HENSEL, F., JUENGST, S., NOLL, F. & WINTER, R. (1985). In *Localization and Metal-Insulator Transitions*, edited by D. ADLER & H. FRITZSCHE. New York: Plenum.
MCLANE, V., DUNFORD, C. L. & ROSE, P. F. (1988). *Neutron Cross Sections*, Vol. 2. London: Academic Press.
MARCH, N. H. (1989). *Phys. Chem. Liq.* **20**, 241-245.
PAALMAN, H. H. & PINGS, C. J. (1962). *J. Appl. Phys.* **33**, 2635-2639.
PETRILLO, C. & SACCHETTI, F. (1990). *Acta Cryst.* A**46**, 440-449.
SOPER, A. K. & EGELSTAFF, P. A. (1980). *Nucl. Instrum. Methods*, **178**, 415-425.
WINTER, R. & BODENSTEINER, T. (1988). *High Press. Res.* **1**, 23-37.
WINTER, R., HENSEL, F., BODENSTEINER, T. & GLASER, W. (1987). *Ber. Bunsenges. Phys. Chem.* **91**, 1327-1330.
ZIMAN, J. M. (1982). *Models of Disorder.* Cambridge Univ. Press.

Acta Cryst. (1992). A**48**, 515-532

Bravais Classes for the Simplest Incommensurate Crystal Phases

BY N. DAVID MERMIN AND RON LIFSHITZ

Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY 14853-2501, *USA*

(*Received* 19 *September* 1991; *accepted* 10 *January* 1992)

Abstract

Through the reformulation of crystallography that treats periodic and quasiperiodic structures on an equal footing in three-dimensional Fourier space, a novel computation is given of the Bravais classes for the simplest kinds of incommensurately modulated crystals: (3+3) Bravais classes in the cubic system and (3+1) Bravais classes in any of the other six crystal systems. The contents of a Bravais class are taken to be sets of ordinary three-dimensional wave vectors inferred from a diffraction pattern. Because no finer distinctions are made based on the intensities of the associated Bragg peaks, a significantly simpler set of Bravais classes is found than Janner, Janssen & de Wolff [*Acta Cryst.* (1983). A**39**, 658-666] find by defining their Bravais classes in higher-dimensional superspace. In our scheme, the Janner, Janssen & de Wolff categories appear as different ways to describe identical sets of three-dimensional wave vectors when those sets contain crystallographic (3+0) sublattices belonging to more than a single crystallographic Bravais class. While such further discriminations are important to make when the diffraction pattern is well described by a strong lattice of main reflections and weaker satellite peaks, by not making them at the fundamental level of the Bravais class, the crystallographic description of all quasiperiodic materials is placed on a single unified foundation.

I. Introduction

Two approaches have been proposed for extending to quasiperiodic structures the conventional crystallographic description of periodic materials. The older superspace approach* retains the fundamental role of periodicity. By regarding quasiperiodic structures as three-dimensional sections of structures periodic in a higher $(3+d)$-dimensional space, it extracts their classification scheme by examining the ordinary crystallographic categories of periodic structures in $(3+d)$ dimensions. The second approach,† developed more recently in response to the discovery of icosahedral and decagonal quasicrystals, abandons the traditional reliance on periodicity and reformulates ordinary crystallography in three dimensions in a way that embraces quasiperiodic materials from the start.

In the three-dimensional approach which dethrones periodicity, a unified crystallography of periodic and quasiperiodic materials emerges as a symmetry-based classification scheme for diffraction patterns consisting of sharp Bragg peaks.‡ When those diffraction patterns can be indexed by three integers, the general scheme reduces to the ordinary crystallographic space-group classification of periodic structures; but the same three-dimensional scheme works just as well for the diffraction patterns

* Our results here bear most directly on the formulations given in de Wolff, Janssen & Janner (1981) and Janner, Janssen & de Wolff (1983). For a recent review see Janner (1991).

† For recent reviews see Rabson, Mermin, Rokhsar & Wright (1991) and Mermin (1992).

‡ The advantages of working in Fourier space even in the periodic case were first emphasized by Bienenstock & Ewald (1962), but it is only in the last dozen years, with the great interest in incommensurately modulated crystals and quasicrystals, that the need has become acute for such a radical reformulation of the foundations of crystallography.

0108-7673/92/040515-18\$06.00

of quasiperiodic structures, which require $3+d$ integers for their indexing.*

In this paper, using the three-dimensional approach, we define and compute the simplest Bravais classes for incommensurately modulated crystals: all $(3+3)$ Bravais classes for cubic crystals and all $(3+1)$ Bravais classes for any of the other crystal systems. In the early 1980's, Janner, Janssen and de Wolff (henceforth JJdW), using the superspace approach, gave the catalogues of $(3+1)$ Bravais classes and space groups and $(3+3)$ cubic Bravais classes, which are now widely used to characterize the structures of incommensurately modulated crystals.† We believe that our approach in three-dimensional Fourier space provides a more direct and intuitive route to such a classification scheme. Furthermore, the scheme that emerges from the three-dimensional approach differs significantly from that of JJdW. In particular, we find a substantially smaller number of distinct Bravais classes and, of course, a corresponding reduction in the number of distinct space groups.‡

There is a simple reason for this difference. We take the view that a Bravais class should characterize only the set of three-dimensional wave vectors determined by a diffraction pattern, without regard to intensities of the associated peaks. The JJdW scheme, on the other hand, assigns one and the same set of three-dimensional wave vectors to more than a single Bravais class, whenever that set contains subsets that are ordinary $(3+0)$-dimensional reciprocal lattices belonging to more than one ordinary crystallographic $(3+0)$ Bravais class.¶ The consequences of these different definitions of Bravais class will emerge in the analysis that follows. We defer a general discussion of their comparative merits to § V.

Our disagreement with JJdW is substantial. Where they give 24 $(3+1)$ Bravais classes categorizing the ways of adding a one-dimensional incommensurate modulation to the 11 non-cubic crystallographic Bravais classes, we find only 16,* all but two of which are trivial (in a sense to be made precise below) extensions of crystallographic Bravais classes. Where they give 14 $(3+3)$ cubic Bravais classes, we find only 9,† all but three of which are trivial extensions of the crystallographic Bravais classes.

In § II we give our definition in three-dimensional Fourier space of a $(3+d)$ Bravais class, noting the single respect in which it is not equivalent to that of JJdW. In § III we derive the 16 $(3+1)$ monoclinic, triclinic, orthorhombic, tetragonal, trigonal and hexagonal Bravais classes and the 9 $(3+3)$ cubic Bravais classes. In § IV we describe how the sets of three-dimensional wave vectors in some of our Bravais classes can be represented in more than one way as a lattice of main reflections and a set of satellites. It is these alternative ways of characterizing such Bravais classes, based not on symmetry but on the relative intensity of the reflections in different orbits of the point group, that leads single Bravais classes emerging from our computation to be listed under more than one heading in the Bravais-class catalog of JJdW. We list our Bravais classes in Tables 1 and 2, and give their relationship to those of JJdW. In § V we discuss why we believe our definition of a $(3+d)$ Bravais class is preferable to that of JJdW as the basis for a unified crystallographic treatment of periodic and quasiperiodic materials.

One can acquire a good sense of our general approach and how it differs from that of JJdW by following only the analysis of the $(3+3)$ cubic Bravais classes (§§ III*A*, III*C* and IV*D*) and skipping the discussions of the other six crystal systems.

II. Preliminary definitions and remarks

Our formulation of crystallography in three-dimensional Fourier space, like the superspace approach, applies to all materials whose diffraction patterns can be described in terms of a set of sharp Bragg peaks – *i.e.* to periodic or quasiperiodic materials. The fundamental concept in our formulation is a set L of three-dimensional wave vectors

* When the point group of the diffraction pattern is one of the crystallographic point groups, we call such quasiperiodic materials incommensurately modulated crystals; when the point group is not crystallographic, we call them quasicrystals if they can be indexed with the minimum number of indices compatible with the point group and, more generally, incommensurately modulated quasicrystals when their indexing is not minimal. See Rokhsar, Mermin & Wright (1987).

† See especially de Wolff, Janssen & Janner (1981), Janner, Janssen & de Wolff (1983) and Yamamoto, Janssen, Janner & de Wolff (1985).

‡ In this paper we examine only the simplest $(3+d)$ Bravais classes. In subsequent papers we derive the space groups associated with these Bravais classes (Lifshitz & Mermin, 1992) and re-examine the broader category of Bravais classes that JJdW call EBC's (elementary Bravais classes) (Mermin & Lifshitz, 1992).

¶ When we wish to emphasize that we are speaking of an ordinary crystallographic reciprocal lattice or Bravais class we characterize it as a $(3+0)$ lattice or Bravais class.

* Grebille, Weigel, Veysseyre & Phan (1990) have noted the corresponding reduction of the 24 JJdW $(3+1)$ Bravais classes to 16 crystallographic four-dimensional Bravais classes, and their Table 3 identifies the same pairs of JJdW classes as our Table 1. We stress, however, that our point is not the redundancy of the JJdW scheme in terms of the Bravais classes of ordinary $(3+d)$-dimensional crystallography. T. Janssen (private communication) has informed us that he and his collaborators have long been aware of this four-dimensional aspect of the redundancy and dismiss it as irrelevant. So do we. Our point is that identical sets of three-dimensional wave vectors are often associated with more than a single JJdW Bravais class; the JJdW Bravais-class assignments are therefore not entirely determined by the locations of the Bragg peaks in ordinary three-dimensional Fourier space.

† We are unaware of anyone having made the analogous (and from our point of view irrelevant) observation in terms of six-dimensional crystallographic Bravais classes.

which is a simple extension of the set of wave vectors that the familiar Laue rules associate with each of the experimentally observed Bragg peaks. We define L to be the set of all integral linear combinations of wave vectors determined by the Bragg peaks.* We are interested in sets L whose three-dimensional vectors can be represented as integral linear combinations of no fewer than $(3+d)$ generating vectors which are linearly independent over the integers. When $d=0$ we have an ordinary crystallographic reciprocal lattice. For quasiperiodic structures d is 1 or greater, and we refer to such a set of three-dimensional wave vectors as a $(3+d)$ lattice [or a lattice of rank $(3+d)$].†

Two remarks about nomenclature:

1. We call the set L of three vectors a 'lattice' because it is the obvious generalization to quasiperiodic materials of the crystallographic reciprocal lattice. In the quasiperiodic case there is no dual direct lattice of translations in real three-dimensional space, and therefore no ambiguity arises from omitting the adjective 'reciprocal'. When we wish to emphasize that the lattice L is in Fourier space we may refer to it as a reciprocal lattice, but we stress that only in the $(3+0)$ case is L dual to a lattice of translations in three-dimensional space.

2. Janner (1991) uses the term 'Z module' for what we would call the lattice, reserving the term lattice for a sublattice of L that is an ordinary crystallographic $(3+0)$ lattice. We do not follow this practice for two reasons. (a) When L contains among its points crystallographic $(3+0)$ lattices from more than one type of $(3+0)$ Bravais class, to single out one for special treatment as 'the lattice' would introduce a distinction between vectors of L that is artificial from the point of view of symmetry, and potentially misleading.‡ When we do wish to single out a particular $(3+0)$ sublattice of L we shall follow JJdW in referring to the sublattice as a 'lattice of main reflections'. (b) In the case of quasicrystals there is no $(3+0)$ lattice at all with the full point-group symmetry and the role played by the crystallographic reciprocal lattice in physical applications is played only by the full set of wave vectors determined by the diffraction pattern. It strikes us as absurd to impose on physicists a nomenclature in which, for example, they would have to describe *umklapp* processes in quasicrystals as those in which the total wave vector is only conserved modulo a vector from the Z module.

The point group G of a $(3+d)$ lattice is the subgroup of $O(3)$ that leaves the lattice invariant. Some lattices are also invariant under certain changes of scale. The only cases we are aware of are quasicrystallographic lattices, in which a non-crystallographic point group G imposes special relations on some of the incommensurate length ratios that characterize the generating vectors. Since we only consider here crystallographic point groups G we shall not assume special ratios between any incommensurate lengths and shall only consider lattices that are not invariant under rescalings.

Our classification scheme rests on the following definition of Bravais class: (a) The Bravais class of a material is entirely determined by the set of three-dimensional wave vectors L; the relative intensities of the Bragg peaks associated with the wave vectors giving rise to L are irrelevant for this purpose. (b) Two $(3+d)$ lattices L with point group G are in the same Bravais class if there is a sequence of $(3+d)$ lattices with point group G that interpolates between them. We shall refer to any particular lattice in a given Bravais class as a 'representative' of that class.

Several comments are required:

1. By an interpolating sequence, we mean a sequence whose adjacent members can be taken as close together as one pleases. There are two technical reasons why we cannot simply interpolate *via* a continuous family of lattices: (i) Isolated members of a continuous family of lattices might necessarily be more symmetric. In the crystallographic case, for example, it may be impossible continuously to deform one rhombohedral $(3+0)$ lattice into another while retaining rhombohedral symmetry without momentarily passing through at least one intermediate cubic lattice. (ii) As one continuously deforms one lattice in a $(3+d)$ Bravais class into another, one will in general be unable to avoid passing through intermediate lattices where certain irrational ratios happen to be rational. Such intermediate lattices will have smaller values of d. An interpolating sequence, however, can avoid the rational values.*

2. Worries about how properly to define proximity of members of the interpolating sequence in view of the fact that no lattice vector of an incommensurately

* Alternatively (and equivalently), L can be viewed as the smallest set of vectors which is closed under subtraction (and hence addition) which contains all the wave vectors determined by the diffraction pattern.

† When d is not zero any wave vector in the lattice will have other wave vectors arbitrarily close to it; this does not mean that measured diffraction patterns can display this property, but merely that for an ideal material more and more peaks will be revealed as the experimental resolution improves. This presents no more of a practical problem for the determination of the lattice than does the fact that only a finite number of peaks are observed in diffraction measurements of ordinary crystals. In both cases it is necessary to determine only a finite number of wave vectors (at least $d+3$, of course) to determine the entire infinite lattice L.

‡ It is precisely the fact that a given $(3+d)$ lattice can, in general, have $(3+0)$ sublattices from more than a single $(3+0)$ Bravais class that accounts for the additional Bravais classes in the JJdW catalog.

* For example, in continuously deforming the $(1+1)$ lattice of integral linear combinations of 1 and a from $a=2^{1/2}$ to $a=3^{1/2}$, one cannot avoid rational values of a, at which the $(1+1)$ lattice degenerates to a $(1+0)$ lattice. But one can connect the two values of a taking arbitrarily small steps that only land on irrational values.

modulated structure has a neighborhood free of other vectors can be circumvented by taking the lattice to be entirely specified by a finite set of integrally independent generating vectors (and an indexing convention, if the generators are not primitive), and defining proximity of lattices by the proximity of their generating vectors, as in the $(1+1)$ example described in the previous footnote.

3. Although part (b) of our definition of Bravais-class equivalence has a geometrical flavor very different from the algebraic definition of JJdW, we emphasize that it is not the source of our disagreement. Each JJdW Bravais class contains exactly the same sets of wave vectors as one of ours, so lattices in each of their Bravais classes satisfy our criterion (b). JJdW list more Bravais classes than we do only because they do not use our criterion (a): exactly the same sets of wave vectors appear in their catalogue under more than one Bravais class.* Bravais classes in the JJdW catalogue implicitly incorporate a further distinction based on Bragg peak intensities.

4. Since the Fourier expansion of the density of a material with a lattice L is given by a set of Fourier coefficients $\rho(\mathbf{k})$ which are non-zero on a set of wave vectors $\mathbf{k}$ whose integral linear combinations give L, our definition makes it possible to interpolate between any two densities in the same Bravais class without ever leaving that class. In the JJdW scheme such an interpolation must at some point cross Bravais-class boundaries, unless the scheme is restricted to a limited class of quasiperiodic densities.†

Most of the Bravais classes we shall find for the $(3+1)$ [or $(3+3)$ cubic] incommensurately modulated structures we shall characterize as 'trivial', a term we define as follows: given any two lattices of vectors in 3 dimensions, L_1 and L_2, we define their sum, L_1+L_2, to be the lattice consisting of sums of all pairs of vectors from L_1 and L_2. We say that a $(3+1)$ Bravais class with point group G is trivial, if any lattice in the class can be expressed as the sum of an ordinary $(3+0)$ crystallographic lattice with point group G, and a set of vectors that constitute a one-dimensional lattice that is independently invariant under G. Similarly, we say that the Bravais class of a cubic $(3+3)$ lattice with point group G (which in general might be the full cubic group $m3m$ or the tetrahedral group $m3$, as noted below) is trivial if it can be represented by the sum of two ordinary $(3+0)$-dimensional crystallographic lattices, each independently invariant under the full cubic group $m3m$.

The trivial Bravais classes in a given crystal system can immediately be inferred from a knowledge of the crystallographic $(3+0)$ Bravais classes. One can, for example, associate with each crystallographic trigonal, tetragonal or hexagonal Bravais class a trivial $(3+1)$ Bravais class whose lattices contain a $(3+0)$ sublattice from the crystallographic class, together with an integrally independent vector along the unique three-, four- or sixfold axis. Only two of the 16 $(3+1)$ Bravais classes in Table 1 are non-trivial: the class labeled M (in the monoclinic system) and the class labeled O (in the orthorhombic system).* The only non-trivial cubic $(3+3)$ Bravais classes are the three in Table 2 with tetrahedral symmetry.

The space groups for a trivial Bravais class turn out to be very simply related to the crystallographic space groups of the Bravais classes of its invariant sublattices.† The crystallographic classification of incommensurately modulated structures would therefore be entirely routine, were it not for the existence of non-trivial Bravais classes. In our scheme the 38 JJdW Bravais classes reduce to 25, all but five of which are trivial.

III. Computation of the Bravais classes

We derive below the $(3+1)$ [or, in the cubic case, $(3+3)$] Bravais classes for each of the seven crystal systems by examining the structure of lattices of three-dimensional wave vectors L that can be indexed by $3+d$ integrally independent vectors, and are invariant under the operations of a point group G belonging to the crystal system. For most of the seven crystal systems‡ the general strategy is as follows:

(i) We identify a particularly simple Bravais class B_P and show that any $(3+d)$ lattice L in the crystal system contains a $(3+d)$ sublattice L_P that is in B_p.§

(ii) We note that the full lattice L can be constructed by adding each of the vectors in L_P to every one of the vectors in a finite subset L_0 of L. We call L_0 the 'modular lattice' of L (adding the phrase 'modulo L_P' if we wish to be absolutely explicit because L_0 is itself closed under subtraction (and addition) if

* We show this in § IV.

† We do not address here the more difficult question of whether one can interpolate between two densities in the same Bravais class that describe impenetrable spheres at a specified set of real-space positions, within a family of such densities. We believe, however, that a fundamental classification scheme ought to be broad enough to encompass materials (for example certain liquid crystals or incommensurate modulations of a continuous electronic charge density) for which such conceivable obstructions to interpolation are irrelevant.

* A trivial $(3+1)$ Bravais class that contains crystallographic $(3+0)$ sublattices from more than a single crystallographic Bravais class can be described in a way that makes it appear non-trivial, as in seven of the eight redundant JJdW Bravais classes listed on the right of Table 1.

† We discuss this in Lifshitz & Mermin (1992).

‡ In the triclinic and (planar) monoclinic systems the symmetry is so low that a more direct approach can be taken.

§ We call the class B_P (P for primitive) because B_P contains what we shall call the $P+1$ or ($P+P$ cubic) lattices.

these operations are defined modulo the vectors of L_P.*

(iii) We note that since the sublattices L_P for different L are all in the same Bravais class, two lattices L will be in the same Bravais class if their modular lattices L_0 are in the same Bravais class - *i.e.* if there is a family of modular lattices that interpolates between them.

(iv) Because the modular lattices contain only a small number of points [at most 16 in any of the $(3+1)$ cases and 64 in the cubic $(3+3)$ case], one can catalog their Bravais classes by an exhaustive enumeration of the possibilities.

(v) For given L_P, one checks for a further (entirely routine) equivalence of Bravais classes of lattices L associated with distinct modular lattices L_0 when there are different but obviously equivalent ways to represent L in terms of an L_P and a modular L_0.

In preparation for the analysis that follows, it may help to illustrate these concepts with some familiar crystallographic examples.†

Example 1: $(3+0)$ *Bravais classes in the cubic system.* Every lattice in the cubic system contains a simple cubic sublattice L_P in the primitive (P) Bravais class. If we represent L_P as the set of vectors, all of whose Cartesian components are even integers, then the modular lattices L_0 are sets of vectors, each of whose components can be either 1 or 0 - *i.e.* the components are integers modulo 2. The cubic $(3+0)$ Bravais classes are associated with the following modular lattices L_0:

(a) *P lattice.* L_0 can contain only the vector $\mathbf{0}$, in which case we have a P lattice (with lattice constant 2). A second choice for L_0 contains all eight possible vectors, in which case we have a P lattice again (with lattice constant 1). This is an example of the routine equivalence one has to watch out for in step (v) above. The formal basis for this (informally obvious) equivalence is that one can interpolate between the lattice L with L_0 consisting of all eight vectors and the one with the L_0 containing only the $\mathbf{0}$ vector with a symmetry-preserving isotropic expansion by a factor of 2. When alternative ways arise of representing a Bravais class by a modular lattice L_0 we shall always choose the L_0 with the smallest number of vectors.‡

(b) I^* (F) *lattice.*† L_0 consists uniquely of the two vectors 000 and 111. Note that, if arithmetic is done modulo 2, these two vectors do indeed constitute a lattice, because one gets no further vectors by taking any integral linear combinations of them. Note that the modular lattice L_0 can be viewed geometrically as the conventional two-site 'basis' when one chooses to represent the I^* lattice as primitive cubic with two sites per unit cell.

(c) F^* (I) *lattice.* L_0 consists uniquely of the four vectors 000, 110, 101 and 011. Note again that this set contains all integral linear combinations (modulo 2) of its four vectors, and can be viewed geometrically as the conventional four-site 'basis' employed when one represents the F^* lattice as primitive cubic with four sites per unit cell.

Example 2: $(3+0)$ *Bravais classes in the orthorhombic system.* Every $(3+0)$ lattice in the orthorhombic system contains a simple orthorhombic sublattice L_P in the primitive (P) Bravais class. If we represent L_P as the set of vectors whose Cartesian components are even integral multiples of three unrelated lengths a, b and c, then the modular lattices L_0 contain vectors whose components are multiples of these three lengths by either 1 or 0. If we denote the vector $n_1 a\mathbf{x} + n_2 b\mathbf{y} + n_3 c\mathbf{z}$ by $n_1 n_2 n_3$ then we can describe the modular lattices L_0 associated with the four orthorhombic Bravais classes as follows:

(a) I^* (F) *and* F^* (I) *lattices.* As in the cubic case, in the I^* Bravais class L_0 can only contain the two vectors 000 and 111, and in the F^* class only the four vectors 000, 110, 101 and 011.

(b) *P lattice.* Here there are eight routinely equivalent L_0 [in the sense of step (v) above]. Taking L_0 to contain only 0 gives the P lattice with lattice constants $2a$, $2b$ and $2c$. We get the P lattice with the lattice constant along $\mathbf{x}$ reduced from $2a$ to a by taking L_0 to contain 000 and 100, and similarly for $\mathbf{y}$ and $\mathbf{z}$. We can get the P lattice with the lattice constants along both $\mathbf{y}$ and $\mathbf{z}$ reduced from $2b$ and $2c$ to b and c by taking L_0 to contain the four vectors 000, 010, 001 and 011 (with two more possibilities arising from cyclic permutations of the axes). And, finally, as in the cubic case, if we take L_0 to contain all eight points, we get back the original P lattice, uniformly scaled down by a factor of 2.

(c) *C lattice.* If the preferred direction is along $\mathbf{z}$ then the C lattice arises when L_0 contains the two vectors 000, 110 and also (contracted by a factor of

* Those with a taste for group theoretic jargon might note that if L is viewed as an Abelian group, then L_P is a subgroup and L_0 is the group of cosets L/L_P. Others (like ourselves) might feel that modular arithmetic does more to illuminate the concept of cosets than the other way around.

† These standard crystallographic facts could also, of course, be derived as special cases of our more general derivation of the $(3+d)$ Bravais classes.

‡ It may seem perverse to introduce at all this redundancy in the description of the P lattice, but it emerges naturally, as we shall see below, when we derive Bravais classes in cases where the answer is not already known.

† Since we work entirely in reciprocal space, it is awkward and, in the incommensurately modulated case, a potential source of confusion to identify a $(3+0)$ Bravais class by the direct lattice, thereby describing the lattice that is body centered in reciprocal space as an F lattice in the face-centered cubic Bravais class. We prefer to denote such lattices and Bravais classes in the cubic and orthorhombic systems by a letter indicating the centering in Fourier space. We avoid a clash with the conventional notation by affixing the usual asterisk denoting reciprocal space as a superscript.

two along **c**) when L_0 contains the four vectors 000, 110, 001 and 111. Analogous pairs of modular lattices L_0 give the centered orthorhombic lattice with the preferred direction along **x** (often called the A lattice) or **y** (B lattice).

These examples should make it clear that the method by which we shall extract the $(3+d)$ Bravais classes is nothing more than a formalization of the common practice of viewing the $(3+0)$ Bravais classes in terms of primitive lattices with or without various kinds of centerings, in which we exploit the fact that the centering points must always have a lattice structure modulo the primitive lattice that is itself invariant under the point group G.

In subsection A we examine those features of $(3+d)$ orthorhombic and cubic symmetry which lead to the primitive sublattices L_P. (We later apply minor variations of the same arguments to the remaining crystal systems.) We then extract the orthorhombic $(3+1)$ Bravais classes in subsection B, the cubic $(3+3)$ Bravais classes in subsection C, the tetragonal and axial monoclinic $(3+1)$ Bravais classes in subsection D, the hexagonal and trigonal $(3+1)$ Bravais classes in subsection E and the triclinic and planar monoclinic $(3+1)$ Bravais classes in subsection F.

The Bravais classes derived in this section are summarized in Tables 1 and 2.

A. Features common to the orthorhombic and cubic cases

Since lattices are closed under subtraction, any lattice contains the negative of each of its vectors, and the point group G of any $(3+d)$ lattice must contain the inversion i. As a result, the point group of a $(3+d)$ lattice in the orthorhombic system is necessarily the full orthorhombic group mmm; the cubic system, however, admits the possibility [not realized in the $(3+0)$ case] of $(3+d)$ lattices with either the full cubic point groups $m3m$, or the smaller tetrahedral point group $m3$ (which also contains i). Lattices with any of these three point groups will have among their point-group symmetries three mutually perpendicular axes of twofold symmetry, **a**, **b** and **c**.

Any lattice with three such axes contains the sum of any of its vectors with the image of that vector under any of the twofold rotations – *i.e.* it contains twice the projection of any of its vectors on each of the twofold axes. The subset L_c of L consisting of twice the projections on the c axis, $2P_c\mathbf{k}$, of all $\mathbf{k}$ in L is a $(1+d_c)$ lattice* and as such it can be primitively indexed by $1+d_c$ of its vectors; *i.e.* one can choose $1+d_c$ integrally independent incommensurate length scales $k_1, \ldots, k_{1+d_c}$ so that L_c consists of all integral

* For the moment we let d_c be general; we will soon specialize to the case of interest, $d_c = 1$, $d_a = d_b = 0$ (or, in the cubic case, $d_a = d_b = d_c = 1$).

Table 1. *The* 16 $(3+1)$ *Bravais classes*

The JJdW symbols and number are given in the second column and (when JJdW describe the same set of lattices of three-dimensional wave vectors as two different Bravais classes) the third. Except for the monoclinic M and orthorhombic O classes, all the Bravais classes are trivial – *i.e.* a representative lattice can be taken to be the sum of a crystallographic $(3+0)$ lattice and a one-dimensional lattice, both invariant under the point group of the Bravais class. We designate the trivial Bravais classes by a symbol of the form $X+1$, where X specifies the $(3+0)$ Bravais class of the crystallographic $(3+0)$ lattice and 1 symbolizes the invariant 1 lattice with a subscript specifying its orientation (along **c** or in the ab plane) in the one (monoclinic) case where relevant orientation is not determined by the point group. The redundant JJdW symbols (in braces) disguise the triviality of the lattices in the $(3+1)$ Bravais classes by focusing on an alternative class of $(3+0)$ sublattices; lattices in the $(3+1)$ Bravais class are not simply sums of the alternative sublattices with an invariant one-dimensional lattice, as revealed by the non-zero 'rational parts' in the star-generating vectors given on the right side of the JJdW symbols. The two non-trivial Bravais classes are both represented by the modular lattice [0000 1010 0101 1111] given in (6) – *i.e.* their diffraction patterns can be indexed as all integral linear combinations $n_1\mathbf{a}+n_2\mathbf{b}+n_3k\mathbf{c}+n_4k'\mathbf{c}$ in which n_1 and n_3 have the same parity, as do n_2 and n_4. The same merging of JJdW $(3+1)$ Bravais classes, when viewed as Bravais classes of ordinary four-dimensional crystallography, has been noted in Table 3 of Grebille, Weigel, Veysseyre & Phan (1990), but they do not discuss the significance of the identification in three dimensions or note the triviality of all but two of the resulting Bravais classes.

Triclinic				
$P+1$	$P(\alpha\beta\gamma)$	1		
Monoclinic				
$P+1_{ab}$	$P2/m(\alpha\beta0)$	2		
$C+1_{ab}$	$B2/m(\alpha\beta0)$	4	$P2/m(\alpha\beta\frac{1}{2})$	3
$P+1_c$	$P2/m(00\gamma)$	5		
$C+1_c$	$B2/m(00\gamma)$	7	$P2/m(\frac{1}{2}0\gamma)$	6
M	$B2/m(0\frac{1}{2}\gamma)$	8		
Orthorhombic				
$P+1$	$Pmmm(00\gamma)$	9		
I^*+1	$Fmmm(00\gamma)$	17	$Pmmm(\frac{1}{2}\frac{1}{2}\gamma)$	11
F^*+1	$Immm(00\gamma)$	12	$Cmmm(10\gamma)$	14
$C+1$	$Cmmm(00\gamma)$	13		
$A+1$	$Ammm(00\gamma)$	15	$Pmmm(0\frac{1}{2}\gamma)$	10
O	$Ammm(\frac{1}{2}0\gamma)$	16	$Fmmm(10\gamma)$	18
Tetragonal				
$P+1$	$P4/mmm(00\gamma)$	19		
$I+1$	$I4/mmm(00\gamma)$	21	$P4/mmm(\frac{1}{2}\frac{1}{2}\gamma)$	20
Trigonal				
$R+1$	$R\bar{3}m(00\gamma)$	22	$P\bar{3}1m(\frac{1}{3}\frac{1}{3}\gamma)$	23
Hexagonal				
$P+1$	$P6/mmm(00\gamma)$	24		

Table 2. *The nine* $(3+3)$ *Bravais classes with point groups in the cubic system*

The first six have full cubic symmetry; the last three only tetrahedral symmetry. All the Bravais classes with full cubic symmetry are trivial sums of $(3+0)$ cubic Bravais classes, which we designate as $X+Y$, where X and Y specify the two $(3+0)$ Bravais classes. The JJdW symbols and numbers are given in the second column and (when a Bravais class occurs under more than one name in their catalog) in the third and fourth. (We enclose the redundant JJdW symbols in braces.) The only non-trivial Bravais classes are the three with the tetrahedral point group $m3$ (though the triviality of the full cubic Bravais class I^*+F^* is obscured when it is described by the JJdW symbol in the fourth column). The non-trivial Bravais class T_0 is represented by the modular lattice $L_0=$ [000, 000 110, 011 011, 101 101, 110], the class T_1 by the sum L_0+[000, 000 111, 000] and the class T_2 by the sum L_0+[000, 000 111, 000 000, 111 111, 111].

Cubic							
$P+P$	**17**	$Pm3m(\alpha 00)$	**208**				
I^*+I^*	**18**	$Fm3m(\alpha\alpha\alpha)$	**217**				
F^*+F^*	**19**	$Im3m(0\beta\beta)$	**213**				
$P+I^*=I^*+P$	**20**	$Pm3m(\alpha\alpha\alpha)$	**215**	{ $Fm3m(\alpha 00)$	**211** }		
$P+F^*=F^*+P$	**21**	$Pm3m(0\beta\beta)$	**212**	{ $Im3m(\alpha 00)$	**210** }		
$I^*+F^*=F^*+I^*$	**22**	$Im3m(\alpha\alpha\alpha)$	**216**	{ $Fm3m(0\beta\beta)$	**214** }	{ $Pm3m(\alpha\frac{1}{2}\frac{1}{2})$	**209** }
Tetrahedral							
T_0	**23**	$Pm3(\frac{1}{2}\beta\beta+\frac{1}{2})$	**206**				
$T_1=T_0+I^*$	**24**	$Fm3(1\beta\beta+1)$	**207**	{ $Pm3(\alpha\frac{1}{2}0)$	**204** }		
$T_2=T_0+I^*+I^*$	**25**	$Fm3(\alpha 10)$	**205**				

linear combinations of the vectors $k_1\mathbf{c}, \ldots, k_{1+d_c}\mathbf{c}$. Similar remarks hold for L_a and L_b, with $d=d_a+d_b+d_c$.

The fact that the indexing can be taken to be primitive is a special case of the fact that any vector space over the integers of dimension $1+d_c$ can be expressed as the set of all integral linear combinations of a suitably chosen basis of $1+d_c$ vectors. Note that two lattices that differ only in the values of the mutually incommensurate length scales $k_1, \ldots, k_{1+d_c}$ that characterize the primitive basis for the sublattice L_c (and similarly for L_a and L_b) are in the same Bravais class (for essentially the same reasons that any two triclinic three lattices are in the same class).*

Because twice the projection of any vector in L on the axes $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ is in the sublattices L_a, L_b and L_c, it follows that any vector of L can be expressed as an integral or half-integral linear combination of the vectors $k_1\mathbf{c}, \ldots, k_{1+d_c}\mathbf{c}$ and the analogous two sets for the axes $\mathbf{a}$ and $\mathbf{b}$, and that all integral (but not necessarily all half-integral) linear combinations are present. It is convenient to restate this conclusion in the form it assumes when the axes are rescaled by a factor of 2:

* In the cubic (as opposed to the orthorhombic) case, one can and should always associate the same set of length scales with each of the three sublattices L_a, L_b and L_c.

Any cubic or orthorhombic $(3+d)$ lattice can be expressed as a set of integral linear combinations of integrally independent vectors along three orthogonal directions, with an even sublattice* L_P that is primitively generated. Note that this generalizes to the $(3+d)$ case the form of L_P we described in the crystallographic examples above, and explains why L_P arises naturally with even indexing.

The cubic and orthorhombic $(3+d)$ lattices can therefore be viewed as the translations through all vectors of the primitive even sublattice L_P of the set L_0 of vectors indexed only by 0's or 1's. The modular lattice L_0 is closed under subtraction when arithmetic is performed on its components modulo 2, as an immediate consequence of the closure of the full lattice L under ordinary subtraction. Since the sublattices L_P of any two lattices L with the same G and same d_a, d_b and d_c are clearly in the same Bravais class, classifying distinct lattices L by Bravais class, reduces to classifying the distinct modular lattices L_0. The modular lattices inherit from the full lattice L the property that they belong to the same Bravais class if they differ only in the choice of primitive vectors along the axes.

At this point we specialize to the cases of orthorhombic $(3+1)$ and cubic $(3+3)$ lattices.

* By the even sublattice, we mean the sublattice of vectors all of whose indices are even.

B. The orthorhombic case

We take the two incommensurate length scales k and k', in terms of which the even sublattice is primitively generated, to be associated with the axis **c**, and index the projections of lattice vectors along the c axis by $n_3k+n'_3k'$. Note that two lattices L (or two modular lattices L_0) that differ only in the interchange of n_3 and n'_3 for all their vectors belong to the same Bravais class, since this merely corresponds to interchanging the roles of $2k$ and $2k'$ as primitive generators of L_c.* More generally, a new Bravais class does not result from a transformation of all the n_3 and n'_3 induced by a replacement of $2k$ and $2k'$ by any of their linear combinations with integral coefficients that continue to generate L_c primitively, since this merely changes the basis in terms of which the lattice L is described, or interchanges two lattices within the same Bravais class. The effect of such a linear transformation on vectors of the modular lattice L_0 is either to interchange n_3 with n'_3, to replace either n_3 or n'_3 with $n_3+n'_3$ (keeping the other index unchanged), or to combine the interchange and the replacement. Thus the Bravais class is unchanged by subjecting the two indices n_3 and n'_3 of every vector in the modular lattice to any of the transformations:

$$n_3, n'_3 \quad\rightarrow\quad \begin{array}{l} n_3,\ n_3+n'_3 \\ n_3+n'_3,\ n'_3 \\ n'_3,\ n_3 \\ n_3+n'_3,\ n_3 \\ n'_3,\ n_3+n'_3. \end{array} \tag{1}$$

We use the term 'reindexing' to refer to this freedom to replace the indices specifying L_0 by any of these linear combinations, without altering the Bravais class. If two $(3+1)$ orthorhombic Bravais classes are characterized by modular lattices L_0 that differ only by a reindexing transformation, then the two classes contain identical sets of lattices and must be identified, unless one discriminates between Bravais classes by means of peak intensities as well as peak locations. Keeping these reindexing transformations in mind, we now enumerate the distinct modular lattices L_0 and hence the distinct Bravais classes of orthorhombic $(3+1)$ lattices.

Evidently there are five trivial orthorhombic $3+1$ Bravais classes, associated with the four ordinary orthorhombic $(3+0)$ Bravais classes. [The centered orthorhombic $(3+0)$ class gives rise to two $(3+1)$ classes, since it alone has a preferred direction among **a**, **b** and **c**, which can either be along (C lattice) or orthogonal to (A or B lattice) the direction of the incommensurate modulation.] We call these lattices $P+1$, F^*+1 (or $I+1$), I^*+1 (or $F+1$), $C+1$ and $A+1$ (or $B+1$).† We now show that in addition there is just a single non-trivial Bravais class of orthorhombic $(3+1)$ lattices.‡

Note that a lattice L belongs to a trivial Bravais class if and only if the associated modular lattice L_0 does. A Bravais class of modular lattices is trivial if and only if it contains lattices L_0 in which all vectors are of the form

$$n_1n_2n_3 0, \tag{2}$$

or in which every vector appears as a member of a pair of vectors differing only in their fourth components,§ so that L_0 is the sum of a lattice of the form (2) with the lattice [0000 0001].

It is convenient¶ to separate out the two-dimensional sublattice L_0^{ab} of L_0 spanned by **a** and **b**, which contains all modulo 2 vectors of the form $n_1n_2 00$. Because we are doing arithmetic modulo 2, there are just five possibilities†† for L_0^{ab}:

$$\begin{array}{c} [0000]; \qquad [0000\ 1000]; \\ [0000\ 0100]; \qquad [0000\ 1100]; \\ [0000\ 1000\ 0100\ 1100]. \end{array} \tag{3}$$

Consider next the set of vectors in L_0 whose third and fourth components are 1, 0. Because L_0 is a lattice, one easily establishes that if this set is not empty, it is given by adding to every vector in L_0^{ab} a vector of the form $n'_1n'_2 10$, where $n'_1n'_2 00$ (which is only determined to within an additive vector from L_0^{ab}) can be taken to be either 0000 or a vector not in L_0^{ab}. In the same way, if L_0 contains any vectors whose third and fourth components are 0, 1, then the set of them is just L_0^{ab} shifted by a vector $n''_1n''_2 01$, and those, if any, with third and fourth components 1, 1 are L_0^{ab} shifted by a vector $n'''_1n'''_2 11$. If two of the types are present then the third (which contains their sums) must also be. If all three types are present then

* JJdW do not make such an identification of Bravais classes. If the Bravais class is determined entirely by the lattice of wave vectors, however, the identification is unavoidable, since one can interpolate through incommensurate pairs of scales between the pair k, k' and the pair k', k, without changing the symmetry or rank of L.

† As noted earlier, the asterisk (*) is to emphasize that the centering is specified in Fourier space.

‡ JJdW list ten Bravais classes of orthorhombic $(3+1)$ lattices instead of our six. In § IV we show that four pairs of their Bravais classes contain identical lattices of wave vectors, and that each of their ten Bravais classes contains the same set of lattices as one of our six.

§ The second case can be converted back to the first case by rescaling the c axis by a factor of 2.

¶ From this point on the analysis makes no further use of the orthogonality of the axes **a** and **b** and therefore, as we shall note in subsection D, applies equally well to the axial monoclinic case.

†† We specify the vector $n_1\mathbf{a}+n_2\mathbf{b}+n_3k\mathbf{c}+n'_3k'\mathbf{c}$ by listing $n_1n_2n_3n'_3$, which we separate by commas only when it would be confusing not to do so. When we wish to emphasize that a set of vectors constitutes a modular lattice we enclose the set in square brackets.

we can pick the shift vectors to satisfy

$$n_1'n_2'10+n_1''n_2''01 \equiv_2 n_1'''n_2'''11, \tag{4}$$

where $\equiv_2$ indicates equality modulo 2.

The general form of L_0 is thus

(a) L_0^{ab} alone.

(b) L_0^{ab} augmented by shifting every vector in L_0^{ab} by a single vector of one of the three types

$$n_1'n_2'10 \quad n_1''n_2''01 \quad n_1'''n_2'''11, \tag{5}$$

where, because of the invariance of the Bravais class under the reindexing transformations (1), the shift can always be represented by the first type.

(c) L_0^{ab} augmented by shifting every vector in L_0^{ab} by a single vector of every one of the three types.

Cases (a) and (b) clearly yield only trivial $(3+1)$ lattices, so non-trivial $(3+1)$ lattices can be only of type (c), with the shift vectors related by (4). If n_1'' and n_2'' are zero, so that L_0^{ab} contains the vector 0001, then the $(3+1)$ lattice is again trivial. Because of reindexing equivalence, this case generates the same Bravais class as those given by choosing the primed or triple primed pair to vanish, so this leaves only the case in which the first two components of every one of the vectors (5) are not both zero, and all three pairs of components are different. The only possibility is thus $n_1'n_2'=10$, $n_1''n_2''=01$, and $n_1'''n_2'''=11$, or permutations of these assignments, which yield the same Bravais classes, since they differ only by permutations of the third and fourth components, which can be accomplished by a reindexing transformation. Since none of these three pairs of indices can be in L_0^{ab},* that lattice can contain only the point 00, and we arrive at a modular sublattice consisting of just four points:

$$L_0=[0000 \;\; 1010 \;\; 0101 \;\; 1111]. \tag{6}$$

Equation (6) specifies the modular lattice of the unique non-trivial orthorhombic $(3+1)$ Bravais class, which we call O.† Its non-triviality follows from the fact that none of the five reindexing transformations (1) performed on the last two indices of the vectors in (6) can reduce L_0 to the trivial form

$$[0000 \;\; n_1n_2n_30 \;\; 0001 \;\; n_1n_2n_31] \tag{7}$$

(or a form in which all four fourth components are 0).

C. *The cubic case*

If a lattice has cubic symmetry its point group G must contain in addition to the twofold axes **a**, **b** and **c** (now specified by vectors of the same lengths), a threefold axis, which we can take to be associated with cyclic† permutations of **a**, **b** and **c**.

Because of the threefold axis, the projections of the lattice vectors on each of the three twofold axes can be characterized by the same sets of incommensurate lengths. The simplest case is the $(3+3)$ lattice where there is a pair of such lengths, and a vector in L has the general form

$$(n_1k+n_1'k')\mathbf{a}+(n_2k+n_2'k')\mathbf{b}+(n_3k+n_3'k')\mathbf{c}, \tag{8}$$

which we shall sometimes find it more convenient to write in the alternative form

$$(n_1n_2n_3)k+(n_1'n_2'n_3')k', \tag{9}$$

or, suppressing explicit reference to the two length scales, in six-vector form

$$n_1n_2n_3,\; n_1'n_2'n_3', \tag{10}$$

or, suppressing reference to individual components, in the vector forms

$$k\mathbf{n}+k'\mathbf{n}' \tag{11}$$

or

$$\mathbf{n},\mathbf{n}'. \tag{12}$$

When it is convenient to focus on the three components rather than the two length scales, we shall use Greek letters to indicate numbers of the form $nk+n'k'$, and write vectors in L as

$$\alpha\beta\gamma;\; \alpha=n_1k+n_1'k',\; \beta=n_2k+n_2'k',\; \gamma=n_3k+n_3'k'. \tag{13}$$

Note that all of the forms (8)-(13) also describe the modular lattice, provided the n_i and n_i' are all restricted to the values 0 or 1 and vector arithmetic is performed modulo 2.

The freedom to choose a primitive basis for the $(1+1)$ sublattices on the axes now leads to the identification of Bravais classes whose modular lattices differ only by the vector generalization of the reindexing transformations (1) applied to every point:

$$\mathbf{n},\mathbf{n}' \;\rightarrow\; \begin{array}{l} \mathbf{n},\mathbf{n}+\mathbf{n}' \\ \mathbf{n}+\mathbf{n}',\mathbf{n}' \\ \mathbf{n}',\mathbf{n} \\ \mathbf{n}+\mathbf{n}',\mathbf{n} \\ \mathbf{n}',\mathbf{n}+\mathbf{n}'. \end{array} \tag{14}$$

Evidently, there are six trivial Bravais classes, given by the six distinct sums of ordinary cubic P, I^* (F)

* Recall that if a pair was in L_0^{ab} we took it to be zero.

† Its name(s) in the JJdW catalog can be found in Table 1.

† If G contains all permutations it is the full cubic $m3m$; if it contains only cyclic permutations it is the tetrahedral subgroup $m3$. As it happens, all ordinary $(3+0)$ lattices with cubic symmetry always have $G=m3m$; as JJdW have noted, some $(3+3)$ lattices may also have the lower (tetrahedral) symmetry.

or F^* (I) lattices.† We shall show that there are, in addition, just three non-trivial Bravais classes of cubic (3+3) lattices,‡§ each with the tetrahedral point group $m3$.

To extract the distinct Bravais classes of modular lattices L_0 [and hence of cubic (3+3) lattices L] we first show that any modular lattice must be a sum of a rather small number of particular modular sublattices. We then consider all the distinct classes one can arrive at by adding such sublattices.

If $\alpha\beta\gamma$ is an arbitrary vector of an arbitrary cubic (3+3) modular lattice L_0, then cubic or tetrahedral symmetry requires L_0 also to contain $\beta\gamma\alpha$ and $\gamma\alpha\beta$; because L_0 is a lattice it must, in addition, contain all possible sums¶ of these three. This leads to at most eight members of L_0, implied by the membership in L_0 of $\alpha\beta\gamma$:

$$\begin{gathered} 000;\ \alpha\beta\gamma;\ \beta\gamma\alpha;\ \gamma\alpha\beta; \\ \alpha+\beta,\ \beta+\gamma,\ \gamma+\alpha; \\ \beta+\gamma,\ \gamma+\alpha,\ \alpha+\beta; \\ \gamma+\alpha,\ \alpha+\beta,\ \beta+\gamma; \\ \alpha+\beta+\gamma,\ \alpha+\beta+\gamma,\ \alpha+\beta+\gamma. \end{gathered} \tag{15}$$

No more are implied because further modulo 2 sums of pairs of the eight reduce back to one of them, but there could be fewer, since for particular values of α, β and γ the eight vectors need not all be distinct.

We denote the modular sublattice generated in this way from a single vector $\alpha\beta\gamma$ by $\{\alpha, \beta, \gamma\}$. If there are no special relations between α, β and γ then the modular sublattice $\{\alpha, \beta, \gamma\}$ will contain eight distinct elements. It can, however, always be expressed as the sum of the two-element sublattice

$$[000;\ \alpha+\beta+\gamma,\ \alpha+\beta+\gamma,\ \alpha+\beta+\gamma] \tag{16}$$

and the four-element sublattice

$$\begin{gathered}[000;\ \alpha+\beta,\ \beta+\gamma,\ \gamma+\alpha; \\ \beta+\gamma,\ \gamma+\alpha,\ \alpha+\beta;\ \gamma+\alpha,\ \alpha+\beta,\ \beta+\gamma].\end{gathered} \tag{17}$$

The first of these is of the general form

$$\{\eta\eta\eta\} = [000 \quad \eta\eta\eta]. \tag{18}$$

The second has the general form

$$\{\varphi\psi\chi\} = [000 \quad \varphi\psi\chi \quad \psi\chi\varphi \quad \chi\varphi\psi],\ \varphi+\psi+\chi \equiv_2 0. \tag{19}$$

We have thus established that every vector in a cubic (3+3) modular lattice L_0 can be taken to be a member of a sublattice that is either of the form (18) or (19) or the sum of two such sublattices. Consequently, L_0 itself can be represented as a sum of (possibly many) sublattices of the forms (18) or (19).

These sublattices are easily enumerated. Because we work with integers modulo 2, each Greek letter can represent only one of the four numbers

$$0,\ k,\ k',\ k+k'. \tag{20}$$

There are thus just three different two-element sublattices of the form (18):

$$\{k(111)\}, \quad \{k'(111)\} \quad \text{and} \quad \{(k+k')(111)\}, \tag{21}$$

which we refer to collectively as I^* sublattices, since in the cubic (3+0) case such a modular sublattice generates a lattice that is body centered (I) in reciprocal (*) space.†

To enumerate the distinct forms of the four-element modular sublattices (19), consider first the case where at least one of φ, ψ or χ is zero. It suffices to consider only one to be zero, since if two are so is the third and the lattice degenerates to the zero lattice $\{0\}$. The two non-zero numbers must be the same (since their modulo 2 sum is zero) and there are thus just three possible modular lattices,

$$\{k(110)\}, \quad \{k'(110)\}, \quad \{(k+k')(110)\}, \tag{22}$$

which we refer to collectively as F^* sublattices [since in the cubic (3+0) case such a modular lattice generates a lattice that is face centered (F) in reciprocal (*) space.‡

† As noted in the analogous orthorhombic case, exchanging which lattice is associated with k and which with k' does not change the Bravais class. The JJdW scheme does not identify two such Bravais classes, even though they specify identical sets of lattices of three-dimensional wave vectors.

‡ Quasicrystallographers should note that the three Bravais classes that characterize icosahedral quasicrystals are examples of the three tetrahedral (3+3) lattices, with a special value $\tau = \frac{1}{2}(5^{1/2}+1)$ for the ratio k/k' that increases the symmetry from tetrahedral to icosahedral. See Rokhsar, Mermin & Wright (1987).

§ JJdW list 14 Bravais classes of cubic (3+3) lattices instead of our nine: ten with full cubic symmetry and four tetrahedral. Three of the extra cubic classes come from assigning the trivial sum $P+I^*$ of a P and I^* lattice to two different Bravais classes (and similarly for $P+F^*$ and I^*+F^*). In § IV we identify the remaining redundant cubic class and the redundant tetrahedral class.

¶ One of the conveniences of arithmetic modulo 2 is that there is no difference between sums and differences: $n \equiv_2 -n$.

† The three lattices L that have a single one of the I^* sublattices as their entire modular lattice L_0 are all related by one of the reindexing transformations (14) and therefore belong to the same Bravais class. We must nevertheless keep in mind all three forms when building up more elaborate modular lattices by adding together sublattices, since the transformation must be applied to all the vectors in a modular lattice and cannot be applied independently to each modular sublattice.

‡ The three lattices L that have a single one of the F^* sublattices as their entire modular lattice L_0 are all related by the reindexing transformations (14) and therefore belong to the same Bravais class. But as noted above for the I^* sublattices, we must keep in mind all three forms when building up more elaborate modular lattices.

To complete the enumeration of the four-element sublattices (19) it remains only to consider the case in which none of φ, ψ or χ are zero. Since we are doing integral arithmetic modulo 2, the vanishing of $\varphi+\psi+\chi$ requires each to be the sum of the other two, and therefore all three must be different if none is to be zero. Since there are only three non-zero choices, we have just two possibilities:

$$\{k, k', k+k'\} \quad \text{or} \quad \{k', k, k+k'\}. \qquad (23)$$

The two cases differ by a non-cyclic permutation of the axes **a**, **b** and **c** - *i.e.* by an operation of $m3m$ that is absent from $m3$. One easily verifies that each type is invariant under any of the reindexing transformations (14).† A modular lattice having just one of these as a sublattice will have only tetrahedral symmetry, so we call them T sublattices. Since the T sublattices are the only ones in our set of modular sublattices without full $m3m$ symmetry, two modular lattices L_0 that differ only in which of the two T lattices they have as a sublattice are related by a 90° rotation and therefore belong to the same Bravais class. We must therefore keep in mind both forms of T lattice only when both are present as sublattices of L_0.

We now enumerate the Bravais classes of the modular lattices [and hence the general cubic (3+3) Bravais classes] according to which of the I^*, T or F^* lattices they contain as sublattices.

1. If L_0 contains only 000, then the full lattice L is just the sum of two incommensurate (3+0) P lattices (each consisting of points with all even coordinates). We call this trivial Bravais class $P+P$. Note that one also gets $P+P$ (each consisting of points with all integral coordinates) when L_0 contains all $2^6=64$ possible points, as well as when L_0 contains all $2^3=8$ possible multiples of k only or k' only (or, as a consequence of reindexing, $k+k'$ only). These cases, examples of point (v) in our initial summary of the method, will emerge later on in our enumeration.

2. If L_0 contains only a single one of the I^* sublattices given in (21) (as noted above it does not then matter which), then L is just the sum of incommensurate (3+0) P and I^* lattices. The order is immaterial and we may call the resulting trivial Bravais class $P+I^*$ or I^*+P (or $P+F$ or $F+P$).

3. If L_0 contains only a single one of the F^* sublattices given in (22) (as noted above it does not matter which) then L is just the sum of incommensurate (3+0) P and F^* lattices. The order is immaterial and we may call the resulting trivial Bravais class $P+F^*$ or F^*+P (or $P+I$ or $I+P$).

4. If L_0 contains only a single T sublattice (23) (as noted above it does not matter which) then L has only tetrahedral symmetry and is a non-trivial (3+3) cubic lattice, which we call T_0.†

If a modular lattice L_0 contains both types of T sublattice then it must contain their sum, and by listing the sums of the 16 pairs of vectors from the two types one immediately establishes that L_0 must also contain all three of the F^* sublattices. In the same way, one establishes that if L_0 contains any two of the three F^* sublattices, then it must contain the third and also both T sublattices. Finally, if L_0 contains one T and one F^* sublattice it again must contain all sublattices of both types.

Thus, if L_0 contains any of the T or F^* sublattices, it contains either a single one of them, or all five. There can therefore be only one more Bravais class containing none of the I^* sublattices:

5. If L_0 is the sum of all five T and F^* sublattices then it is easily verified to be the trivial sum of two (3+0) F^* lattices, a Bravais class we call F^*+F^* (or $I+I$).

We next note that if a modular lattice L_0 does contain any of the I^* sublattices, then it contains either a single one or all three. Case 2 above took L_0 to consist of a single I^* sublattice, so there is at most one additional Bravais class containing none of the T or F^* sublattices.

6. If L_0 is the sum of all three I^* sublattices then it is easily verified to be the trivial sum of two (3+0) I^* lattices, a Bravais class we call I^*+I^* (or $F+F$).

We are left with the modular lattices that contain at least one of the I^* and at least one of the T or F^* sublattices. We first consider the result of combining just a single sublattice from each of these two groups. If we keep all five varieties of the T and F^* sublattices, then reindexing permits us to consider only a single specimen of the I^* sublattices, which we can take to be $\{k(111)\}$. As noted above, it also suffices to consider a single one of the two T sublattices, and we therefore have just four cases to examine. Combining $\{k(111)\}$ with the F^* sublattice $\{k(110)\}$ gives us just the trivial $P+P$ lattice again (this time in a version in which the k sublattice has all integral coordinates and the k' sublattice only even coordinates). Combining $\{k(111)\}$ with the F^* sublattice $\{(k+k')(110)\}$ gives us back $P+F^*$ (in the version in which P occurs with all integral coordinates). The remaining two possibilities give us something new.

† The non-zero vectors of the first type, for example, are $k(101)+k'(011)$, $k(110)+k'(101)$ and $k(011)+k'(110)$. Any of the reindexing transformations applied to all three simply permutes them.

† The non-triviality of T_0 follows from the fact that if it were the sum of two (3+0) lattices with full cubic symmetry it would have to have full cubic symmetry itself, since all four threefold axes would have to coincide to maintain the tetrahedral symmetry. It can, however, be viewed as a sum of two rhombohedral (3+0) lattices, with lattice constants and angles cunningly adjusted to give the larger tetrahedral symmetry group to the sum. This view of the T_0 lattice (and the other two tetrahedral lattices that emerge below) has been exploited to construct a very simple computation of the icosahedral space groups (Mermin, 1992), and is similarly well suited for computing the (3+3) cubic space groups on the three tetrahedral lattices. (See Lifshitz & Mermin, 1992.)

7. Combining $\{k(111)\}$ with the F^* sublattice $\{k'(110)\}$ gives us the trivial sum of $(3+0)$ I^* and F^* lattices, a Bravais class we call I^*+F^* or F^*+I^* (or $F+I$ or $I+F$).

8. Combining $\{k(111)\}$ with the T sublattice $\{(k, k', k+k')\}$ gives us a second non-trivial lattice with tetrahedral symmetry, which we call T_1.†

There remain only modular lattices that contain either all three of the I^* sublattices (*i.e.* that contain I^*+I^*) or all five of the T or F^* sublattices (*i.e.* that contain F^*+F^*). (If all three I^* and all five T or F^* sublattices are present, then L_0 contains all 64 points and we have $P+P$ again.) Since either of the modular sublattices I^*+I^* or F^*+F^* is invariant under the reindexing transformations (14), it is sufficient to consider combining F^*+F^* with just a single specimen of the I^* sublattice, and I^*+I^* with just a single specimen of the F^* or T sublattices. But combining F^*+F^* with the I^* sublattice $\{k(111)\}$ just gives another version of $P+F^*$, and combining I^*+I^* with the F^* sublattice $\{k(110)\}$ just gives $P+I^*$, so there is only one additional case.

9. Combining I^*+I^* with the T sublattice $\{(k, k', k+k')\}$ gives us a third non-trivial tetrahedral lattice which we call T_2.‡

This completes the enumeration of the nine cubic Bravais classes.

D. *The tetragonal and axial monoclinic cases*

Tetragonal $(3+1)$ lattices must have the unique incommensurate direction along the fourfold c axis, since otherwise the fourfold symmetry would require a $(3+d)$ lattice with $d>1$. Monoclinic lattices, on the other hand, have point group $G=2/m$, and can therefore have a unique direction either along or perpendicular to the twofold c axis. Monoclinic $(3+1)$ lattices with the unique direction along $\mathbf{c}$ (axial monoclinic) and all tetragonal $(3+1)$ lattices can be classified by essentially the same analysis we used in the orthorhombic case, once one notes the following.

As in the orthorhombic and cubic cases, twice the projection of any vector of L along the c axis is itself in L. Therefore, as argued in subsection A above, the set of projections of all vectors along that axis can be expressed as a set of linear combinations of two vectors $k\mathbf{c}$ and $k'\mathbf{c}$ with an even sublattice that is primitively indexed. Furthermore, since all lattices have inversion symmetry, the plane perpendicular to the c axis is a mirror plane, and therefore L contains twice the projection of any of its vectors in that plane. Since $2P_\perp L$ is itself a two-dimensional lattice (with fourfold symmetry in the tetragonal case and only the minimum twofold symmetry in the monoclinic case), it can always be primitively indexed in terms of two vectors $\mathbf{a}$ and $\mathbf{b}$ (which are orthonormal in the tetragonal case and arbitrary in the monoclinic case). We can again scale those lattices so that $P_\perp L$ can be indexed by integral linear combinations of $\mathbf{a}$ and $\mathbf{b}$ in such a way that the even sublattice is primitively indexed. We are thus back to a study of the modular lattices L_0 with integral coordinates taken modulo 2.

The analysis of the modular sublattices in the axial monoclinic case is identical to our analysis of the orthorhombic case in subsection B above. We conclude that aside from the two trivial lattices - sums of either the monoclinic P (to which orthorhombic P or C degenerate) or monoclinic C lattices (to which orthorhombic I^* or F^* degenerate) with incommensurate one-dimensional lattices along $\mathbf{c}$ - there is a third non-trivial lattice whose modular lattice L_0 is given by (6).† We call the trivial lattices‡ $P+1_c$ and $C+1_c$ and the non-trivial lattice M.

In the tetragonal case the analysis is again identical to that for the orthorhombic case, except that we must additionally impose fourfold symmetry in the plane perpendicular to $\mathbf{c}$, which restricts us to modular lattices that contain $n_2n_1n_3n_3'$ whenever they contain $n_1n_2n_3n_3'$. The non-trivial lattice (6) does not satisfy this condition, and is therefore excluded. The only tetragonal $(3+1)$ lattices are thus the two trivial extensions of the P and I $(3+0)$ lattices,§ which we call $P+1$ and $I+1$.

E. *The trigonal and hexagonal cases*

We can discuss together the trigonal and hexagonal $(3+1)$ Bravais classes as classes of lattices L with point groups having a threefold axis which may or may not also be sixfold, taken to be along $\mathbf{c}$. If $d=1$ the modulation can only be along the threefold axis. The threefold symmetry also requires L to contain three times the projection of any of its vectors along the threefold axis. Consequently, the $(1+1)$ lattice L^c of projections of vectors in L along the c axis can be expressed as integral linear combinations $nk\mathbf{c}+n'k'\mathbf{c}$ with primitive indexing for the subset of points having both n and n' multiples of three. Thus the two components along $\mathbf{c}$ of vectors in the modular lattice L_0 can be taken from the integers modulo 3, which we represent by the three numbers 1, 0 and $\bar{1}=-1$.

The horizontal components of vectors in the modular lattice L_0 are treated exactly as in the crystallographic case. One first notes that the sublattice L^{ab} of L in the ab plane is a triangular lattice generated primitively by two vectors $\mathbf{a}$ and $R\mathbf{a}=\mathbf{b}$, with R

† T_1 cannot be equivalent to T_0 since their modular lattices have eight and four elements, respectively. [Equivalences as in step (v) above can only change the number of vectors in a cubic modular lattice by factors of eight.]

‡ Its modular lattice has 16 elements, and is therefore not equivalent to either of the other two.

† This conclusion agrees with JJdW.

‡ The subscript c is to distinguish these from the trivial planar monoclinic lattices $P+1_{ab}$ and $C+1_{ab}$, discussed below.

§ Here we disagree with JJdW, who list a third type.

a 120° rotation. We can therefore take the lattice L_P, with respect to which the modular lattice L_0 is defined, to be the hexagonal $P+1$ lattice generated primitively by **a**, **b**, $3k\mathbf{c}$ and $3k'\mathbf{c}$. If **k** is any vector of L, then $(1-R)\mathbf{k}$ is in the ab plane. It follows that the projection $P_{ab}\mathbf{k}$ of any vector **k** of L in the ab plane is either itself in L^{ab} or becomes a vector of L^{ab} when acted upon by $(1-R)$. As a result, if $P_{ab}\mathbf{k}$ is not in L^{ab} then it can be taken, up to an additive vector of L^{ab}, to be either **d** or $-\mathbf{d}=\bar{\mathbf{d}}$, where $\mathbf{d}=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$. Consequently, L_0^{ab}, the sublattice of the modular lattice L_0 in the ab plane, is either the single vector **0** or the three vectors **d**, **0** and $-\mathbf{d}$.

If L_0^{ab} contains all three vectors, then the Bravais class is just a trivial sum of a $(3+0)$ hexagonal P lattice [with three times the density of vectors in the ab plane as the hexagonal $(3+0)$ sublattice L_P] with an incommensurate 1 lattice along c. Non-trivial $(3+1)$ lattices can thus arise only if L_0^{ab} contains the **0** vector alone. In that case the modular lattice will contain at most a single vector for each of the nine choices for the third and fourth components of its vector. It therefore either can be a set of three vectors of the form

$$[0000\ \ \mathbf{u}n_3n_3'\ \ -\mathbf{u}\bar{n}_3\bar{n}_3'] \tag{24}$$

or can be expressed as the set of all nine integral linear combinations modulo 3 of two vectors of the form

$$\mathbf{v}01 \quad \text{and} \quad \mathbf{w}10, \tag{25}$$

where **v** and **w** can each be one of the three vectors **d**, **0** or $-\mathbf{d}$.

In the former case, the lattice is again trivial, since a reindexing transformation can always be found to make all fourth components zero. Therefore, a non-trivial modular lattice must contain vectors of both forms (25) along with all their modulo 3 linear combinations. If either **v** or **w** is zero then L_0 is once again trivial,* so there are only two distinct candidates for a non-trivial modular lattice:

$$L_0=\{\mathbf{d}10\ \ \mathbf{d}01\} \quad \text{or} \quad L_0=\{\mathbf{d}10\ \ \bar{\mathbf{d}}01\}, \tag{26}$$

where here the curly brackets indicate the lattice generated by all modulo 3 integral linear combinations of the vectors within them. The first of these can be written as the sum

$$L_0=[0000\ \ \mathbf{d}10\ \ \bar{\mathbf{d}}\bar{1}0]+[0000\ \ 00\bar{1}1\ \ 001\bar{1}], \tag{27}$$

while the second is

$$L_0=[0000\ \ \mathbf{d}10\ \ \bar{\mathbf{d}}\bar{1}0]+[0000\ \ 0011\ \ 00\bar{1}\bar{1}]. \tag{28}$$

But by reindexing we can alter (27) [or (28)] by adding each fourth component (or the negative of each fourth component) to each third component. In either case this gives

$$L_0=[0000\ \ \mathbf{d}10\ \ \bar{\mathbf{d}}\bar{1}0]+[0000\ \ 0001\ \ 000\bar{1}], \tag{29}$$

which is just the trivial sum of a $(3+0)$ rhombohedral R lattice with an incommensurate 1 lattice along **c** (consisting of all integral multiples of $k'\mathbf{c}$).

Consequently, the only two hexagonal and trigonal $3+1$ Bravais classes are the trivial $P+1$ and $R+1$ classes.*

F. The triclinic and planar monoclinic cases

The symmetry of lattices in these Bravais classes is so low that they are better analyzed directly, without the intermediary of the modular sublattices.

Lattices L in the triclinic $(3+1)$ Bravais class are generated by four integrally independent non-coplanar vectors bearing no special relations to one another, so that the point group G of L contains only the inversion. Since any $(3+1)$ lattice (in any Bravais class) can be generated primitively by four vectors, and since all $(3+1)$ lattices have at least the triclinic point group G, it follows from the definition of Bravais class equivalence in § II that all triclinic $(3+1)$ lattices are in the same Bravais class.†

The planar monoclinic Bravais class contains lattices generated by three integrally independent vectors in the ab plane and a fourth vector not in the plane of the first three. The point group G contains a twofold axis **c** perpendicular to the ab plane. Because there are no special relations between the generating vectors in the ab plane, the two-dimensional sublattice L^{ab} can be primitively generated by three vectors **a**, **b** and **d**. The full $(3+1)$ lattice, as in the $(3+0)$ case, is given by the sum of L^{ab} and the 1 lattice consisting of integral multiples of a vector $\mathbf{c}+\mathbf{s}$, where the vector **s** is in the ab plane and only determined to within an additive vector of L^{ab}. Twofold symmetry about the axis **c** requires $2\mathbf{s}$ to be in the $(2+1)$ sublattice L^{ab}. If $2\mathbf{s}=0$, then the resulting structure can be viewed as a $P+1_{ab}$ lattice – the sum of a $(3+0)$ monoclinic P lattice with all integral multiples of an integrally independent vector in the ab plane. If $2\mathbf{s}$ is non-zero then **s** must be a linear combination of **a**, **b** and **d**, with coefficients which can be taken to be either 0 or $\frac{1}{2}$, so that $2\mathbf{s}$ is an integral linear combination with coefficients that are either 0 or 1. As a result, we can find a new set of three primitive generating vectors for L^{ab}, one of which is $2\mathbf{s}$ itself. The lattice L therefore contains a $(3+0)$ centered monoclinic sublattice consisting of the sum of a $(2+0)$ centered rectangular lattice in the plane of **c** and **s** and a 1 lattice in a general direction in the ab plane. The full $(3+1)$ lattice L is the sum of this

* It is explicitly trivial when $\mathbf{v}=0$, and seen to be trivial after a reindexing transformation that interchanges the third and fourth components when $\mathbf{w}=0$.

* JJdW give a third.

† JJdW agree.

centered monoclinic C lattice and a second 1 lattice in the ab plane. We denote the Bravais class by $C+1_{ab}$. These two trivial lattices are the only monoclinic $(3+1)$ lattices with the incommensurate direction lying in the ab plane.*

This completes the enumeration of the 25 $(3+1)$ [or $(3+3)$ cubic] Bravais classes. They are listed in Tables 1 and 2, along with the 38 JJdW Bravais classes that reduce to them, as we now show.

IV. Lattices of main reflections

Usually the diffraction pattern of an incommensurately modulated structure is characterized by a strong set of main reflections and a weaker set of satellites.† The main reflections are associated with a basic $(3+0)$ lattice characterizing the unmodulated material, and the satellites arise from a weak incommensurate distortion of the material such as might, for example, result from one or more 'frozen in' phonons in an otherwise perfect crystal. Since the distinction between main reflections and satellite peaks is based on the intensities of the diffraction peaks, and not on their positions, it has not played a role in our construction of the Bravais classes.

When a diffraction pattern does display an obvious set of main reflections, however, this can be of great help in identifying its $(3+d)$ Bravais class even though that Bravais class is determined only by the peak positions, since lattices in the $(3+d)$ Bravais class characterizing the material must have sublattices in the $(3+0)$ Bravais class of the sublattice of main reflections. Noting this constraint can reduce the number of candidates for the full $(3+d)$ Bravais class. For each $(3+d)$ Bravais class it is therefore useful to examine which $(3+0)$ Bravais classes a $(3+0)$ sublattice of a $(3+d)$ lattice in the class can belong to.‡§

In recording the $(3+0)$ Bravais classes of the sublattices contained in the lattices from a given $(3+d)$ Bravais class, we recover the classification scheme of JJdW. When the lattices in one of our $(3+d)$ Bravais classes contain only $(3+0)$ sublattices from a single $(3+0)$ Bravais class, then our Bravais class can be identified with a single one of the JJdW classes. When, however, the lattices in one of our Bravais classes have $(3+0)$ sublattices from more than a single $(3+0)$ Bravais class, then our $(3+d)$ Bravais classes can be identified with correspondingly many of the JJdW classes; each of these JJdW classes contains identical lattices of wave vectors, but displays them from a perspective that emphasizes the different $(3+0)$ sublattices they contain.

A. Lattices of main reflections in the orthorhombic, tetragonal and axial monoclinic cases

1. *Orthorhombic case.* We show below that two of the six orthorhombic Bravais classes ($P+1$ and $C+1$) contain $(3+1)$ lattices with $(3+0)$ sublattices from a unique $(3+0)$ Bravais class. The non-trivial Bravais class O, however, and the three trivial classes I^*+1, F^*+1 and $A+1$ contain $(3+1)$ lattices that have $(3+0)$ sublattices from two distinct $(3+0)$ Bravais classes. This accounts for the extra four JJdW Bravais classes.

(*a*) A lattice in the I^*+1 ($F+1$) Bravais class can be described by the modular lattice

$$[0000\ 1110], \tag{30}$$

which represents it as the (trivial) sum of a $(3+0)$ I^* lattice and an incommensurate 1 lattice along $\mathbf{c}$ (with lattice constant $2k'$).† A reindexing transformation that interchanges the third and fourth components does not change the Bravais class, but converts (30) into

$$[0000\ 1101]. \tag{31}$$

This now represents the lattice as the sum of a $(3+0)$ P lattice (given by the even sublattice L_P)‡ and the 1 lattice consisting of arbitrary integral multiples of $\mathbf{a}+\mathbf{b}+k'\mathbf{c}$. JJdW would describe this as a modulation vector with a 'rational part' not along $\mathbf{c}$. None of the other reindexing transformations (1) give $(3+0)$ sublattices in any other $(3+0)$ Bravais classes. These two forms of the I^*+1 Bravais class appear as two distinct Bravais classes in the catalog of JJdW: the first as $Fmmm(00\gamma)$ (No. 17) and the second as $Pmmm(\frac{1}{2}\frac{1}{2}\gamma)$ (No. 11).

(*b*) A lattice in the F^*+1 ($I+1$) Bravais class can be described by the modular lattice

$$[0000\ 1100\ 1010\ 0110], \tag{32}$$

* JJdW list three.

† This is not the case for quasicrystals (when viewed as incommensurately modulated structures that have additional symmetries because of special values of the incommensurate parameters) or for incommensurate intergrowth compounds, and it need not be the case for compositionally (or 'substitutionally') modulated structures.

‡ In extracting the $(3+0)$ Bravais classes that can be associated in this way with a given $(3+d)$ Bravais class, the procedure is simplest if one chooses the modular lattice with the smallest number of vectors whenever a $(3+d)$ Bravais class can be described by several distinct modular lattices [as in point (v), § III].

§ We are, of course, only interested in those $(3+0)$ sublattices that are maximal, *i.e.* that are not sublattices of larger $(3+0)$ sublattices.

† Because all vectors in the 1 lattice are $\mathbf{0}$ modulo the even sublattice L_P, the 1 lattice does not appear explicitly in (30). To emphasize its presence one could rewrite (30) as [0000 1110]+[0000]. A similar remark applies to the other trivial Bravais classes, and also to Bravais classes containing $(3+0)$ P sublattices, when they contain only the $\mathbf{0}$ vector modulo L_P.

‡ Here, as remarked upon in the preceding footnote, the $(3+0)$ P lattice does not appear explicitly, since it contains only the $\mathbf{0}$ vector modulo L_P. To emphasize its presence one could rewrite (31) as [0000]+[0000 1101].

which represents it as the (trivial) sum of a $(3+0)$ F^* lattice and an incommensurate one-dimensional lattice along $\mathbf{c}$ (with lattice constant $2k'$). Interchanging the third and fourth components (a reindexing transformation that does not alter the Bravais class) changes this to

$$[0000\ 1100\ 1001\ 0101], \tag{33}$$

which we can express as the sum of two smaller modular lattices:

$$[0000\ 1100]+[0000\ 1001]. \tag{34}$$

In this form the first modular lattice describes a sublattice in the $(3+0)$ C Bravais class, and the second adds to it the 1 lattice of integral multiples of $\mathbf{a}+k'\mathbf{c}$. None of the other reindexing transformations lead to any other $(3+0)$ sublattices, so we arrive at two ways of viewing the F^*+1 Bravais class: the first occurs in the JJdW catalog as $Immm(00\gamma)$ (No. 12) and the second as $Cmmm(10\gamma)$ (No. 14).

(c) A lattice in the $A+1$ Bravais class can be described by the modular lattice

$$[0000\ 0110]. \tag{35}$$

The reindexing transformation that interchanges the third and fourth components changes this to

$$[0000\ 0101], \tag{36}$$

which describes the sum of a $(3+0)$ P lattice (given by the even sublattice L_P) with the 1 lattice of integral multiples of $\mathbf{b}+k'\mathbf{c}$. None of the other reindexing transformations lead to any other $(3+0)$ sublattices and we have two alternative descriptions of the $A+1$ Bravais class, which occur in JJdW as $Ammm(00\gamma)$ (No. 15) and $Pmmm(0\frac{1}{2}\gamma)$ (No. 10).

(d) The single non-trivial orthorhombic Bravais class O has the modular lattice given by (6):

$$[0000\ 1010\ 0101\ 1111], \tag{37}$$

which can also be written as

$$[0000\ 1010]+[0000\ 0101]. \tag{38}$$

In this form it is seen to contain a $(3+0)$ centered lattice (in the B setting) and can be viewed as the sum of such a B lattice with the 1 lattice of integral multiples of $\mathbf{b}+k'\mathbf{c}$. If, however, we apply to (37) the reindexing transformation that adds the third component to the fourth, we get

$$[0000\ 1011\ 0101\ 1110], \tag{39}$$

which can be written as

$$[0000\ 1110]+[0000\ 0101]. \tag{40}$$

This displays the O lattice as the sum of a $(3+0)$ I^* (F) lattice and a 1 lattice of integral multiples of $\mathbf{b}+k'\mathbf{c}$. The other reindexing transformations give no other $(3+0)$ sublattices (though they can transform the B setting to the A setting) and we have the JJdW Bravais classes $Ammm(\frac{1}{2}0\gamma)$ (No. 16) and $Fmmm(10\gamma)$ (No. 18).

The $P+1$ Bravais class can be represented by the modular lattice containing only 0, which clearly generates no other $(3+0)$ sublattices under reindexing, and the $C+1$ Bravais class can be represented by [0000 1100] which is also invariant under reindexing. These two therefore admit $(3+0)$ sublattices from only a single $(3+0)$ Bravais class, and correspond to unique Bravais classes of JJdW: $Pmmm(00\gamma)$ (No. 9) and $Cmmm(00\gamma)$ (No. 13).

2. *Tetragonal case.* These results are immediately carried over to the tetragonal case, where the orthorhombic $P+1$ and $C+1$ $(3+1)$ Bravais classes become identified, as do I^*+1 and F^*+1. (The orthorhombic $A+1$ and O Bravais classes do not exist in the tegragonal system.)

The tetragonal $P+1$ Bravais class has therefore a unique representation which is JJdW's $P4/mmm(00\gamma)$ (No. 19). The centered tetragonal $I+1$ Bravais class, however, inherits from its orthorhombic parent a pair of representations: $I4/mmm(00\gamma)$ (No. 21) or $P4/mmm(\frac{1}{2}\frac{1}{2}\gamma)$ (No. 20).

3. *Axial monoclinic case.* In the monoclinic case, the $P+1_c$ Bravais class again contains a unique class of $(3+0)$ sublattices, and therefore can be described only as JJdW's $P2/m(00\gamma)$ (No. 5). The $C+1_c$ Bravais class, however, has the modular lattice

$$[0000\ 1010], \tag{41}$$

which displays a $(3+0)$ centered monoclinic sublattice. Interchanging the third and fourth components gives

$$[0000\ 1001], \tag{42}$$

which now describes the sum of a monoclinic $(3+0)$ P lattice and the 1 lattice of integral multiples of $\mathbf{a}+k'\mathbf{c}$. Thus the $C+1_c$ Bravais class appears in JJdW both as $B2/m(00\gamma)$ (No. 7) and as $P2/m(\frac{1}{2}0\gamma)$ (No. 6).

The non-trivial monoclinic M lattice has the modular lattice

$$[0000\ 0101\ 1010\ 1111], \tag{43}$$

which can be written as

$$[0000\ 1010]+[0000\ 0101]. \tag{44}$$

This describes the sum of a $(3+0)$ C lattice with the 1 lattice of integral multiples of $\mathbf{b}+k'\mathbf{c}$, which appears in the JJdW catalog as $B2/m(0\frac{1}{2}\gamma)$ (No. 8). Various reindexing transformations only reveal other centered monoclinic $3+0$ sublattices.

B. Lattices of main reflections in the trigonal and hexagonal cases

Since the $P+1$ Bravais class can be represented with a modular lattice consisting of 0 alone, it has no $(3+0)$ sublattice other than the P lattice and occurs only as $P6/mmm(00\gamma)$ (No. 24) of JJdW. The $R+1$ Bravais class, however, can be described most simply in terms of the modular lattice:

$$[0000\ \mathbf{d}10\ \bar{\mathbf{d}}\bar{1}0], \qquad (45)$$

which describes the sum of a $(3+0)$ R lattice and the 1 lattice of integral multiples of $3k'\mathbf{c}$. This is JJdW's $R\bar{3}m(00\gamma)$ (No. 22). Interchanging the third and fourth components gives

$$[0000\ \mathbf{d}01\ \bar{\mathbf{d}}0\bar{1}], \qquad (46)$$

which now describes the sum of a $(3+0)$ P lattice and the 1 lattice of integral multiples of $k'\mathbf{c}+\mathbf{d}$, which is JJdW's $P\bar{3}1m(\frac{1}{3}\frac{1}{3}\gamma)$ (No. 23).

C. Lattices of main reflections in the planar monoclinic case

Lattices in the monoclinic $P+1_{ab}$ Bravais class have no $(3+0)$ sublattices other than the P lattice, and the class appears in JJdW only as $P2/m(\alpha\beta 0)$ (No. 2). The $C+1_{ab}$ Bravais class, however, can be represented with the modular lattice

$$[0000\ 1010], \qquad (47)$$

where we have taken the third position to describe the c axis and have associated the first, second and fourth positions with the three integrally independent vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{d}$ in the ab plane, so that (47) describes the trivial sum of a centered monoclinic lattice and the 1 lattice (not shown explicitly) consisting of even multiples of $\mathbf{d}$ $(=\alpha\mathbf{a}+\beta\mathbf{b})$ given by JJdW as $B2/m(\alpha\beta 0)$ (No. 4). If we reindex in the ab plane by interchanging the first and fourth components we change (47) to

$$[0000\ 0011], \qquad (48)$$

which describes the sum of a $(3+0)$ P lattice (not shown explicitly) and the 1 lattice of integral multiples of $\mathbf{c}+\mathbf{d}$, which is JJdW's $P2/m(\alpha\beta\frac{1}{2})$ (No. 3).

D. Lattices of main reflections in the cubic case

As with the $(3+1)$ lattices, the question of what lattices of main reflections can be associated with the nine cubic $(3+3)$ Bravais classes is simply the question of what $(3+0)$ sublattices of the form

$$n_1n_2n_3,\ 000 \qquad (49)$$

are contained in the $(3+3)$ lattices in the class. One verifies easily that the trivial Bravais classes $P+P$, $P+F^*$, $P+I^*$, I^*+I^* and F^*+F^* admit no $(3+0)$ sublattices beyond those appearing explicitly in their designations. As a result, the $P+P$, I^*+I^* and F^*+cF^* Bravais classes correspond to the unique JJdW classes $Pm3m(\alpha 00)$ (No. 208), $Fm3m(\alpha\alpha\alpha)$ (No. 217) and $Im3m(0\beta\beta)$ (No. 213). However, JJdW list both forms of the other two as separate Bravais classes: $P+F^*$ appears as both $Pm3m(0\beta\beta)$ (No. 212) and $Im3m(\alpha 00)$ (No. 210); and $P+I^*$ as $Pm3m(\alpha\alpha\alpha)$ (No. 215) and $Fm3m(\alpha 00)$ (No. 211).

More interesting is the Bravais class F^*+I^*. Lattices in this Bravais class, in addition to containing a $(3+0)$ F^* sublattice, corresponding to JJdW's $Im3m(\alpha\alpha\alpha)$ (No. 216), and a $(3+0)$ I^* sublattice, corresponding to $Fm3m(0\beta\beta)$ (No. 214), also contain a primitive $(3+0)$ sublattice. To see this, note that F^*+I^* is characterized by the eight-element modular lattice:

$$\begin{aligned}&[000,000\ \ 110,000\ \ 101,000\ \ 011,000]\\ &\quad+[000,000\ \ 000,111]\\ &\qquad=[000,000\ \ 110,000\ \ 101,000\ \ 011,000\\ &\qquad\quad 000,111\ \ 110,111\ \ 101,111\ \ 011,111]. \qquad (50)\end{aligned}$$

This is in the same $(3+3)$ Bravais class as the form it assumes under the reindexing transformation $\mathbf{n},\mathbf{n}'\to\mathbf{n},\mathbf{n}+\mathbf{n}'$:

$$\begin{aligned}&[000,000\ \ 110,110\ \ 101,101\ \ 011,011\\ &\ 000,111\ \ 110,001\ \ 101,010\ \ 011,100]. \qquad (51)\end{aligned}$$

This has a $(3+0)$ sublattice consisting of the $\mathbf{0}$ vector alone. It describes the sum of the primitive even sublattice L_P (represented implicitly by $[000,000]$) and another sublattice given by all integral linear combinations of the three vectors†

$$011,100\ \ 101,010\ \ 110,001, \qquad (52)$$

since these are easily verified to form a basis (modulo 2) for the full set of eight modulo 2 vectors (51). This is precisely what JJdW call $Pm3m(\alpha\frac{1}{2}\frac{1}{2})$ (No. 209).

Thus each of the ten cubic $(3+3)$ Bravais classes of JJdW with $m3m$ symmetry coincides (trivially, except for No. 209) with one of our six trivial Bravais classes. We can also reduce to three their four tetrahedral Bravais classes.

The lattices in the Bravais class T_0 have the four-element modular lattice (23):

$$[000,000\ \ 110,011\ \ 011,101\ \ 101,110]. \qquad (53)$$

The reindexing transformations (14) simply permute the vectors in this set or rotate them through 90°. None of them alter the fact that the only lattice of main reflections that can be found in the lattices of this Bravais class is the $(3+0)$ P lattice, and therefore

† In the notation of III.C we would describe this second sublattice simply as $\{110,001\}$.

the $(3+3)$ lattice (53) can be uniquely characterized as a P lattice of main reflections with satellites at the points generated by all integral linear combinations of the three non-zero vectors in (53).† JJdW give this as $Pm3(\frac{1}{2}\beta\beta+\frac{1}{2})$ (No. 206).

Lattices in the Bravais class T_1 have eight-element modular lattices given by adding to (53) one of the I^* lattices (21). The various forms allowed by reindexing correspond to the three possible representations for the I^* lattice:

$$\begin{aligned}&[000,000\ \ 111,000];\\&[000,000\ \ 000,111];\\&[000,000\ \ 111,111].\end{aligned}\qquad(54)$$

The first form represents T_1 as an I^* lattice of main reflections, with satellites at the points about the main reflections generated by all linear combinations of the three non-zero vectors in (53). This is JJdW's $Fm3(1\beta\beta+1)$ (No. 207). The second and third forms of the I^* lattice yield modular lattices in which only the zero vector has a vanishing component along k', so the lattices of main reflections are the $(3+0)$ P lattice L_P, and the entire set of eight modulo 2 vectors describe the shifts. Depending on whether we use the second or third form of I^* these can be represented as all integral linear combinations of either 101, 100 or 010, 100 and their cyclic permutations.‡ The second alternative appears on JJdW's list as $Pm3(\alpha\frac{1}{2}0)$ (No. 204).

The Bravais class T_2 has a 16-element modular lattice given by adding to T_0 the modular lattice I^*+I^*:

$$[000,000\ \ 000,111\ \ 111,000\ \ 111,111].\qquad(55)$$

Since this structure is invariant under any of the reindexing transformations and since T_0 is either invariant or rotated by the transformations, T_2 can only have a single representation in terms of a basic lattice, and this representation is immediately extracted by viewing T_2 as the sum of an $I^*(3+0)$ lattice of main reflections with the satellites described by a $T_1(3+3)$ lattice in the form we identified above as JJdW's $Pm3(\alpha\frac{1}{2}0)$. This immediately gives JJdW's $Fm3(\alpha 10)$ (No. 205).

The $(3+0)$ sublattices contained in the $(3+d)$ lattices of each of our 25 Bravais classes are summarized in Table 1 [$(3+1)$ lattices] and Table 2 [$(3+3)$ cubic lattices], which specify them by listing to which of the 38 categories in the JJdW catalog of Bravais classes they correspond.

† In the notation of III.C we would describe the modular lattice characterizing the satellites as {110, 011}.

‡ In the notation of III.C as {101, 100} or {010, 100}.

V. Concluding remarks

It is unquestionably useful and important to note the various ways of describing each of our $(3+d)$ Bravais classes in terms of $(3+0)$ lattices of main reflections and satellite peaks. It should be recognized, however, that these are merely alternative descriptions of one and the same class of lattices of wave vectors. It is, of course, a matter of convention whether one chooses (as JJdW do) to label these different representations of identical classes of lattices as distinct Bravais classes or to regard them (as we do) as different descriptions of a single Bravais class. What is not a matter of convention, however, is the fact that the JJdW use of the term leads one to a scheme in which distinct Bravais classes contain identical collections of lattices ('Z modules') of three-dimensional wave vectors - an identity that de Wolff, Janssen & Janner (1981) and Janner, Janssen & de Wolff (1983) never explicitly state.

In support of our convention, we would argue that to use the term 'Bravais class', as JJdW do, in a manner that requires one to specify the intensities as well as the positions of the Bragg peaks, is to introduce a degree of imprecision into a set of categories that would otherwise be rigorously based on symmetry alone, and to provide those categories with an unnecessary complexity.

(1) Using the JJdW convention one must arbitrarily specify how much more intense the main reflections must be than the satellite peaks for the scheme to be applicable.

(2) Under the JJdW convention, cases that fail to reveal a pronounced lattice of main reflections (such as certain compositionally modulated structures or quasicrystals) must unnecessarily be provided with a different crystallographic taxonomy. Resemblances across categories (such as that between the tetrahedral and icosahedral Bravais classes noted in footnote ‡ on p. 524) are obscured.

(3) One can specify densities that interpolate continuously between two distinct JJdW Bravais classes without ever changing their symmetry or the rank of their lattices.

(4) If one fails to recognize that distinct JJdW Bravais classes contain identical lattices of three-dimensional wave vectors, when one computes the space groups associated with each Bravais class one is led to unnecessary additional calculations and a further redundancy of description.*

(5) As remarked upon above, the character of the associated space groups is related in a very elementary way to the character of the associated crystallographic space groups for all the trivial $(3+1)$ [or $(3+3)$ cubic]

* We examine this in Lifshitz & Mermin (1992), where we construct the space groups for all of the 25 Bravais classes derived here.

Bravais classes. The JJdW scheme, by presenting seven of the trivial $(3+1)$ [and one of the trivial $(3+3)$ cubic] Bravais classes in a second non-trivial guise, obscures the simplicity of the space groups associated with these redundant Bravais classes, when lattices of main reflections favor the description in terms of non-trivial representatives.*

(6) While recognizing the dangers of imperfect analogies, we would like to illustrate, in the more familiar context of periodic crystals, what we believe to be the central issue. Consider an orthorhombic ordinary crystal which is soft along the *c* direction, so that the periodic density variations are much stronger in the horizontal *ab* plane than along the vertical *c* axis, resulting in a basic 'lattice of main reflections' in the *ab* plane with much weaker 'satellites' displaced along **c**. Suppose we have two such materials. In the first, the two-dimensional lattice of main reflections is centered rectangular and the satellites lie directly above or below its points. In the second, the two-dimensional lattice of main reflections is primitive rectangular, and the satellites are displaced from its points by multiples of $\mathbf{c}+\frac{1}{2}\mathbf{b}$. It is certainly useful for any number of purposes to view the first structure as a centered rectangular lattice of main reflections with satellites shifted in the purely vertical direction and the second as a primitive rectangular lattice of main reflections with satellites shifted vertically with an additional horizontal shift by a vector not in the basic lattice. But from the crystallographic point of view the reciprocal lattices of both structures are centered orthorhombic, the first in the *C* setting and the second in the *A* setting. While it is very useful to have descriptions from the point of view of both settings, crystallography does not treat them as distinct Bravais classes nor distinguish two corresponding types of space groups. It is the same with the extra Bravais classes of JJdW: they are useful and important categories to note, but are better regarded as different manifestations of the smaller number of $(3+1)$-Bravais classes enumerated here.

* This is examined in Lifshitz & Mermin (1992), where we also expand on the following point: A space-group-classification scheme based on our definition of Bravais class must clearly have the property that two JJdW Bravais classes that we identify should have the same number of space groups. This rule is often but not always satisfied in the JJdW catalogue of space groups. This is because in our scheme (but not in the scheme of JJdW) the further subdivision of a Bravais class of lattices into space groups also makes no reference to peak intensities beyond requiring that the intensities should be the same at wave vectors in the orbit of any point-group operation.

We have benefited from comments on an earlier draft by S. van Smaalen, A. Yamamoto, T. Janssen and D. Grebille. NDM is indebted to Juan Pérez Mato for inviting him to participate in the Bilbao Conference on Quasicrystals and Incommensurately Modulated Structures (May, 1991), and remembers with pleasure conversations with A. Janner during a very cold and rainy conference excursion that stimulated him to extend the application of generalized three-dimensional crystallography from quasicrystals to incommensurately modulated structures. This work was supported by the National Science Foundation through grant DMR 89-20979.

References

Bienenstock, A. & Ewald, P. P. (1962). *Acta Cryst.* **15**, 1253-1261.

Grebille, D., Weigel, D., Veysseyre, R. & Phan, T. (1990). *Acta Cryst.* **A46**, 234-240.

Janner, A. (1991). In *Methods of Structural Analysis of Modulated Structures and Quasicrystals*, edited by J. M. Pérez-Mato, F. J. Zúñiga & G. Madariaga, pp. 64-79. Singapore: World Scientific.

Janner, A., Janssen, T. & de Wolff, P. M. (1983). *Acta Cryst.* **A39**, 658-666, 667-670, 671-678.

Lifshitz, R. & Mermin, N. D. (1992). To be submitted to *Acta Cryst.* A.

Mermin, N. D. (1992). *Rev. Mod. Phys.* **64**, 3-49.

Mermin, N. D. & Lifshitz, R. (1992). To be submitted to *Acta Cryst.* A.

Rabson, D. A., Mermin, N. D., Rokhsar, D. S. & Wright, D. C. (1991). *Rev. Mod. Phys.* **63**, 699-733.

Rokhsar, D. S., Mermin, N. D. & Wright, D. C. (1987). *Phys. Rev.* **B35**, 5487-5495.

Wolff, P. M. de, Janssen, T. & Janner, A. (1981). *Acta Cryst.* **A37**, 625-636.

Yamamoto, A., Janssen, T., Janner, A. & de Wolff, P. M. (1985). *Acta Cryst.* **A41**, 528-530.