(1) Of the 16 general rank-4 Bravais classes, 14 have lattices that are simply the sum of a rank-3 crystallographic lattice and a one-dimensional lattice that is independently invariant under all point-group operations.* As a result, the space groups in all these cases can be trivially inferred from the Fourier-space forms of the ordinary rank-3 space groups, exactly as we have done above for the hexagonal and trigonal systems. The $(3+1)$ settings of these space groups used to describe modulated crystals then emerge straightforwardly by the application of a more limited set of scale-equivalence transformations to the general gauge-equivalence classes.

(2) By working with a smaller number of Bravais classes (16 instead of the 24 settings), one avoids a considerable redundancy of both calculation and description.

We emphasize the generality of our approach. By first focusing on only the gauge-equivalence classes of phase functions, we give the results of the nontrivial part of the calculation in a form that applies to arbitrary quasiperiodic crystals of the appropriate symmetry and rank. By deferring to the end the book-keeping question of which space groups to further identify through scale equivalence, we retain the freedom to use whatever transformations are appropriate to the material of interest, making straightforward the treatment of materials even when they fail to fit neatly into any of the conventional categories (modulated crystals, intergrowth compounds, quasicrystals *etc.*) and allowing for a unified description of materials that might interpolate between quite different categories. As a further demonstration of the power of the more general approach, we discuss in a companion paper (Lifshitz & Mermin, 1994) the Bravais classes and space groups of hexagonal and trigonal quasiperiodic crystals of arbitrary finite rank.

Whether one chooses to call the categories designed for modulated crystals superspace groups or different settings of general rank-4 space groups is, of course, a nomenclatural question; but that these categories are more easily used and derived from the latter point of view seems to us indisputable.

* There are two exceptions, one in the monoclinic system and one in the orthorhombic system. A lattice of either type, however, can be viewed as the sum of two two-dimensional lattices, each independently invariant under the point-group operations leading to a similar simplification.

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Bravais Classes and Space Groups for Trigonal and Hexagonal Quasiperiodic Crystals of Arbitrary Finite Rank

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Abstract

To demonstrate the power of the Fourier-space approach to crystallography, the Bravais classes and space groups of hexagonal and trigonal quasiperiodic crystals are derived for lattices of arbitrary finite rank. The specification of the space groups for each Bravais class is given by an elementary extension of

the rank-4 case. The conventional classification of incommensurately modulated hexagonal and trigonal crystals, previously derived using the superspace approach for Bravais classes up to rank $(3+3)$ [Janner, Janssen & de Wolff (1993). *Acta Cryst.* A**39**, 658–666] and for superspace groups of rank $(3+1)$ [de Wolff, Janssen & Janner (1981). *Acta Cryst.* A**37**, 625–636], is easily extracted from the general classification for modulations of any finite rank.

I. Introduction

We show here that a modest extension of the analysis in the preceding paper* yields the Bravais classes and space groups for trigonal and hexagonal quasiperiodic crystals of arbitrary finite rank. We describe the rank-n Bravais classes in §II and derive them in the Appendix. We derive the space groups associated with each Bravais class in §III.

The possible subdivisions of space groups and Bravais classes into settings that identify different sublattices of wave vectors as lattices of main reflections are much more extensive than in the rank-4 case because there are no longer any *a priori* grounds for restricting lattices of main reflections to rank-3 sublattices. If, for example, we wished to consider the categories of rank-5 quasiperiodic crystals with weak satellites requiring two additional vectors for their indexing, these would be given by the $(5+2)$ settings of the general rank-7 space groups. It is straightforward to extract these settings for any case of interest. We illustrate how to do this in §IV for the important case of rank-3 lattices of main reflections, recovering the 'Bravais classes for incommensurate crystal phases' of Janner, Janssen & de Wolff (1983) (henceforth JJdW) for ranks 4 to 6 and deriving their generalizations to any arbitrary finite rank. We also derive the $(3+d)$ settings of the space groups, extending the tabulated 'superspace groups for incommensurate crystal structures with a one-dimensional modulation' of de Wolff, Janssen & Janner (1981) for the trigonal and hexagonal crystal systems to modulations of any finite rank.

II. Bravais classes

We follow the three-dimensional geometric approach used in LM, describing the Bravais classes in terms of a two-dimensional horizontal sublattice H of wave vectors perpendicular to the threefold (or sixfold) axis and in terms of stacking vectors. We first describe the Bravais classes of two-dimensional lattices with sixfold symmetry that can be horizontal sublattices of the full three-dimensional lattice. These Bravais classes are clearly distinct if we follow Mermin & Lifshitz (1992) in taking classes to be distinct if it is impossible to interpolate between them through a sequence of lattices all with the same point group and rank. In the Appendix (parts A and B), we prove that there are no additional Bravais classes.

It is always possible to take the two-dimensional horizontal sublattice H to be primitively generated by pairs of wave vectors $\mathbf{a}_i$ and $\mathbf{b}_i$, of equal length, separated by 120°. Each such pair generates a sixfold star of vectors given by $\pm\mathbf{a}_i$, $\pm\mathbf{b}_i$ and $\pm(\mathbf{a}_i+\mathbf{b}_i)$.

Symmetry distinguishes two ways of orienting the stars:

(*a*) If every star has the same orientation or if each star has one of two orientations separated by 30°, then the two-dimensional horizontal sublattice is invariant under the full three-dimensional point group $6/mmm$. We say that such sublattices are of type $[i,j]$, where i and j are even integers giving the number of primitive vectors in the plane generating stars of each orientation. The rank of the horizontal sublattice is then $i+j$. We include a single set of star directions in the case $[i,0]$.

(*b*) If there is at least one pair of stars separated by an angle of less than 30°, then the symmetry of the two-dimensional sublattice is reduced to $6/m$. One can interpolate between any two such sublattices having the same number of stars without any change of symmetry. Consequently, any relation between the orientations of any other stars in the family is accidental. The types of sublattices are now distinguished only by the total number of primitive vectors in the plane. We denote horizontal sublattices of this type by the symbol $[i]$, with i an even number greater than two, giving the rank of the sublattice.

Three-dimensional lattices with horizontal sublattices of distinct types obviously belong to distinct Bravais classes. Further subdivisions of the Bravais classes for the full lattice are determined by the additional primitive generating vectors with nonzero vertical components – the stacking vectors.

As in the periodic (rank-3) case, the stacking vectors can be either vertical or staggered. We show in part C of the Appendix that primitive generating vectors can always be chosen so that the horizontal shift of a staggered stacking vector has the form

$$\mathbf{h}_i = \tfrac{2}{3}\mathbf{a}_i + \tfrac{1}{3}\mathbf{b}_i, \qquad (1)$$

where $\mathbf{a}_i$ and $\mathbf{b}_i$ are one of the pairs of primitive generators of the horizontal sublattice.

If all stacking vectors are vertical, the point group of the full lattice remains that of the two-dimensional sublattice: $6/mmm$ if the two-dimensional sublattice is of type $[i,j]$ and $6/m$ if it is of type $[i]$. The full Bravais class is then determined by the type of the

* Lifshitz & Mermin (1994, hereinafter LM), which treats only the rank-4 case. We assume the reader is familiar with the concepts of Fourier-space crystallography described in that paper.

horizontal sublattice and the total number of vertical stacking vectors.

If there are staggered stacking vectors, then, as in the rank-4 case, one requires at most one for each pair of horizontal generating vectors. When the two-dimensional sublattice is of the type $[i,j]$, the existence of just one staggered stacking vector reduces the rotational symmetry to threefold and removes one of the mirrors, reducing the point group of the full lattice to $\bar{3}m$. The vertical mirror that remains still provides enough symmetry to maintain the stars in just two orientations because an infinitesimal rotation of any one star would further reduce the symmetry to $\bar{3}$. The $\bar{3}m$ symmetry is preserved by additional stacking vectors, provided their horizontal shifts are all associated through (1) with stars of the same orientation. If, however, there are two staggered vectors with horizontal shifts associated with stars of different orientations, then the point group is reduced to $\bar{3}$ and there are no longer symmetry-based grounds for the stars to have just two orientations. Thus, when two-dimensional lattices of the type $[i,j]$ are stacked, staggered stacking vectors can be associated with only one of the groups of stars. If an attempt is made to associate staggered vectors with stars from both groups, then the two-dimensional sublattice $[i,j]$ will be unstable against a deformation to type $[i+j]$.

In summary (see Table 1), the Bravais classes of the hexagonal and trigonal crystals of arbitrary finite rank are characterized as follows.

(*a*) *Horizontal sublattice of type* $[i,j]$. The horizontal primitive vectors give stars of no more than two orientations, 30° apart. We identify the Bravais class by the symbol $[i,j]S^kV^l$, where i and j are the (even) numbers of horizontal-sublattice generating vectors giving stars in each orientation and k and l are the numbers of staggered and vertical stacking vectors.* If there are no staggered stacking vectors, then we may take $i \geq j$.† If there are staggered stacking vectors, then all must be associated with stars of the same orientation and we adopt the convention that these stars are given by the first group of i horizontal generating vectors in the square brackets (so that $k \leq i/2$). The symmetry of the full lattice is $6/mmm$ if staggered stacking vectors are absent and $\bar{3}m$ if they are present. The rank is $n = i + j + k + l$.

(*b*) *Horizontal lattice of type* $[i]$. The horizontal primitive vectors give stars with unrelated orientations (so there must be at least two stars). We identify the Bravais class by the symbol $[i]S^kV^l$, where $i \geq 4$ is the (even) number of horizontal-sublattice generating vectors, $k \leq i/2$ is the number of staggered stacking vectors and l is the number of vertical stacking vectors. The symmetry of the full lattice is $6/m$ if there are not any staggered stacking vectors and $\bar{3}$ if there are. The rank is $n = i + k + l$.

The enumeration of these possibilities for any given rank n is straightforward and is illustrated in the first two columns of Table 2, which lists the trigonal and hexagonal Bravais classes from rank 3 to rank 7.

Table 1. *The hexagonal and trigonal Bravais classes of arbitrary finite rank and their point groups*

The notation is explained in §II. When the horizontal sublattice is of type $[i,j]$, our convention is that i is associated with the staggered stacking vectors if there are any, and $i \geq j$ otherwise. If there are no staggered stacking vectors and the horizontal sublattice is of type $[i,j]$, then the lattice has the full hexagonal point group $6/mmm$. The existence of staggered stacking vectors reduces the rotational symmetry to threefold and removes one of the vertical mirrors. Horizontal sublattices of type $[i]$ have no vertical mirror symmetry.

Bravais class	$[i,j]S^kV^l$	$[i]S^kV^l$
No staggered stacking vectors ($k=0$)	$6/mmm$	$6/m$
At least one staggered stacking vector ($k>0$)	$\bar{3}m$	$\bar{3}$

III. Space groups

1. *Gauge-equivalence classes of phase functions*

As in the rank-4 case, the gauge-equivalence classes in the general case can be read directly from Tables 3 and 4 of LM which give the gauge-equivalence classes in the rank-3 periodic case. (1) As in the periodic case, a gauge can be picked in which the phases at all horizontal lattice-generating vectors are zero. (2) Each staggered vector and its corresponding pair of generators in the horizontal plane form an independent rank-3 trigonal R sublattice on which the phases are determined independently of their determination at the other lattice-generating vectors. Therefore, the phases at each staggered stacking vector can be taken directly from Table 4 of LM for the rank-3 R lattice. (3) The phases at all the vertical stacking vectors are determined independently of any of the other phases. They can therefore be taken directly from Table 3 of LM which gives the gauge-equivalence classes for the rank-3 hexagonal P lattice.

The resulting tabulation of gauge-equivalence classes is given in parts I of Tables 3–5 of this paper.

* If k or l are 0, we omit the S or V from the symbol.

† The symbol $[i,j]$ is omitted in the discussion in LM of the rank-3 and rank-4 cases because it is always [2,0].

Table 2. *An explicit catalog of the Bravais classes of trigonal and hexagonal lattices for ranks* 3–7 *and their* (3 + *d*) *settings*

The table of Bravais classes for arbitrary rank n is constructed by simply enumerating the cases in §II for which $i+j+k+l=n$. The $(3+d)$ settings are found by applying the general rules of §IV.1 and Table 6. The Bravais classes are grouped in the table by their rank and further subgrouped by the number of generating vectors in the horizontal sublattice (or, equivalently, by the number of incommensurate stacking vectors). The first column lists the Bravais classes using the notation $[i,j]S^kV^l$ or $[i]S^kV^l$ described in §II. The second column gives the point group of the lattices in each Bravais class according to the general rules of Table 1. The third column lists the possible $(3+d)$ settings useful in describing incommensurately modulated periodic crystals. The notation for the different settings is described in §IV. 1 and summarized in Table 6. The last column lists the same settings using the superspace notation of JJdW (1983) where they are characterized as '$(3+d)$ Bravais classes' and listed up to rank 6. We have made the obvious generalization of the JJdW notation to rank 7 but do not recommend it. In LM, we used the symbols SV or $R+1$ and VV or $P+1$ for the two rank-4 Bravais classes.

Bravais Class	Point Group	(3+*d*) Settings	JJdW Symbol
		rank–3	
$[2,0]S[R]$	$\bar{3}m$		
$[2,0]V[P]$	$6/mmm$		
		rank–4	
$[2,0]SV$	$\bar{3}m$	$R,\ P_S$	$R\bar{3}m(00\gamma),\ P\bar{3}1m(\frac{1}{3}\frac{1}{3}\gamma)$
$[2,0]V^2$	$6/mmm$	P	$P6/mmm(00\gamma)$
		rank–5	
$[2,0]SV^2$	$\bar{3}m$	$R,\ P_S$	$R\bar{3}m(00\gamma,00\nu),\ P\bar{3}1m(\frac{1}{3}\frac{1}{3}\gamma,00\nu)$
$[2,0]V^3$	$6/mmm$	P	$P6/mmm(00\gamma,00\nu)$
$[4,0]S$	$\bar{3}m$	$R,\ P^S$	$R\bar{3}m(\alpha00),\ P\bar{3}1m(\alpha\alpha\frac{1}{3})$
$[4,0]V$	$6/mmm$	P	$P6/mmm(\alpha00)$
$[2,2]S$	$\bar{3}m$	$R,\ P^S$	$R\bar{3}m(\alpha\alpha0),\ P\bar{3}m1(\alpha0\frac{1}{3})$
$[2,2]V$	$6/mmm$	P	$P6/mmm(\alpha\alpha0)$
$[4]S$	$\bar{3}$	$R,\ P^S$	$R\bar{3}(\alpha\beta0),\ P\bar{3}(\alpha\beta\frac{1}{3})$
$[4]V$	$6/m$	P	$P6/m(\alpha\beta0)$
		rank–6	
$[2,0]SV^3$	$\bar{3}m$	$R,\ P_S$	$R\bar{3}m(00\gamma,00\nu,00\theta),\ P\bar{3}1m(\frac{1}{3}\frac{1}{3}\gamma,00\nu,00\theta)$
$[2,0]V^4$	$6/mmm$	P	$P6/mmm(00\gamma,00\nu,00\theta)$
$[4,0]S^2$	$\bar{3}m$	$R,\ P_S^S$	$R\bar{3}m(\alpha0\gamma),\ P\bar{3}1m(\alpha\alpha\frac{1}{3},\frac{1}{3}\frac{1}{3}\gamma)$
$[4,0]SV$	$\bar{3}m$	$R,\ P_S,$	$R\bar{3}m(\alpha00,00\gamma),\ P\bar{3}1m(\alpha00,\frac{1}{3}\frac{1}{3}\gamma),$
		$P^S,\ P$	$P\bar{3}1m(\alpha\alpha\frac{1}{3},00\gamma),\ P\bar{3}1m(\alpha\alpha\gamma)$
$[4,0]V^2$	$6/mmm$	P	$P6/mmm(\alpha0\gamma)$
$[2,2]SV$	$\bar{3}m$	$R,\ P_S,$	$R\bar{3}m(\alpha\alpha0,00\gamma),\ P\bar{3}1m(\alpha\alpha0,\frac{1}{3}\frac{1}{3}\gamma),$
		$P^S,\ P$	$P\bar{3}m1(\alpha0\frac{1}{3},00\gamma),\ P\bar{3}m1(\alpha0\gamma)$
$[2,2]V^2$	$6/mmm$	P	$P6/mmm(\alpha\alpha\gamma)$
$[4]S^2$	$\bar{3}$	$R,\ P_S^S$	$R\bar{3}(\alpha\beta\gamma),\ P\bar{3}(\alpha\beta\frac{1}{3},\frac{1}{3}\frac{1}{3}\gamma)$
$[4]SV$	$\bar{3}$	$R,\ P_S,$	$R\bar{3}(\alpha\beta0,00\gamma),\ P\bar{3}(\alpha\beta0,\frac{1}{3}\frac{1}{3}\gamma),$
		$P^S,\ P$	$P\bar{3}(\alpha\beta\frac{1}{3},00\gamma),\ P\bar{3}(\alpha\beta\gamma)$
$[4]V^2$	$6/m$	P	$P6/m(\alpha\beta\gamma)$

Table 2. (*cont.*)

Bravais Class	**Point Group**	**(3+*d*) Settings**	**JJdW Symbol**
			rank–7
$[2,0]SV^4$	$\bar{3}m$	R,	$R\bar{3}m(00\gamma, 00\nu, 00\theta, 00\mu)$,
		P_S	$P\bar{3}1m(\frac{1}{3}\frac{1}{3}\gamma, 00\nu, 00\theta, 00\mu)$
$[2,0]V^5$	$6/mmm$	P	$P6/mmm(00\gamma, 00\nu, 00\theta, 00\mu)$
$[4,0]S^2V$	$\bar{3}m$	R, P^S_S,	$R\bar{3}m(\alpha 0\gamma, 00\nu)$, $P\bar{3}1m(\alpha 0\frac{1}{3}, \frac{1}{3}\frac{1}{3}\gamma, 00\nu)$,
		P_S	$P\bar{3}1m(\alpha\alpha\gamma, \frac{1}{3}\frac{1}{3}\nu)$
$[4,0]SV^2$	$\bar{3}m$	R, P_S,	$R\bar{3}m(\alpha 00, 00\gamma, 00\nu)$, $P\bar{3}1m(\alpha 00, \frac{1}{3}\frac{1}{3}\gamma, 00\nu)$,
		P^S, P	$P\bar{3}1m(\alpha\alpha\frac{1}{3}, 00\gamma, 00\nu)$, $P\bar{3}1m(\alpha\alpha\gamma, 00\nu)$
$[4,0]V^3$	$6/mmm$	P	$P6/mmm(\alpha 0\gamma, 00\nu)$
$[2,2]SV^2$	$\bar{3}m$	R, P_S,	$R\bar{3}m(\alpha\alpha 0, 00\gamma, 00\nu)$, $P\bar{3}1m(\alpha\alpha 0, \frac{1}{3}\frac{1}{3}\gamma, 00\nu)$,
		P^S, P	$P\bar{3}m1(\alpha 0\frac{1}{3}, 00\gamma, 00\nu)$, $P\bar{3}m1(\alpha 0\gamma, 00\nu)$
$[2,2]V^3$	$6/mmm$	P	$P6/mmm(\alpha\alpha\gamma, 00\nu)$
$[4]S^2V$	$\bar{3}$	R, P^S_S,	$R\bar{3}(\alpha\beta\gamma, 00\nu)$, $P\bar{3}(\alpha\beta\frac{1}{3}, \frac{1}{3}\frac{1}{3}\gamma, 00\nu)$,
		P_S	$P\bar{3}(\alpha\beta\gamma, \frac{1}{3}\frac{1}{3}\nu)$
$[4]SV^2$	$\bar{3}$	R, P_S,	$R\bar{3}(\alpha\beta 0, 00\gamma, 00\nu)$, $P\bar{3}(\alpha\beta 0, \frac{1}{3}\frac{1}{3}\gamma, 00\nu)$,
		P^S, P	$P\bar{3}(\alpha\beta\frac{1}{3}, 00\gamma, 00\nu)$, $P\bar{3}(\alpha\beta\gamma, 00\nu)$
$[4]V^3$	$6/m$	P	$P6/m(\alpha\beta\gamma, 00\nu)$
$[6,0]S$	$\bar{3}m$	R, P^S	$R\bar{3}m(\alpha 00, \beta 00)$, $P\bar{3}1m(\alpha\alpha\frac{1}{3}, \beta 00)$
$[6,0]V$	$6/mmm$	P	$P6/mmm(\alpha 00, \beta 00)$
$[4,2]S$	$\bar{3}m$	R, P^S_1,	$R\bar{3}m(\alpha 00, \beta\beta 0)$, $P\bar{3}1m(\alpha\alpha\frac{1}{3}, \beta\beta 0)$,
		P^S_2	$P\bar{3}m1(\alpha 0\frac{1}{3}, \beta\beta 0)$
$[2,4]S$	$\bar{3}m$	R, P^S	$R\bar{3}m(\alpha\alpha 0, \beta\beta 0)$, $P\bar{3}m1(\alpha 0\frac{1}{3}, \beta 00)$
$[4,2]V$	$6/mmm$	P_1, P_2	$P6/mmm(\alpha 00, \beta\beta 0)$, $P6/mmm(\alpha\alpha 0, \beta\beta 0)$
$[6]S$	$\bar{3}$	R, P^S	$R\bar{3}(\alpha\beta 0, \delta\epsilon 0)$, $P\bar{3}(\alpha\beta 0, \delta\epsilon\frac{1}{3})$
$[6]V$	$6/m$	P	$P6/m(\alpha\beta 0, \delta\epsilon 0)$

For each Bravais class, one needs to consider only the point groups that are subgroups of the point group of the lattices in the class, as given in Table 1.

2. *Identification of gauge-equivalence classes under scale equivalence*

As in our treatment of the rank-4 case, we consider integral linear combinations of the stacking vectors with determinant ± 1 that give alternative sets of stacking vectors differing from the original set only by rescalings of their vertical components. Gauge-inequivalent phase functions that differ only by these transformations belong in the same scale-equivalence class.

We make these further identifications by building up the general transformations out of transformations of pairs of stacking vectors, using the same 2×2 matrices of determinant ± 1 used in the rank-4 case in §VI of LM. There we found that, except for the point groups $6mm$ and $6/mmm$, which we consider below, only one of the two stacking vectors need have nonzero phases, the phases associated with the other being reducible to zero by appropriate

Table 3. *Gauge-equivalence classes and space groups of arbitrary finite rank in the hexagonal system and their settings for modulated periodic crystals*

The hexagonal point groups are compatible with lattices containing only vertical stacking vectors: Bravais classes of types $[i,j]V^{l}$ and $[i]V^{l}$. All point groups are compatible with Bravais classes of type $[i,j]V^{l}$. If the Bravais class is $[i]V^{l}$, one need only consider the point groups $6/m$, $\bar{6}$ and 6.

The gauge-equivalence classes are given in part I of the table. They are specified by a set of phases: the values of a representative set of phase functions for the point-group generators at the primitive generating vectors of the lattices. A gauge is used in which all phases unspecified in the table are zero. The possible nonzero phases are only at the vertical stacking vectors $\mathbf{c}^{\alpha}$ ($\alpha = 1 \dots l$) and only associated with the sixfold rotation r or the vertical mirror m. These phases are taken directly from Table 3 of LM which gives the gauge-equivalence classes for the rank-3 hexagonal P lattice.

Part II of the table lists the space groups of arbitrary finite rank arrived at by identifying scale-equivalent gauge-equivalence classes. Again, only nonzero phases are given. Phases characterizing a given space group are on a horizontal row, enclosed in brackets when more than one phase is needed. (The absence of such brackets in part I of the table indicates that any selection of phases from each possible column gives a distinct gauge-equivalence class.) In all but the last case in the right-hand column, only a single stacking vector has nonzero phases. The nonzero phases describing hexagonal space groups of arbitrary rank are identical to those given in Table 5 of LM for the case of rank 4, since all additional lattice-generating vectors can be assigned zero phases.

Part III of the table lists the different settings of the space groups in the modulated case, where one singles out a rank-3 sublattice of main reflections, which must be taken from one of the P settings (P_1 or P_2). We take $\mathbf{c}^1$ to be the generator of the lattice of main reflections. All other stacking vectors describe satellite peaks. The settings are separated vertically into sets that correspond to settings of the general space groups listed in the same order in part II. All settings except for the last one in the right-hand column involve nonzero phases at only two stacking vectors, which are identical to the phases that specify the settings for rank 4. The last setting appears only in lattices with rank 5 or more.

Parts II and III of the table apply to lattices with more than one stacking vector. If a lattice has only a single stacking vector, then the space groups and the $(3+d)$ settings are identical to the gauge-equivalence classes, as they are in the rank-3 case. In particular, enantiomorphic pairs of space groups *are* distinct when there is only one stacking vector.

G	$\bar{6}$	6 622	$\bar{6}2m$ $\bar{6}m2$	$6/m$	$6mm$ $6/mmm$
Phases	—	$\Phi_r(\mathbf{c}^{\alpha})$	$\Phi_m(\mathbf{c}^{\alpha})$	$\Phi_r(\mathbf{c}^{\alpha})$	$\Phi_r(\mathbf{c}^{\alpha})$ $\Phi_m(\mathbf{c}^{\alpha})$
I. Gauge		0	0	0	0 0
Equiva-		$\frac{1}{6}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$ $\frac{1}{2}$
lence		$\frac{2}{6}$			
Classes		$\frac{3}{6}$			
		$\frac{4}{6}$			
		$\frac{5}{6}$			
Phases	—	$\Phi_r(\mathbf{c}^1)$	$\Phi_m(\mathbf{c}^1)$	$\Phi_r(\mathbf{c}^1)$	$\Phi_r(\mathbf{c}^1)$ $\Phi_m(\mathbf{c}^1)$ $\Phi_r(\mathbf{c}^2)$ $\Phi_m(\mathbf{c}^2)$
II. General		0	0	0	[0 0 0 0]
Rank-n		$\frac{1}{6}$	$\frac{1}{2}$	$\frac{1}{2}$	[$\frac{1}{2}$ 0 0 0]
Space		$\frac{2}{6}$			[0 $\frac{1}{2}$ 0 0]
Groups		$\frac{3}{6}$			[$\frac{1}{2}$ $\frac{1}{2}$ 0 0]
					[0 $\frac{1}{2}$ $\frac{1}{2}$ 0]
Phases	—	$\Phi_r(\mathbf{c}^1)$ $\Phi_r(\mathbf{c}^2)$	$\Phi_m(\mathbf{c}^1)$ $\Phi_m(\mathbf{c}^2)$	$\Phi_r(\mathbf{c}^1)$ $\Phi_r(\mathbf{c}^2)$	$\Phi_r(\mathbf{c}^1)$ $\Phi_m(\mathbf{c}^1)$ $\Phi_r(\mathbf{c}^2)$ $\Phi_m(\mathbf{c}^2)$ $\Phi_r(\mathbf{c}^3)$ $\Phi_m(\mathbf{c}^3)$
III. Settings		[0 0]	[0 0]	[0 0]	[0 0 0 0 0 0]
of					
General		[$\frac{1}{6}$ 0]	[$\frac{1}{2}$ 0]	[$\frac{1}{2}$ 0]	[$\frac{1}{2}$ 0 0 0 0 0]
Space		[$\frac{2}{6}$ $\frac{1}{6}$]	[0 $\frac{1}{2}$]	[0 $\frac{1}{2}$]	[0 0 $\frac{1}{2}$ 0 0 0]
Groups		[$\frac{3}{6}$ $\frac{1}{6}$]			
for		[$\frac{4}{6}$ $\frac{1}{6}$]			[0 $\frac{1}{2}$ 0 0 0 0]
Modul-		[$\frac{5}{6}$ 0]			[0 0 0 $\frac{1}{2}$ 0 0]
ated		[0 $\frac{1}{6}$]			
Crystals					[$\frac{1}{2}$ $\frac{1}{2}$ 0 0 0 0]
		[$\frac{2}{6}$ 0]			[0 0 $\frac{1}{2}$ $\frac{1}{2}$ 0 0]
		[$\frac{4}{6}$ 0]			
		[0 $\frac{2}{6}$]			[0 $\frac{1}{2}$ $\frac{1}{2}$ 0 0 0]
					[$\frac{1}{2}$ 0 0 $\frac{1}{2}$ 0 0]
		[$\frac{3}{6}$ 0]			[$\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ 0 0 0]
		[0 $\frac{3}{6}$]			[0 0 0 $\frac{1}{2}$ $\frac{1}{2}$ 0]

Table 4. *Gauge-equivalence classes and space groups of arbitrary finite rank in the trigonal system for lattices containing only vertical stacking vectors (Bravais classes of types* $[i,j]V^l$ *and* $[i]V^l$*) and their settings for modulated periodic crystals*

All trigonal point groups are compatible with Bravais classes of type $[i,j]V^l$. If the Bravais class is $[i]V^l$, one need only consider the point groups $\bar{3}$ and 3. The structure and conventions are the same as for Table 3. The nonzero phases describing these space groups and their P settings (P_1 or P_2) for modulated periodic crystals are identical to those given in Table 6 of LM for the rank-4 case, since all additional lattice-generating vectors can be assigned zero phases.

G	$\bar{3}$	3, 321, 312	$\bar{3}m1$, $3m1$, $\bar{3}1m$, $31m$
Phases	—	$\Phi_r(\mathbf{c}^\alpha)$	$\Phi_m(\mathbf{c}^\alpha)$
I. Gauge		0	0
Equivalence		$\frac{1}{3}$	$\frac{1}{2}$
Classes		$\frac{2}{3}$	
Phases	—	$\Phi_r(\mathbf{c}^1)$	$\Phi_m(\mathbf{c}^1)$
II. General Rank-n		0	0
Space Groups		$\frac{1}{3}$	$\frac{1}{2}$
Phases	—	$\Phi_r(\mathbf{c}^1)$ $\Phi_r(\mathbf{c}^2)$	$\Phi_m(\mathbf{c}^1)$ $\Phi_m(\mathbf{c}^2)$
III. Settings of General		[0 0]	[0 0]
Space Groups			
for Modulated Crystals		[$\frac{1}{3}$ 0]	[$\frac{1}{2}$ 0]
		[$\frac{2}{3}$ 0]	[0 $\frac{1}{2}$]
		[0 $\frac{1}{3}$]	

linear transformations. In the case of arbitrary rank, we can make the same argument, picking one stacking vector and using it sequentially to form new linear combinations of each of the others at which all the phase functions are zero.* As a result, for all the point groups except $6mm$ and $6/mmm$, the space groups for any number of stacking vectors are exactly the same as in the rank-4 case: the nonzero phases can be associated with a single stacking vector. Unless all stacking vectors are staggered, that single vector can be taken to be vertical and the phases are exactly as for the rank-3 periodic P lattice (Table 3 of LM), except for the simplifying identification of enantiomorphic pairs that exists when the rank exceeds 3. If all stacking vectors are staggered, then the phases at the stacking vector with nonzero phase are exactly as for the rank-3 periodic R lattice (Table 4 of LM). This is shown in parts II of Tables 3–5 of this paper.

It remains to consider the point groups $6mm$ and $6/mmm$. These allow only vertical stacking vectors and allow nonzero values for both Φ_r and Φ_m. There are only three choices for the possible nonzero pairs of phases $[\Phi_r,\Phi_m]$ at each stacking vector: $[0\frac{1}{2}]$, $[\frac{1}{2}0]$, and $[\frac{1}{2}\frac{1}{2}]$. We can, therefore, reduce the maximum number of vectors with nonzero phases to three, by selecting one with each of the three types of phases and simply adding it to any other vector of that type.* If stacking vectors with all three types of phases are present, we can also reduce both phases at one of the remaining three to zero by adding to it the sum of the other two. To group the gauge-equivalence classes into space groups, we need therefore consider only a pair of vertical stacking vectors with nonzero phases, just as in the rank-4 case. Therefore, for the remaining point groups, $6mm$ and $6/mmm$, the space groups for any number of stacking vectors are also exactly the same as in the rank-4 case. The nonzero phases can be associated with a pair of vertical stacking vectors and are given in the column on the right of part II of Table 3.

IV. Settings for the (3 + d) modulated case

We stress that, in contrast to the rank-4 case, the (3 + d) settings are just one example of the settings in which one can display the general space groups,

* The procedure we followed in the rank-4 case works in exactly the same way even when applied to two *staggered* stacking vectors, a possibility that first arises in rank 6.

* The result is zero because phase arithmetic is modulo unity.

Table 5. *Gauge-equivalence classes and space groups of arbitrary finite rank in the trigonal system for lattices containing at least one staggered stacking vector (Bravais classes of types $[i,j]S^kV^l$ and $[i]S^kV^l$ with $k > 0$) and their settings for modulated periodic crystals*

All trigonal point groups are compatible with Bravais classes of type $[i,j]S^kV^l$. If the Bravais class is $[i]S^kV^l$, one need only consider the point groups $\bar{3}$ and 3.

The structure and conventions are the same as for Table 3, except that the settings of the space groups for modulated crystals occupy parts III–V, corresponding to the three types of settings for the Bravais classes: P, R and P^S. (The entries for P apply equally well to the P_1, P_2, and P_S settings and those for P^S apply equally well to P^S_1, P^S_2 and P^S_S.)

The phases in part I for the gauge-equivalence classes are identical to those in Table 4 of LM giving the gauge-equivalence classes for the rank-3 trigonal R lattice.

When the point group is 3 or 32 and the lattice has no vertical stacking vectors, there are only symmorphic space groups (*i.e.* all phases can be taken to be zero). The table entries only apply when there is at least one vertical stacking vector.

When the point group is $\bar{3}m$ or $3m$, $\Phi_m(\mathbf{c}')$ denotes the nonzero phase associated with a stacking vector that can be taken to be either vertical or staggered if both possibilities are available. The simplest convention is to take it to be vertical whenever possible.

We take the generator of the lattice of main reflections to be $\mathbf{c}^1$ for the P settings, $\mathbf{c}_s^1$ for the R settings and $\mathbf{c} = 3\mathbf{c}_s^1 - 2\mathbf{a} - \mathbf{b}$ for the P^S settings, where $\mathbf{a}$ and $\mathbf{b}$ are the horizontal generating vectors associated with $\mathbf{c}_s^1$. In the P^S settings the phase of the stacking vector for the lattice of main reflections is also assigned to two satellite stacking vectors. $\mathbf{c}_s^1$ and $(\mathbf{c}_s^1 - \mathbf{a})$, as noted in § IV.2. The P^S settings are possible only in ranks greater than 4.

G	$\bar{3}$	3 32	$\bar{3}m$	$3m$
Phases	—	$\Phi_r(\mathbf{c}^\alpha)$	$\Phi_m(\mathbf{c}_s^\beta)$	$\Phi_m(\mathbf{c}^\alpha)$
I. Gauge		0	0	0
Equivalence		$\frac{1}{3}$	$\frac{1}{2}$	$\frac{1}{2}$
Classes		$\frac{2}{3}$		
Phases	—	$\Phi_r(\mathbf{c}^1)$	$\Phi_m(\mathbf{c}')$	
II. General Rank-n		0	0	
Space Groups		$\frac{1}{3}$	$\frac{1}{2}$	
Phases	—	$\Phi_r(\mathbf{c}^1)$	$\Phi_m(\mathbf{c}^1)$	$\Phi_m(\mathbf{c}')$
III. P Settings of General		0	[0	0]
Space Groups				
for Modulated Crystals		$\frac{1}{3}$	[$\frac{1}{2}$	0]
		$\frac{2}{3}$	[0	$\frac{1}{2}$]
Phases	—	$\Phi_r(\mathbf{c}^1)$	$\Phi_m(\mathbf{c}_s^1)$	$\Phi_m(\mathbf{c}')$
IV. R Settings of General		0	[0	0]
Space Groups				
for Modulated Crystals		$\frac{1}{3}$	[$\frac{1}{2}$	0]
			[0	$\frac{1}{2}$]
Phases	—	$\Phi_r(\mathbf{c}^1)$	$\Phi_m(\mathbf{c})$	$\Phi_m(\mathbf{c}')$
V.· P^S Settings of General		0	[0	0]
Space Groups				
for Modulated Crystals		$\frac{1}{3}$	[$\frac{1}{2}$	0]
			[0	$\frac{1}{2}$]

useful in the case when the modulated structure is a periodic crystal. More general $(m + d)$ settings would be useful if one wished to describe weak modulations of a general quasiperiodic crystal of rank m. We focus here on the $(3 + d)$ settings because these are currently the ones of practical importance and because this enables us to establish the relation of our own approach to that of JJdW, who have computed the settings of the general Bravais classes for $d = 1, 2, 3$.*

* The settings for the Bravais classes were derived using the superspace approach and appear in JJdW (1983) as '$(3 + d)$ Bravais classes'. The associated 'superspace groups for modulated crystals' – the $(3 + d)$ settings of the general space groups – have only been given for the $(3 + 1)$ case (de Wolff, Janssen & Janner, 1981). See also Janssen, Janner, Looijenga-Vos & de Wolff (1992).

1. *Settings of the general Bravais classes*

A rank-3 sublattice, serving as a lattice of main reflections, is itself either a trigonal or a hexagonal (periodic) lattice and as such must include one star of horizontal generating vectors and a single stacking vector. There are three distinct possibilities for the stacking vector of main reflections: (1) it can be a vertical stacking vector from the full lattice; (2) it can be three times the vertical part of a staggered stacking vector of the full lattice; (3) it can be a staggered stacking vector of the full lattice. Cases (1) and (2) have P lattices of main reflections and case (3) has R lattices. We distinguish the settings of types (1) and (2) by calling them P and P^S settings, respectively.

In specifying, for any given Bravais class, which of the P, P^S and R settings can be realized and in how many distanct ways, it is enough to consider Bravais classes of type $[i,j]$ since the settings of a Bravais class of type $[i]$ are identical to those of type $[i,0]$.*

Case (1): *P settings.* When the stacking vector of main reflections is a vertical stacking vector of the full lattice, there can be up to three distinct choices for the star of main reflections. If the star is associated with a staggered stacking vector, we have a P_S setting. If it is not, then there can, in general, be two additional settings, depending on which set of stars the star of main reflections is taken from. We denote the two settings P_1 and P_2, depending on whether the star of main reflections is taken from the set specified by i or j in the $[i,j]$ symbol. When only one possibility is available (*i.e.* when $j=0$, or when $i=j$ and there are no staggered stacking vectors), the subscript may be omitted.

Case (2): *P^S settings.* When the stacking vector of main reflections is three times the vertical part of a staggered stacking vector $\mathbf{c}_s$ of the full lattice, the star of main reflections can be from any horizontal star of the full lattice except the one associated with $\mathbf{c}_s$. If the full lattice has a second staggered stacking vector $\mathbf{c}_s'$, then its associated star gives a setting we call P^S_S. If the star of main reflections is not associated with another staggered stacking vector, then, as in case (1), there are in general two settings, P^S_1 and P^S_2, which may be denoted simply P^S when only one possibility is available.

Case (3): *R settings.* The lattice of main reflections can be an R lattice whenever the full lattice contains at least one staggered stacking vector. The star of main reflections must then be the one uniquely associated with that staggered vector and there is just one such setting.

The settings are summarized in full generality in Table 6 and are listed in the third column of Table 2 for all Bravais classes from ranks 4 to 7.

2. *Settings of the general space groups*

Case (1): *all point groups except* 6*mm and* 6/*mmm*. These point groups assign nonzero phases to only a single point-group generator.

Case (1*A*): *R and P settings.* If the Bravais class of the main reflections is given by the R, P_1, P_2 or P_S setting of the general Bravais class, then the stacking vector for the main reflections, whose phases must not be altered by the transformations that establish scale equivalence, is one of the vertical or staggered generating vectors of the full lattice. Since the transformations that act only on the satellite stacking vectors are entirely unrestricted, the analysis of the phase functions associated with the satellite stacking vectors is identical to our analysis of *unrestricted* scale equivalence that led to the general space groups. In that case, we found that all but a single stacking vector could be given zero phases. The analysis of the *restricted* scale equivalence for that single satellite stacking vector and the stacking vector for the main reflections is then identical to the analysis we performed in the rank-4 case, leading directly to the settings given in parts III of Tables 3 and 4 and in parts III and IV of Table 5.

Case (1*B*): *P^S settings.* If the Bravais class of main reflections is given by the settings P^S_1, P^S_1 or P^S_S – possibilities that do not arise in the rank-4 case – then the stacking vector for the main reflections is three times the vertical component of one of the staggered stacking vectors $\mathbf{c}_s$ for the full lattice. If $\mathbf{a}$ and $\mathbf{b}$ are the horizontal generating vectors associated with $\mathbf{c}_s$, then the stacking vector for the main reflections is

$$\mathbf{c} = 3\mathbf{c}_s - 2\mathbf{a} - \mathbf{b} \qquad (2)$$

and among the generating vectors for the satellites there are two with nonzero horizontal components that can be taken to be

$$\mathbf{s}_1 = \mathbf{c}_s, \quad \mathbf{s}_2 = \mathbf{c}_s - \mathbf{a}. \qquad (3)$$

Since the only nonzero phase $\mathbf{c}_s$ can have* is $\Phi_m(\mathbf{c}_s) \equiv \frac{1}{2}$ and since all phase functions vanish in the horizon-

* Whether the stars are all aligned (type $[i,0]$) or not aligned at all (type $[i]$) is irrelevant to the settings because in either case the only grounds for distinguishing among stars is whether or not they are associated with a staggered vector.

* See part I of Table 5.

Table 6. *The* $(3+d)$ *settings of the hexagonal and trigonal Bravais classes* $[i,j]\ S^kV^l$ *of rank* $i+j+k+l = 3+d$

Definitions of the seven settings are given in §IV.1. The settings for lattices of type $[i]S^kV^l$ are the same as those for lattices of type $[i,0]S^kV^l$. The subscripts 1 and 2 can be omitted when a Bravais class only admits one of the two settings they distinguish. For a Bravais class to have all seven settings, we require $k \geq 2$, $i \geq 6$, $j \geq 2$ and $l \geq 1$, so the one of least rank with all seven is the Bravais class $[6,2]S^2V$ of rank 11.

Settings	Conditions on $[i,j]S^kV^l$
P_1	$l>0,\ i>2k$
P_2	$l>0,\ j>0,\ i\neq j$ if $k=0$
P_S	$l>0,\ k>0$
P^S_1	$k>0,\ i>2k$
P^S_2	$k>0,\ j>0$
P^S_S	$k>1$
R	$k>0$

tal plane, the possible phases of the stacking vector for the main reflections and these two generating vectors for the satellites are not independent:

$$\Phi_m(\mathbf{c}) \equiv \Phi_m(\mathbf{s}_1) \equiv \Phi_m(\mathbf{s}_2) \equiv 0 \text{ or } \tfrac{1}{2}. \qquad (4)$$

Note that in this case the phases available to **c**, the generating vector for a P lattice of main reflections, must be taken from the set of phases appropriate to the rank-3 R lattice.

Having noted that $\Phi_m(\mathbf{c})$ is restricted by (4) and that its value entirely determines the phases at the satellite generating vectors $\mathbf{s}_1$ and $\mathbf{s}_2$, we can proceed with the remaining satellite stacking vectors just as we did for the other four settings, concluding that all but one of the remaining satellite stacking vectors can be assigned zero phases.

When the point groups are 3 and 32, there are no nonvanishing mirror phase functions and the above complication does not arise. In this case, the settings of the space groups are exactly as given for the R settings: a nonzero phase can be associated with a single vertical satellite stacking vector, if one exists.

When the point groups are $\bar{3}m$ or $3m$, then, in addition to the two possible values of the phases in (4), we need to consider the possible values of 0 or $\frac{1}{2}$ for the phase of a single additional stacking vector for the satellites, whether it is staggered or vertical.* These four possibilities yield only three settings, the one with both phases $\frac{1}{2}$ being scale-equivalent to the one where the phases in (4) are $\frac{1}{2}$ and the phase of the additional stacking vector is 0.

The P^S settings of the space groups are summarized in part V of Table 5.

Case (2): *point groups* $6mm$ and $6/mmm$ (*only P settings are possible*). When the point group is $6mm$ or $6/mmm$, all stacking vectors are vertical, so the complications of the P^S settings do not arise, but now both Φ_r and Φ_m can be nonzero. Evidently, if there are just two stacking vectors, the settings are exactly as in the rank-4 case. When there are three or more, let $\mathbf{c}^1$ be the one that indexes the main reflections. Scale-equivalence transformations that act only on the remaining stacking vectors are entirely unrestricted and therefore the analysis of the scale-equivalence classes of phase functions associated with the remaining stacking vectors is identical to our analysis of *unrestricted* scale equivalence, which led to the phases that characterize the general space groups. Thus, we can index the satellites in such a way that at most two of the satellite stacking vectors $\mathbf{c}^2$ and $\mathbf{c}^3$ have nonzero phases and the possible choices for those phases are the same five sets that part II of Table 3 assigns to $\mathbf{c}^1$ and $\mathbf{c}^2$ in the general space groups.

* It would be simplest to choose it to be a vertical vector if one is available.

In four of those five sets, one of the two stacking vectors $\mathbf{c}^2$ and $\mathbf{c}^3$ is assigned zero phases. If we take that one to be $\mathbf{c}^3$, then, in determining restricted scale equivalence, we need only examine restricted scale-equivalence transformations that act on the stacking vector of main reflections $\mathbf{c}^1$ and the satellite stacking vector $\mathbf{c}^2$. But this is exactly the procedure we followed in LM to determine the settings for modulated crystals in the rank-4 case, where we found the ten settings listed in Table 5 of LM. These same sets of phases, with phases 0 assigned to $\mathbf{c}^3$, form the first ten entries in the right-hand column of part III of Table 3.

The eleventh entry arises from the fifth possible assignment of phases to the satellite stacking vectors $\mathbf{c}^2$ and $\mathbf{c}^3$, in which $[\Phi_r, \Phi_m]$ has the value $[0,\frac{1}{2}]$ at $\mathbf{c}^2$ and $[\frac{1}{2},0]$ at $\mathbf{c}^3$. The accompanying phases at the stacking vector of main reflections $\mathbf{c}^1$ can independently have the full set of values $[0,0]$, $[0,\frac{1}{2}]$, $[\frac{1}{2},0]$ or $[\frac{1}{2},\frac{1}{2}]$. The restricted scale-equivalence transformations allow us to add $\mathbf{c}^1$ to either of the satellite stacking vectors $\mathbf{c}^2$ or $\mathbf{c}^3$ and to add one of $\mathbf{c}^2$ or $\mathbf{c}^3$ to the other. As a result, except when $\mathbf{c}^1$ has both phases 0, we can again reduce the phase associated with one of the two satellite stacking vectors to zero, thereby establishing scale equivalence with one of the ten cases already listed. For each point group, there is thus only one additional setting beyond the ten we found in the rank-4 case. This is a setting of the fifth general space group in part II of Table 3. The setting has nonzero phases only at the two stacking vectors $\mathbf{c}^2$ and $\mathbf{c}^3$ and is listed as the last entry in part III of Table 3.

V. Concluding remarks

The conventional approach to the crystallographic classification of modulated materials relies on analytical tools developed to describe real-space periodicity and treats quasiperiodic materials by embedding them in a higher-dimensional superspace where they can be viewed as three-dimensional slices of a periodic structure. Superspace crystallography therefore relies on the abstract algebraic formulation of crystallography necessary when dealing with periodic structures in more than three dimensions. As currently formulated, it is also strongly biased toward quasiperiodic materials that are modulated crystals, because of the manner in which it performs the embedding.

The Fourier-space approach permits one to retain the powerful tool of three-dimensional geometric intuition and is nonprejudicial among the different classes of quasiperiodic materials. It gives a scheme that is easier to derive and more generally applicable, from which the conventional categories of modulated crystals can be reached as convenient settings for the general categories, useful in that special case.

In this application of Fourier-space crystallography, we have given the classification of hexagonal and trigonal quasiperiodic crystals of arbitrary finite rank to demonstrate the power and simplicity of the approach. We have constructed the Bravais classes as an elementary geometrical exercise in three-dimensional space and have found the space groups associated with each Bravais class in a manner hardly more elaborate than that used in the rank-4 case. In both the rank-4 and rank-n cases, the crucial part of the calculation has already been accomplished when one derives, in their Fourier-space forms, the ordinary rank-3 crystallographic space groups.

The specification of these results in a form tailored to the description of modulated crystals is simply a matter of listing the settings of the general space groups and Bravais classes. A crucial part of our simplification lies in not specializing to the modulated case (which breaks the symmetry of the problem by singling out a particular rank-3 sublattice for special treatment) until the end of the calculation. While our results are equivalent to the conventional description of modulated crystals in all cases for which that description has been worked out, they apply to a much broader range of quasiperiodic crystals, as well as to modulated crystals of arbitrary rank.

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APPENDIX

Bravais classes of trigonal and hexagonal lattices of arbitrary finite rank

We justify here the assertions made in §II about the Bravais classes of finite rank lattices with hexagonal or trigonal symmetry. When a lattice L in three dimensions has axial symmetry, it is conveniently characterized in terms of its two-dimensional sublattice H, perpendicular to the n-fold axis, and a *modular lattice* L/H of vectors defined only to within an additive vector of H. The notation reflects the fact that, if L is considered as an Abelian group under addition, then L/H is just the quotient group modulo the subgroup H. The rank of L is just the sum of the ranks of H and L/H. We refer to the generators of L/H as *stacking vectors* because the full lattice L can be viewed as a set of lattice planes given by shifting H by all integral linear combinations of the stacking vectors.

Viewed as a two-dimensional lattice, the sublattice H can have the two-dimensional point group $6mm$ or 6. In §A, we derive the Bravais classes of two-dimensional lattices of finite rank with point group $6mm$; in §B, we derive the Bravais classes when the point group is 6. In §C, we derive the ways in which these two-dimensional sublattices can be stacked to give the full three-dimensional lattice.

A. Two-dimensional lattices with point group 6mm

We first categorize a general two-dimensional lattice H of finite rank with $6mm$ symmetry in terms of a family of stars all with the same orientation. We then note that this description is equivalent to the $[i,j]$ Bravais classes described in §II, based on families of stars with two distinct orientations.

1. *A description with a single family of stars*. Let $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$ be unit vectors, 120° apart, on invariant lines of two vertical mirrors m_a and m_b. Expand a vector $\mathbf{v}$ in the lattice H as

$$\mathbf{v} = \alpha\hat{\mathbf{a}} + \beta\hat{\mathbf{b}} \tag{5}$$

(with coefficients α and β that are not necessarily rational). Twice the projections of $\mathbf{v}$ onto $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$ must also be in H, since they can be expressed as

$$\begin{aligned} 2P_a\mathbf{v} &= \mathbf{v} + m_a\mathbf{v} = (2\alpha - \beta)\hat{\mathbf{a}}, \\ 2P_b\mathbf{v} &= \mathbf{v} + m_b\mathbf{v} = (2\beta - \alpha)\hat{\mathbf{b}}. \end{aligned} \tag{6}$$

The subset H_a of H consisting of $2P_a\mathbf{v}$ for all $\mathbf{v}$ in H is a one-dimensional lattice of finite rank k (since the full lattice is of finite rank) and can therefore be primitively indexed by k of its vectors; *i.e.* one can choose k integrally independent lengths $\alpha^{(1)}, \dots, \alpha^{(k)}$ so that H_a consists of all integral linear combinations of the vectors $\mathbf{a}_1 = \alpha^{(1)}\hat{\mathbf{a}}, \dots, \mathbf{a}_k = \alpha^{(k)}\hat{\mathbf{a}}$. By symmetry, H_b can be primitively generated by the vectors $\mathbf{b}_1 = \alpha^{(1)}\hat{\mathbf{b}}, \dots, \mathbf{b}_k = \alpha^{(k)}\hat{\mathbf{b}}$. Note that two-dimensional lattices of rank $2k$ that differ only in the mutually incommensurate lengths $\alpha^{(1)}, \dots, \alpha^{(k)}$ that characterize the primitive bases for the sublattices H_a and H_b are in the same Bravais class [for essentially the same reasons that two orthorhombic P lattices with different lattice constants (a, b and c) belong to the same Bravais class].

We can expand the vectors (6) in these bases for the one-dimensional sublattices:

$$\begin{aligned} (2\alpha - \beta)\hat{\mathbf{a}} &= \sum_{i=1}^{k} n_i\mathbf{a}_i = \left(\sum_{i=1}^{k} n_i\alpha^{(i)}\right)\hat{\mathbf{a}}, \\ (2\beta - \alpha)\hat{\mathbf{b}} &= \sum_{i=1}^{k} m_i\mathbf{b}_i = \left(\sum_{i=1}^{k} m_i\alpha^{(i)}\right)\hat{\mathbf{b}}. \end{aligned} \tag{7}$$

Solving for α and β enables us to express the original arbitrary vector $\mathbf{v}$ in H as

$$\mathbf{v} = \sum_{i=1}^{k} [(\tfrac{2}{3}n_i + \tfrac{1}{3}m_i)\mathbf{a}_i + (\tfrac{1}{3}n_i + \tfrac{2}{3}m_i)\mathbf{b}_i], \qquad (8)$$

where all the n_i and m_i are integers.

All vectors with integral coefficients for the $\mathbf{a}_i$'s and the $\mathbf{b}_i$'s are in H, since they are sums of vectors in H_a and H_b. From (8), we learn that the lattice may also contain vectors whose coefficients are multiples of $\frac{1}{3}$, as long as the sum of the coefficients of $\mathbf{a}_i$ and $\mathbf{b}_i$ for each i is an integer. It is convenient to restate this conclusion in the form it assumes when the axes are rescaled by a factor of three:

Any two-dimensional hexagonal lattice of rank $2k$ and point group $6mm$ can be expressed as a set of integral linear combinations of k integrally independent parallel vectors, $\mathbf{a}_1,...,\mathbf{a}_k$ and their images under a 120° rotation, $\mathbf{b}_1,...,\mathbf{b}_k$, where: (1) for each i the sum of the coefficients of $\mathbf{a}_i$ and $\mathbf{b}_i$ is a multiple of three; (2) vectors with all coefficients multiples of three are in the lattice and constitute a sublattice, H_P.

The two-dimensional hexagonal lattices with point group $6mm$ can therefore be viewed as the translations through all vectors of the sublattice H_P of a finite set of vectors H_0, which can contain only vectors whose coefficients for each pair of generators $\mathbf{a}_i$ and $\mathbf{b}_i$ are 00, $1\bar{1}$, or $\bar{1}1$.* H_0 is the modular lattice† H/H_P; it is closed under addition and subtraction modulo the lattice H_P (*i.e.* when arithmetic is performed on its components modulo 3) as a consequence of the closure of the full lattice under ordinary addition and subtraction. Since all sublattices H_P of the same rank are in the same two-dimensional Bravais class, classifying these two-dimensional lattices into Bravais classes reduces to classifying the corresponding modular lattices.

2. *Proof by induction that all Bravais classes of two-dimensional hexagonal lattices with* 6*mm symmetry are of type* $[i,j]$. Note first the elementary geometrical fact that a pair of star vectors with a three-element modular lattice (00, $1\bar{1}$ and $\bar{1}1$) generate exactly the same rank-2 lattice as a pair of star vectors rotated through 30° and scaled down by $3^{1/2}$, with a modular lattice containing only 00. As a result, to establish the validity of the description in §II of the horizontal sublattice in terms of two families of star vectors at 30°, we need only show that a basis of identically oriented star-generating vectors can be chosen for H_P, in terms of which the modular lattice H_0 reduces to a sum of modular lattices (each consisting of either 00 alone or the three vectors 00, $1\bar{1}$ and $\bar{1}1$) associated with each pair $\mathbf{a}_m$, $\mathbf{b}_m$.

* It is convenient to write $\bar{1}$ for -1.

† Modular lattices were used in a similar manner to enumerate Bravais classes of quasiperiodic crystals by Mermin & Lifshitz (1992).

This is trivially the case when the rank is 2, since there is then only one pair $\mathbf{a}$, $\mathbf{b}$. Suppose it has been established for rank $2k$. Then, with a modular lattice H_0 of rank $2(k+1)$ it is possible to choose the first k pairs $\mathbf{a}_m$, $\mathbf{b}_m$ so that the sublattice of H_0 spanned by them is of type $[i,j]$ (*i.e.* H_0 is the sum of j three-element modular lattices). If the $(k+1)$th pair $\mathbf{a}_{k+1}$, $\mathbf{b}_{k+1}$ does not appear in the expansion of any vector of H_0, then H_0 is of type $[i+2,j]$. Otherwise there must be at least one vector in H_0 of the form $\mathbf{u} + \mathbf{a}_{k+1} - \mathbf{b}_{k+1}$, where $\mathbf{u}$ is a vector spanned by only the first k pairs of generating vectors. It follows that H_0 must be the sum of a modular lattice of type $[i,j]$, with a three-element modular lattice that can be taken to be $[0,\ \mathbf{u}+\mathbf{a}_{k+1}-\mathbf{b}_{k+1},\ -\mathbf{u}-\mathbf{a}_{k+1}+\mathbf{b}_{k+1}]$. If $\mathbf{u}$ is zero, then H_0 is of type $[i,j+2]$. If $\mathbf{u}$ is not zero, then define

$$\mathbf{a}'_{k+1} = \mathbf{a}_{k+1} + \tfrac{2}{3}P_a\mathbf{u}, \quad \mathbf{b}'_{k+1} = \mathbf{b}_{k+1} - \tfrac{2}{3}P_b\mathbf{u}. \qquad (9)$$

Because $\mathbf{u}$ has components 0, $1\bar{1}$ or $\bar{1}1$ along each of the first k pairs of star vectors, $-P_b\mathbf{u}$ is simply a 120° rotation of $P_a\mathbf{u}$, and $\mathbf{a}'_{k+1}$ and $\mathbf{b}'_{k+1}$ are an alternative pair of primitive star vectors for H. Since (2/3) $(P_a\mathbf{u} + P_b\mathbf{u}) = \mathbf{u}$, the three-element modular lattice becomes $[0,\ \mathbf{a}'_{k+1}-\mathbf{b}'_{k+1},\ -\mathbf{a}'_{k+1}+\mathbf{b}'_{k+1}]$ and H_0 is again of type $[i,j+2]$.

B. Lattices with point group 6

If the two-dimensional point group is only 6, we must show that the lattice can be primitively generated by pairs of vectors of equal length, separated by 120°. Such a lattice of finite rank i belongs to the Bravais class $[i]$ described in §II.

Let $\mathbf{a}'$ be a vector in H and let $\mathbf{b}' = r\mathbf{a}'$ be its image under a 120° rotation r. Consider the sublattice H_2 of H consisting of all points that are *rational* linear combinations of $\mathbf{a}'$ and $\mathbf{b}'$. Because H has finite rank, so does H_2, which can therefore be indexed by a finite number of its vectors. Because all such vectors are rational linear combinations of $\mathbf{a}'$ and $\mathbf{b}'$ and because they are finite in number, they can all be expressed as integral linear combinations of two rational linear combinations of $\mathbf{a}'$ and $\mathbf{b}'$ (with sufficiently large denominators). Therefore, H_2 has rank 2. Because it also has sixfold symmetry it can only be a triangular lattice and can therefore indeed be expressed as all integral linear combinations of two vectors $\mathbf{a}$ and $\mathbf{b}$ of equal length, 120° apart.

We take $\mathbf{a}$ and $\mathbf{b}$ to be members of a set of generating vectors for the full lattice H. If we expand every vector of H in this set and drop the two terms in which $\mathbf{a}$ and $\mathbf{b}$ appear, we get a sublattice of H of rank two less than H for which we can repeat the above procedure. Since H is of finite rank, successive repetitions will yield a complete set of primitive generating vectors for H composed of pairs of vectors of equal length 120° apart.

C. The stacking vectors

Because the full lattice L is closed under addition and subtraction, any plane of vectors parallel to the horizontal sublattice H must consist of H itself, shifted by a vector with a nonzero component along the axis of three- or sixfold symmetry. A set of primitive generating vectors for L consists of a set of primitive generating vectors for H and a set of stacking vectors that can be regarded as primitive generating vectors for the modular lattice L/H.

To establish that the stacking vectors can be taken as specified in §II, note first that the projection of L into the horizontal plane, P, is a two-dimensional lattice with sixfold symmetry that contains H. If $P = H$, then no stacking vectors need horizontal components. Staggered stacking vectors – those which necessarily have nonzero horizontal components – are only required if P has vectors not in H. The horizontal parts of such staggered stacking vectors can be specified by a modular lattice $P_0 = P/H$. The projected lattice P is given by the translations of P_0 through all the vectors of H and P_0 is itself a lattice under addition modulo H. The rank of P_0 as a modular lattice is the number of independent staggered stacking vectors.

We must show that a set of generators can be found for P_0 (which generate P_0 under arithmetic modulo H) and for H such that each generator of P_0 has the form

$$\mathbf{h} = \tfrac{2}{3}\mathbf{a}_0 + \tfrac{1}{3}r\mathbf{a}_0, \tag{10}$$

where $\mathbf{a}_0$ and $r\mathbf{a}_0$ are a pair of primitive generators of H, r being a 120° rotation. For each such $\mathbf{h} \in P_0$, there is a staggered stacking vector $\mathbf{c} + \mathbf{h}$ among the primitive generators of L, which establishes our claim in §II.

To establish (10), note first that if $\mathbf{v}$ is any vector of L with vertical and horizontal components $\mathbf{c}$ and $\mathbf{h}$, then threefold symmetry requires H to contain

$$\mathbf{a} = (1 - r)\mathbf{v} = (1 - r)\mathbf{h}. \tag{11}$$

H also contains

$$(1 - r^2)\mathbf{a} = (1 - r^2)(1 - r)\mathbf{h} = 3\mathbf{h}, \tag{12}$$

the last identity following from the fact that $1 + r + r^2 = 0$ in the plane. Thus, vectors in P that differ by multiples of $3\mathbf{h}$ are equivalent modulo H, as are vectors in P related by a 120° rotation. Consequently, P_0 consists of the integral linear combinations with coefficients 1, 0 and -1 of a finite number of incommensurate vectors $\mathbf{h}_1, \ldots, \mathbf{h}_j$.

According to (12), any of these generators of P_0 has the form

$$\mathbf{h} = \tfrac{1}{3}(\mathbf{a} - r^2\mathbf{a}) = \tfrac{2}{3}\mathbf{a} + \tfrac{1}{3}(r\mathbf{a}). \tag{13}$$

If $\mathbf{a}$ and $r\mathbf{a}$ are among the primitive generating vectors of H, then $\mathbf{h}$ has indeed the desired form (10). If $\mathbf{a}$ and $r\mathbf{a}$ are not among the primitive generators of H, then we can express them as integral linear combinations of a pair of primitive generating vectors, $\mathbf{a}_0$ and $r\mathbf{a}_0$:*

$$\begin{aligned} \mathbf{a} &= l\mathbf{a}_0 + m(r\mathbf{a}_0), \\ r\mathbf{a} &= -m\mathbf{a}_0 + (l - m)(r\mathbf{a}_0). \end{aligned} \tag{14}$$

In terms of the primitive generating vectors

$$\mathbf{h} = [(2l - m)/3]\mathbf{a}_0 + [(l + m)/3](r\mathbf{a}_0) = p\mathbf{a}_0 + q(r\mathbf{a}_0). \tag{15}$$

Since $p + q$ is an integer, while p and q themselves are not (since $\mathbf{h}$ is not in H), there must be integers j and k such that

$$p = j \pm \tfrac{1}{3}, \quad q = k \mp \tfrac{1}{3}, \tag{16}$$

so that modulo H we can take $\mathbf{h}$ to be

$$\mathbf{h} = -\tfrac{1}{3}\mathbf{a}_0 + \tfrac{1}{3}r\mathbf{a}_0. \tag{17}$$

If we shift this by $\mathbf{a}_0$, we arrive at the desired form (10).

* We find $\mathbf{a}_0$ and $r\mathbf{a}_0$ by examining the rank-2 sublattice of all points in H that are *rational* linear combinations of $\mathbf{a}$ and $r\mathbf{a}$, as we did in §*B* above.

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