'grid shift vector' $\mathbf{f}$ is

$$\mathbf{f} = \sum f_i \mathbf{b}^{(i)}, \tag{2.6}$$

and (although this will be of no importance in what follows)

$$\varphi(\mathbf{q}) = v^{-1} \int_A \exp(i\mathbf{q} \cdot \mathbf{r}), \tag{2.7}$$

where $A$ is the $(D-2)$-dimensional 'acceptance region' given by the set of all $\sum \lambda_i \mathbf{b}^{(i)}$ with $0 \le \lambda_i < 1$, and $v$ is the volume of the primitive cell of the $D$-dimensional lattice generated primitively by the $(\mathbf{a}^{(i)}, \mathbf{b}^{(i)})$.

## III. Gauge equivalence and grid shifts

In the cases that interest us the result of applying to the tiling any operation $g$ in the point group of the lattice can also be produced by appropriate grid shifts. In determining whether $\rho(g\mathbf{k})$ and $\rho(\mathbf{k})$ are gauge equivalent we shall use a simple condition for gauge

* It is this extension to $D$ dimensions that underlies the interpretation of tilings as projections of higher-dimensional periodic structures, but we make no use of this interpretation here.

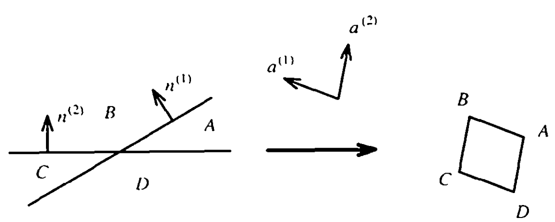


Fig. 1. The intersection of two grid lines from families 1 and 2 determines four grid cells (left); the labeled grid cells correspond to the labeled vertices of a tile (right) whose sides are given by the vectors $\mathbf{a}^{(1)}$ and $\mathbf{a}^{(2)}$ (top).

equivalence of two tilings that differ only in their grid shifts.

Suppose then that two tilings are produced by the same grid wave vectors $\mathbf{k}^{(i)}$ and tiling vectors $\mathbf{a}^{(i)}$, but with grid shifts that differ by $\Delta f_i$. The grid and tiling vectors are restricted only by the orthonormality condition (2.3) and the additional requirement that no two tiling vectors should be the same (or differ only in sign). We prove in this section that two such tilings are gauge equivalent if and only if for every integral linear combination of grid wave vectors that vanishes the corresponding integral linear combinations of grid shifts differ by an integer; *i.e.*

$$\sum n_i \Delta f_i \equiv 0 \quad \text{whenever} \quad \sum n_i \mathbf{k}^{(i)} = 0 \qquad (3.1)$$

(where '≡' means equality modulo unity).*

According to (2.5) the Fourier coefficients for the two tilings are given by

$$\rho(\mathbf{k}) = \sum \exp(i\mathbf{q}\cdot\mathbf{f})\varphi(\mathbf{q}),$$
$$\rho'(\mathbf{k}) = \sum \exp(i\mathbf{q}\cdot\mathbf{f})\exp(i\mathbf{q}\cdot\Delta\mathbf{f})\varphi(\mathbf{q}). \qquad (3.2)$$

Since

$$\Delta\mathbf{f} = \sum \Delta f_i \mathbf{b}^{(i)}, \quad \mathbf{q} = \sum n_i \mathbf{q}^{(i)}, \qquad (3.3)$$

it follows from the orthonormality relations (2.4) that

$$\mathbf{q}\cdot\Delta\mathbf{f} = 2\pi \sum n_i \Delta f_i - \mathbf{k}\cdot\sum \Delta f_i \mathbf{a}^{(i)}. \qquad (3.4)$$

For given $\mathbf{k}$, the second term on the right in (3.4) is explicitly independent of $\mathbf{q}$, and since the sum in (3.2) is over only those $\mathbf{q} = \sum n_i \mathbf{q}^{(i)}$ such that $\sum n_i \mathbf{k}^{(i)} = \mathbf{k}$, the first term on the right in (3.4) will also be independent of $\mathbf{q}$ (mod 1) if (3.1) holds. Consequently (3.1) implies that $\rho'(\mathbf{k})$ and $\rho(\mathbf{k})$ differ only by a phase factor $\exp[2\pi i\chi(\mathbf{k})]$. The linearity (mod 1) of $\chi(\mathbf{k})$ follows directly from the form (3.4) of that phase factor. Thus (3.1) implies gauge invariance.

The converse result, that gauge equivalence implies (3.1), is less trivial, and is essential for establishing that the space-group assignments made below have in fact the largest possible point groups for the specified grid shifts. Suppose then that the two tilings in (3.2) are gauge equivalent, so that (2.1) holds with $\chi(\mathbf{k})$ linear (mod 1). If we shift the grid giving the tiling with density $\rho$ by the grid shift vector

$$\Delta\mathbf{f}^0 = \sum \chi(\mathbf{k}^{(i)})\mathbf{b}^{(i)}, \qquad (3.5)$$

then it follows from the orthonormality relations (2.4) that the Fourier transform of the shifted tiling,

$$\rho''(\mathbf{k}) = \sum \exp(i\mathbf{q}\cdot\mathbf{f})\exp(i\mathbf{q}\cdot\Delta\mathbf{f}^0)\varphi(\mathbf{q}), \qquad (3.6)$$

is the same as that of the tiling with density $\rho'$ given in (2.1) except for the additional phase factor $\exp(i\mathbf{k}\cdot\mathbf{r}_0)$ where

$$\mathbf{r}_0 = -\sum \chi(\mathbf{k}^{(i)})\mathbf{a}^{(i)}. \qquad (3.7)$$

This extra phase simply expresses a translation of the whole tiling through $\mathbf{r}_0$. Thus shifting the $\rho$ tiling by $\Delta\mathbf{f}^0$ gives the same tiling as shifting it by $\Delta\mathbf{f}$, except for a uniform translation in tiling space. In the Appendix, however, we prove when all the tiling vectors $\mathbf{a}^{(i)}$ are distinct that if two grid shifts yield the same aperiodic tiling (except for a translation in tiling space) then the grid shifts can differ only by a uniform translation in grid space:

$$\Delta f_i = \Delta f_i^0 + \mathbf{c}\cdot\mathbf{k}^{(i)} = \chi(\mathbf{k}^{(i)}) + \mathbf{c}\cdot\mathbf{k}^{(i)} \qquad (3.8)$$

for some constant vector $\mathbf{c}$. Since the gauge function $\chi$ is linear in $\mathbf{k}$ (mod unity), (3.1) follows directly from (3.8).

## IV. Some tilings and their space groups

We now apply the criterion of § III to the construction of tilings with the space groups $pnm1$ and $pn1m$ that exist as distinct possibilities when $n = p^k$ for any odd prime $p$.* (We also extract as a byproduct tilings with only $pn$ symmetry.) We first consider the usual case where there is just a single symmetric star of $n$ grid vectors, showing that such a grid can yield the space group $pnm1$ (or $p[2n]mm$) but not $pn1m$ (or $pn$). We subdivide our discussion into two cases, depending on whether $n$ is prime or a non-trivial power of a prime. We then examine the simplest extension of the single symmetric star capable of yielding $pn1m$ (or $pn$) as well as $pnm1$ (or $p[2n]mm$).

### A. One star

The grid wave vectors constitute a single star of vectors of equal length uniformly separated by angles of $2\pi/n$. We take the tiling vectors to be parallel to the grid wave vectors, all with the same length, determined by the orthonormality condition (2.3). We shall assume here, and for the two-star construction described below, that the lattice is the standard lattice $L_{2n}$, consisting of all integral linear combinations of the $n$ grid wave vectors. This is certainly the case for $n = 5$, 7, 9, 11, 13, 17, 19, 25 and 27, since these are all the values of $n$ of the form $p^k$ for which there are no non-standard lattices with $2n$-fold symmetry (Mermin *et al.*, 1987). A sufficient condition for the lattice to be standard, which can be checked numerically in any given case, is that the density Fourier coefficient should be non-zero at a grid wave vector (a primary grid wave vector in the two-star construction). We would be surprised if constructions as

* This result, stated in terms of local isomorphism class rather than gauge equivalence, is proved by Niizeki (1988) in the special case when the grid and tiling vectors are a symmetric star.

* When $n$ is not a prime power the orientation of a star of wave vectors whose integral linear combinations give the entire lattice is not unique, and there is no way to distinguish between the two families of mirrorings that distinguish $pnm1$ (mirrors along the vectors of such a generating star) from $pn1m$ (mirrors perpendicular to the vectors of a generating star). When $n$ *is* a prime power, however, the orientation of a generating star is unique and the distinction can be made (Rokhsar *et al.*, 1988*b*).

simple as those we describe could yield tilings with non-standard lattices, but we have not found a general argument that the lattices must necessarily be standard for general $n$.

When $n$ is odd the point group of the lattice is $[2n]mm$. Point-group operations can permute and/or change the sign of the grid wave vectors. The macroscopic symmetry group $G$ of the tiling can be lower than $[2n]mm$ only if the grid shifts $f_i$ are less symmetric. The effect of a point-group operation on the tiling is entirely produced by the corresponding permutations or changes of sign of those grid shifts.

The condition for $g$ to be in the point group $G$ of the tiling is that $\rho(g\mathbf{k})$ should be gauge equivalent to $\rho(\mathbf{k})$. When $n$ is prime, there is only one linear combination of grid wave vectors that vanishes,

$$\sum_{i=0}^{n-1} \mathbf{k}^{(i)} = 0, \tag{4.1}$$

so the condition (3.1) for gauge equivalence reduces to a single condition on the change of grid shifts that relates $\rho(g\mathbf{k})$ to $\rho(\mathbf{k})$,

$$\sum_{i=0}^{n-1} \Delta f_i \equiv 0. \tag{4.2}$$

When $g$ is a rotation through a multiple of $2\pi/n$ or a mirroring in a line containing one of the grid wave vectors (the case giving $pnm1$) then $g$ simply permutes the grid shifts, (4.2) is always satisfied, and the space group is at least $pnm1$, whatever the choice of grid shifts.

When $g$ is a rotation through an odd multiple of $2\pi/2n$ or a mirroring in a line perpendicular to one of the grid wave vectors (the case giving $pn1m$) then $g$ changes the sign of the grid shifts as well as permuting them, so that (4.2) is satisfied only if

$$\sum_{i=0}^{n-1} f_i = j/2, \quad j \text{ an integer}. \tag{4.3}$$

Since the space group is always at least $pnm1$, when (4.3) holds the space group becomes $p[2n]mm$.

Thus when $n$ is an odd prime number, a single symmetric $n$-fold star of grid vectors will give a quasicrystallographic tiling with space group $pnm1$ whatever the choice of grid shifts unless they satisfy (4.3), in which case the space group is raised to $p[2n]mm$. Tilings with the space groups $pn1m$ and $pn$ cannot be produced by a single star of grid vectors.

Similar conelusions hold when $n$ is a non-trivial power of an odd prime. If $n = p^k$ with $p$ an odd prime, then any sum of grid wave vectors that vanishes can be expressed as an integral liner combination of the $q = p^{k-1}$ linearly independent relations among the grid wave vectors* that express the vanishing of the sum over $q$ distinct $p$-fold stars:

$$\sum_{i=0}^{p-1} \mathbf{k}^{(qi+k)} = 0, \quad k = 0, \ldots, q-1. \tag{4.4}$$

There are thus $q$ conditions on the change of grid shifts that relates $\rho(g\mathbf{k})$ to $\rho(\mathbf{k})$ if $g$ is to be in the point group of the tiling:

$$\sum_{i=0}^{p-1} \Delta f_{qi+k} \equiv 0, \quad k = 0, \ldots, q-1. \tag{4.5}$$

When $g$ is a rotation through a multiple of $2\pi/n$ or a mirroring in a line containing one of the grid wave vectors (the case giving $pnm1$) then its effect on the shifts is simply a permutation of the different $p$-fold stars, and (4.5) requires the sum of the grid shifts associated with each $p$-fold star to be the same (modulo an integer):

$$\sum_{i=0}^{p-1} f_{qi+k} \equiv \sum_{i=0}^{p-1} f_{qi}, \quad k = 0, \ldots, q-1. \tag{4.6}$$

Unless (4.6) holds, the point group $G$ is not even $n$ and the tiling is not quasicrystallographic, the lattice having a higher symmetry than required by the point group (see footnote * on p. 539). When (4.6) does hold the space group is at least $pnm1$.

When $g$ is a rotation through an odd multiple of $2\pi/2n$ or a mirroring in a line perpendicular to a grid wave vector (the case giving $pn1m$) then $g$ changes the signs of the $p$-fold stars as well as permuting them, so that to satisfy (4.5), condition (4.6) requires that

$$\sum_{i=0}^{p-1} f_{qi+k} \equiv j/2,$$

$$k = 0, \ldots, q-1, \quad j \text{ an integer independent of } k. \tag{4.7}$$

Thus when $n$ is a non-trivial power of an odd prime number, a single symmetric $n$-fold star of grid vectors will give a quasicrystallographic tiling only if the sums of the grid shifts associated with each $p$-fold substar are the same. The space group of the quasicrystallographic tiling will then be $pnm1$ unless these grid shift sums are all integral or all half integral, in which case the space group is $p[2n]mm$. Tilings with the space groups $pn1m$ and $pn$ cannot result.

### *B. More than one star*

To get tilings with the space groups $pn1m$ and $pn$ we must increase the set of grid wave vectors to allow for new grid shifts that break the symmetry in such a way as to reduce $p[2n]mm$ to $pn1m$, or $pnm1$ to $pn$. We can do this without changing the lattice* or reducing its symmetry by introducing additional

* The number of independent wave vectors is the Euler function $\varphi(n)$ [see, for example, Lang (1984), pp. 313-314], which is $(p-1)p^{k-1}$ when $n = p^k$.

* This assertion, though highly plausible for general $n$, is subject to the *caveat* given at the beginning of § IV *A*.

$n$-fold stars of wave vectors that are appropriately chosen integral linear combinations of vectors from the original set (which we now refer to as the primary star). We can continue to satisfy the orthonormality condition (2.3) by associating with the new stars of grid vectors new $n$-fold stars of tiling vectors parallel to those grid vectors. We can get a tiling of rhombi by taking all tiling vectors in all stars to have the same length, determining that length from the orthonormality condition (2.3).

In finding the grid shifts for the new non-primary stars, it is useful to work in a gauge in which the grid shifts for the primary star have a particularly simple form. As already noted, when $n = p^k$ the wave vectors within the primary star satisfy precisely $q = p^{k-1}$ independent linear relations with integral coefficients - namely the conditions (4.4) that the sums of the wave vectors in each of the $q$ different $p$-fold substars should vanish. When additional stars are present, a complete (in general overcomplete) set of linear relations is given by adding to the relations (4.4) the relations

$$\bar{\mathbf{k}}^{(i)} = \sum n_{ij}\mathbf{k}^{(j)} \tag{4.8}$$

that express each new grid wave vector as an integral linear combination of grid wave vectors from the primary star.

Since two tilings are gauge equivalent if and only if every integral linear relation satisfied by the grid wave vectors is also satisfied by the differences in the grid shifts relating the tilings, it follows from the relation (4.4) that, given a particular tiling, a necessary condition for a second tiling to be gauge equivalent is that the primary grid shifts within each substar should have the same sum for each of the tilings. If this condition is met, then there will indeed be a set of secondary grid shifts for the second tiling that make it gauge equivalent to the first: namely the (unique) set determined by the additional linear relations

$$\Delta\bar{f}_i \equiv \sum n_{ij}\Delta f_j. \tag{4.9}$$

We can therefore pick a gauge in which the primary grid shifts are *the same* within each primary substar. The condition (4.6) for the tiling to be quasicrystal with $n$-fold symmetry then reduces to the condition that the shifts for primary substars can differ only by integral multiples of $1/p$. Since a change of every shift in a primary substar by $1/p$ is itself a gauge transformation, we can pick a gauge in which the integer is zero, and the grid shifts are then the same within the entire primary star. We take this to be the standard form for the tiling.

The space group of a tiling produced by a single star in standard form will then be $pnm1$ unless the common value $f$ of the grid shifts is an integral multiple of $1/2p$ [*cf.* (4.7)]. When $f = j/2p$ the space group is $p[2n]mm$.

If, however, there are grid wave vectors in addition to those in the primary star, then the condition for $g$ to be in the point group $G$ is augmented by the condition that the changes in grid shifts produced by $g$ should satisfy (4.9). Using the standard form, $f_j = f$, for the grid shifts associated with the $\mathbf{k}^{(j)}$, we conclude from (4.9) that if $g$ is an operation that permutes the $\mathbf{k}^{(j)}$ (a rotation through a multiple of $2\pi/n$ or a mirroring in one of the $\mathbf{k}^{(j)}$) then

$$\Delta\bar{f}_i \equiv 0. \tag{4.10}$$

Since the $2\pi/n$ rotation must be in $G$ we immediately conclude that the grid shifts must also be constant in every non-primary star:

$$\bar{f}_i \equiv \bar{f}. \tag{4.11}$$

If $g$ is a mirroring in one of the $\mathbf{k}^{(i)}$ then (4.10) requires that the value of $\bar{f}$ in a secondary star must be the same as its value in the mirror image of that star. By violating this condition we can produce tilings without that mirror symmetry. The simplest way to do this is with one secondary star that goes into its negative under the mirroring, so that $\Delta\bar{f}_i \equiv 2\bar{f}$. This can be done by taking (4.8) to have the particular form (see Fig. 2)

$$\bar{\mathbf{k}}^{(i)} = \mathbf{k}^{(i+1)} - \mathbf{k}^{(i)}. \tag{4.12}$$

Thus for the mirror to remain in $G$ we must have

$$2\bar{f}_i \equiv 0: \tag{4.13}$$

the grid shift for the secondary star must be equivalent to zero or to $\frac{1}{2}$.

Therefore if the primary grid shift $f$ is not an integral multiple of $1/2p$ (so that the primary shifts satisfy the condition for the space group to be $pnm1$ but not $p[2n]mm$) then unless the secondary grid shift $\bar{f}$ is an integer or half integer the space group of the tiling produced by the total grid is reduced to $pn$. If the primary grid shift *is* a multiple of $1/2p$ (so that the primary grid shifts do satisfy the condition

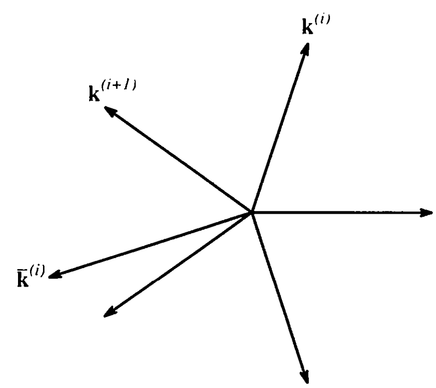


Fig. 2. A secondary star vector $\bar{\mathbf{k}}^{(i)} = \mathbf{k}^{(i+1)} - \mathbf{k}^{(i)}$. The secondary star is invariant under mirrorings perpendicular to primary star vectors and *vice versa*.

Table 2. *Quasicrystallographic space groups for different choices of the primary and secondary grid shifts when n is a power of an odd prime p*

All families in the primary grid have the same shift $f$; all families in the secondary grid have the same shift $\bar{f}$; $l = 0$ or 1; $j = 0, 1, \ldots,$ or $2p-1$.

| | $f = j/2p$ | $f \neq j/2p$ |
|---|---|---|
| $\bar{f} = \ell/2$ | $p[2n]mm$ | $pnm1$ |
| $\bar{f} \neq \ell/2$ | $pn1m$ | $pn$ |

for the space group to be $p[2n]mm$), then unless the secondary grid shift $\bar{f}$ is an integer or half integer the secondary grid reduces the space group of the tiling from $p[2n]mm$ to $pn1m$. For if $g$ is a mirroring perpendicular to one of the primary star wave vectors, then $g$ leaves the secondary star (4.12) invariant, and (4.9), which here reduces to

$$\Delta \bar{f}_i \equiv \Delta f_{i+1} - \Delta f_i, \qquad (4.14)$$

is automatically satisfied:

$$0 \equiv 2f - 2f. \qquad (4.15)$$

Setting $\bar{f}_i \neq l/2$ therefore eliminates only the mirror along the primary star. We therefore have the four cases summarized in Table 2.

## V. Applications: some tilings

We illustrate some of the results of these constructions, first showing what the two-star construction gives in the crystallographic case of threefold symmetry. The argument in the Appendix breaks down when the tiling is crystallographic, but for the grid shifts given in the figure captions, the procedure continues to produce the required space group in the crystallographic case, as can be verified by direct inspection of the tiling. Fig. 3 shows the result of applying the $pn1m$ procedure when $n = 3$, where the outlined primitive cells reveal mirrors along lines joining nearest-neighboring cells, as is required in real space for periodic structures with the space group $p31m$. Fig. 4 does the same for $p3m1$, the real-space mirrors now being along the lines joining next-nearest-neighboring cells. Fig. 5 shows a $p3$ tiling, with no mirror lines.

We next show some quasicrystallographic tilings, first from the familiar single-star construction, then

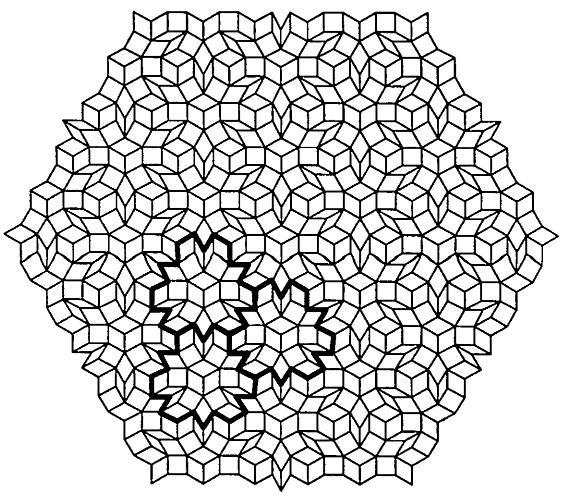

Fig. 3. A $p31m$ tiling in standard form with primary shifts 0·5 and secondary shifts 0·1. A possible unit-cell packing is outlined. Mirrors are along nearest-neighbor lines.

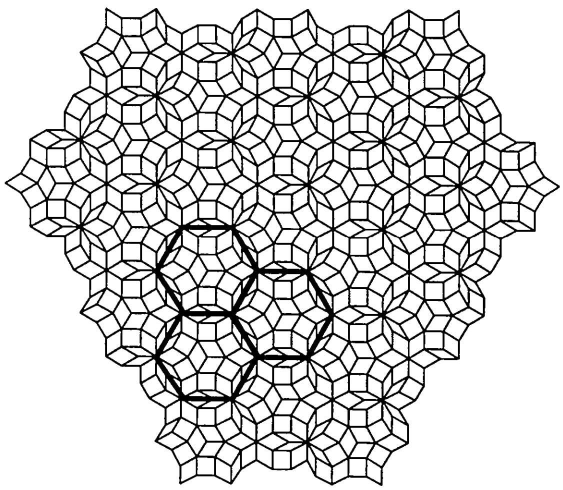

Fig. 4. A $p3m1$ tiling with primary shifts 0·1 and secondary shifts 0·5. Mirrors are along next-nearest-neighbor lines.

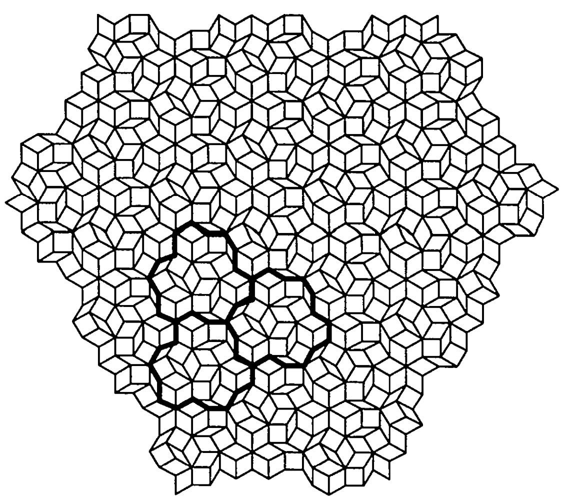

Fig. 5. A $p3$ tiling with primary shifts 0·1 and secondary shifts 0·35. There are no mirrors.

from the two-star construction necessary to produce space groups $p5$ and $p51m$. The Penrose tiling of Fig. 6 comes from a star with $\sum f_i \equiv 0$; we have put it in standard form (all shifts equal) in order to show a point of perfect fivefold symmetry. The space group is $p10mm$. The grid giving Fig. 7 has $\sum f_i \equiv 0{\cdot}75$ and so the tiling has space group $p5m1$. Any choice (mod 1) other than 0 or $\frac{1}{2}$ for $\sum f_i$ yields another $p5m1$ tiling. To produce tilings with space groups $p51m$ and $p5$ we require two stars. Fig. 8 shows a $p51m$ tiling, while Fig. 9 has a tiling with space group $p5$. Again, all the tilings are in standard form. For comparison, we show in Figs. 10 and 11 $p10mm$ and $p5m1$ tilings produced by the same two-star construction that gave Figs. 8 and 9.

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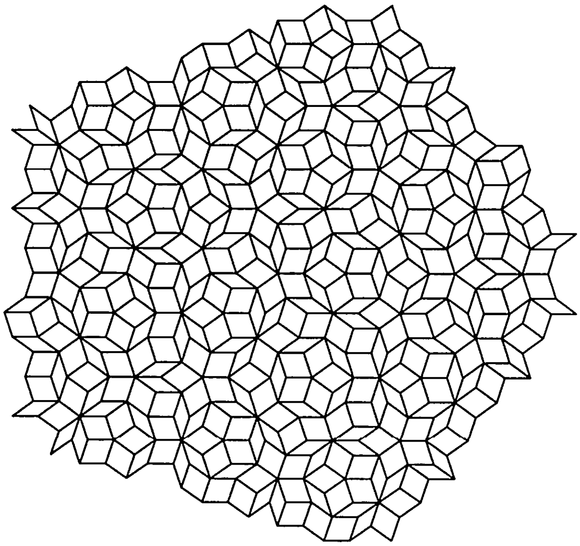

Fig. 6. The Penrose ($p10mm$) tiling with shifts all equal to 0·4; the point of perfect fivefold symmetry here and in Figs. 7–11 is near the upper right-hand corner.

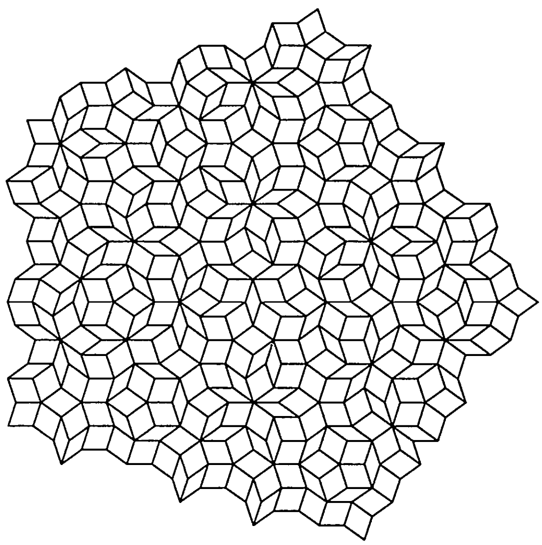

Fig. 7. A one-star tiling ($p5m1$) with shifts all equal to 0·15. Although the space group is determined unambiguously by the Fourier coefficients of the tiling, in contrast to the crystallographic case there is no obvious connection between the real-space structure and such distinctions as that between $p5m1$ and $p51m$.

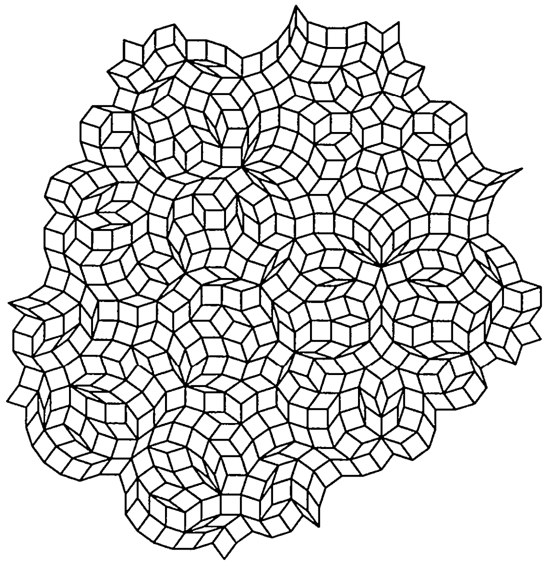

Fig. 8. A two-star tiling ($p51m$) with primary shifts of 0·5 and secondary shifts of 0·13.

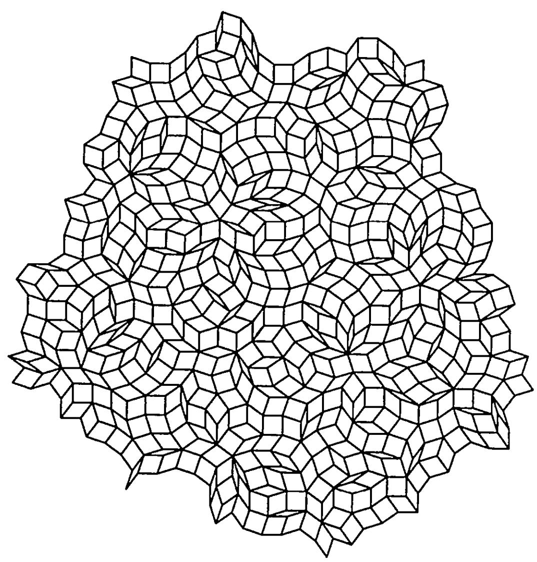

Fig. 9. A two-star tiling ($p5$) with primary shifts of 0·13 and secondary shifts of 0·32.

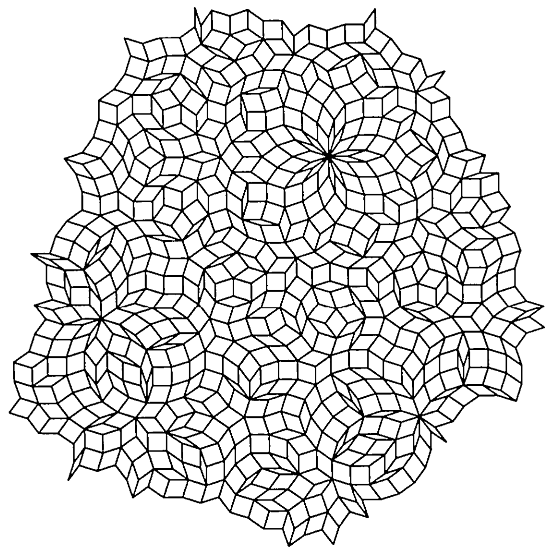

Fig. 10. A two-star tiling ($p10mm$) with primary shifts of 0·4 and secondary shifts of 0·5.

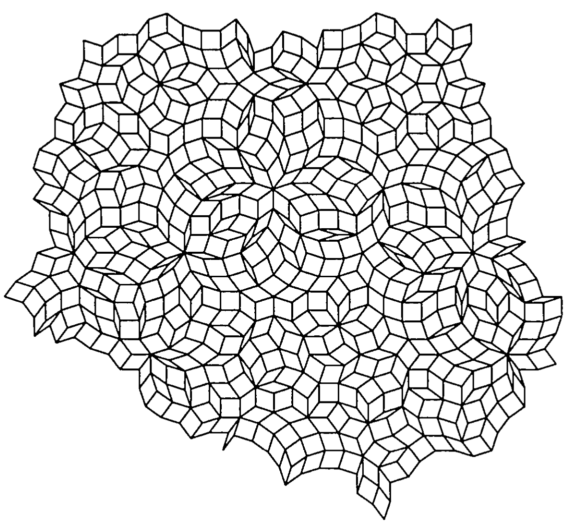

Fig. 11. A two-star tiling ($p5m1$) with primary shifts of 0·13 and secondary shifts of 0·5.

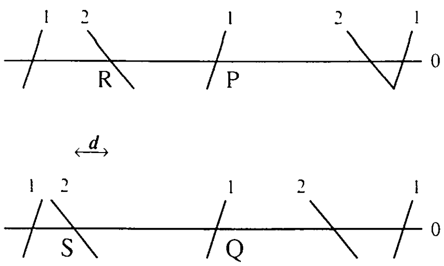


Fig. 12. Portions of corresponding family 0 lines in two grids that yield identical tilings. The numbers label the families of intersecting lines; the labels $P$, $Q$, $R$ and $S$ are as in the text of the Appendix.

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## APPENDIX

We have two grids and their associated tilings, produced by the same sets of wave vectors and tiling vectors, but with possibly different grid shifts. We require all the tiling vectors to be different (and no two equal and opposite) so that a tile of a given shape comes from a grid intersection associated with a unique pair of wave vectors (but we do not require the grid wave vectors all to be different). We prove that if the tilings are aperiodic and the same (except perhaps for a translation in tiling space) then the two grids must be the same except, perhaps, for a translation in grid space; *i.e.* the grid shifts differ by

$$\Delta f_i = \mathbf{c} \cdot \mathbf{k}^{(i)} \qquad (A.1)$$

for some constant vector $\mathbf{c}$. The proof is as follows.

If there are only two grid vectors then the tiling is periodic, so there must be at least three. Because the tiling is aperiodic, it is possible to find three families of lines, perpendicular to $\mathbf{k}^{(0)}$, $\mathbf{k}^{(1)}$ and $\mathbf{k}^{(2)}$, such that the spacing between intersections of family 1 with a family 0 line is incommensurate with the spacing between intersections of family 2 with the family 0 line. We show first that the subgrids of the two grids associated with these three families differ at most by a translation; *i.e.* that the position of the family of lines 2 with respect to families 0 and 1 must be the same in both grids.

Because the two tilings differ by at most a translation, we can find lines in family 0, one from each grid, that have identical sequences of intersections with all the lines from families 1 and 2. Let $P$ and $Q$ be 1-intersections on the two lines about which the sequences of 1- and 2-intersections are identical (Fig. 12). Shift one of the grids by a translation that brings $P$ and $Q$ into coincidence. Then the families of lines 0 and 1 certainly coincide. Supppose the families 2 did not. Let $R$ be the 2-intersection nearest to $P$ in one grid, and let $S$ be the 2-intersection nearest to $P$ (in the same direction as $R$) in the other. Let $d$ be the non-zero distance between $R$ and $S$. There can be no 1-intersection between $R$ and $S$, for if there were then one of the grids would have one more 1-intersection between $P$ and the first 2-intersection than the other had. Continuing away from $P$ in the same direction, this must also be true of the next pair of 2-intersections, and therefore the next after that, and thus it must be true of all subsequent pairs. The same must also be true in the other direction from $P$. We conclude that the line we are considering must contain a set of intervals of length $d$ with the periodicity of the 2-intersections, inside of which no 1-intersection can lie. This, however, is impossible because the period of the 1-intersections is incommensurate with the period of the 2-intersections. Thus $d$ must be zero, the 2-intersections must indeed coincide, and the position of family 2 is fixed with respect to families 0 and 1.

The rest of the proof is simple: any other family 3 that is not parallel to family 0 must have a spacing between intersections along a line in family 0 that is incommensurate with the spacings of either family 1 or of family 2 on family 0 (since if it were commensurate with both then families 1 and 2 would have commensurate spacings). Therefore, by repeating the first part of the argument we can conclude that the position of family 3 is fixed with respect to either family 1 or family 2. In this way the positions of all families are fixed except for those given by families parallel to family 0. But these can now be fixed, in the same way, with respect to families not parallel to 0. Thus the grids are indeed identical except for a possible translation.

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# Crystallography, Geometry and Physics in Higher Dimensions. VI. Geometrical 'WPV' Symbols for the 371 Crystallographic Mono-Incommensurate Space Groups in Four-Dimensional Space


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### Abstract

A geometrical 'WPV' notation for the 371 crystallographic space groups describing mono-incommensurate phases of physical space in four-dimensional space is proposed, which completes the geometrical 'WPV' notation for all crystallographic point symmetry groups. The WPV symbols are given for the 76 mono-incommensurate arithmetic classes, or $Z$ classes. Definitions and some examples of $Z$ classes, Bravais types, Bravais flocks, $Q$ classes (or geometrical classes or point groups), holohedries and crystal families both in the physical space and the superspace $\mathbb{E}^4$ are given.


### Introduction

In a previous paper (Weigel, Phan & Veysseyre, 1987) we have given a simple geometric symbol, the 'WPV' symbol, for each of the 227 crystallographic point symmetry groups (PSGs) of the four-dimensional space $\mathbb{E}^4$. In this article we propose a WPV symbol for 371 crystallographic symmetry space groups (SSGs) belonging to the seven crystal systems of $\mathbb{E}^4$ describing the mono-incommensurate phases of the physical space.

A symmetry space group of the Euclidean space $\mathbb{R}^n$ is the group of all the crystallographic symmetry operations (SOs), or isometries, mapping one crystal structure onto itself. A space group is always an infinite group because a crystal structure has infinitely many symmetry translations. The set of all the translation vectors of $\mathbb{E}^n$ mapping a crystal structure onto itself is the lattice of this structure. A lattice of $\mathbb{E}^n$ is defined by $n$ linearly independent vectors $\mathbf{e}_i$ ($i$ varying from 1 to $n$). So it depends, in the most general case, on $n$ parameters of length and $n(n-1)/2$ parameters of angle.

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