The space groups of icosahedral quasicrystals and cubic, orthorhombic, monoclinic, and triclinic crystals

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In 1962 Bienenstock and Ewald described a simple and systematic method for computing all the crystallographic space groups in Fourier space. Their approach is reformulated and further simplified, starting from the definition of the point group of a structure as the set of operations that take it into something *indistinguishable* and not merely identical to within a translation. The reformulation does not require periodicity, making it possible to define and compute on an equal footing the space groups for crystals, quasicrystals, and incommensurately modulated structures, without having to digress into the crystallography of unphysically many dimensions, and using only simple geometry and the most elementary properties of symmetry groups. The general scheme is illustrated by a unified computation of all the icosahedral, cubic, orthorhombic, monoclinic, and triclinic space groups. The remaining (axial) crystallographic and quasicrystallographic space groups have been discussed in a companion paper.

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I. INTRODUCTION

This essay is intended to serve both a pedagogical and a polemical purpose. I hope to persuade the reader that it was a misfortune of intellectual history that the space-group classification scheme of crystallography was developed in real space to categorize periodic structures, rather than in Fourier space to categorize diffraction patterns consisting of sharp Bragg peaks. This was first remarked upon in a little cited[1] paper by Arthur Bienenstock and P. P. Ewald, 1962. That their work has for thirty years had no impact on textbook treatments of space groups, or on the *International Tables for Crystallography* (International Union of Crystallography, 1987), I attribute in part to the enormous inertia of well established methods and in part to a few unnecessary complexities in their formulation, simple as it was compared with conventional methods.

The misfortune was compounded when people started to extend space-group theory to the classification of incommensurately modulated crystals (de Wolff, Janssen, and Janner, 1981; Janner, Janssen, and de Wolff, 1983a, 1983b, and 1983c; Janner, 1991), and then, more recently, to quasicrystals. (Janssen, 1986). With space groups firmly regarded as giving the categories of periodic materials, it was considered necessary to regard quasiperiodic materials as lower-dimensional slices of periodic higher-dimensional structures, in order to arrive at a space-group classification scheme. Space-group theories for quasiperiodic materials therefore began with an arbitrary and artificial embedding of the structure in a higher-dimensional space and proceeded by developing the appropriate subset of the higher-dimensional space-group scheme, and then, not without hazard, projecting this information back down to the physical number of dimensions.

There is, however, a much simpler approach, based on reformulating the Bienenstock-Ewald method so that it *defines,* as well as efficiently derives, the space-group classification scheme for both periodic and quasiperiodic materials in ordinary three-dimensional reciprocal space. In their approach a fundamental role is played by phase relations between density Fourier coefficients at wave vectors related by point-group symmetries. The key to extending their method to quasiperiodic structures is to note that those phase relations, although usually viewed as consequences of real-space translational symmetry, can also be derived as a direct expression of real-space quasiperiodicity, without any excursion into higher-dimensional space.

In the course of applying this extended Bienenstock-Ewald method to the computation of three-dimensional quasicrystallographic space groups, some refinements have been developed that simplify its application to crystals as well as quasicrystals. Since the space groups for ordinary three-dimensional cystals are easier to construct in three-dimensional Fourier space than in three-dimensional real space, and since that three-dimensional construction applies to quasiperiodic as well as periodic structures, there is no reason to continue to extract the classification scheme for quasiperiodic structures by embedding them in a higher number of dimensions. The motivation for doing so—to take advantage of periodicity in the higher-dimensional space—vanishes when one abandons an obsolete formulation of crystallography that relies unnecessarily on periodicity.

Thus I maintain that the world deserves to learn how to construct space groups for both periodic and quasiperiodic materials in three-dimensional Fourier space. There is, however, a barrier of unfamiliarity to be overcome. It is the purpose of this paper and an earlier companion paper to provide an assault on that barrier. In Rabson, Mermin, Rokhsar, and Wright (1991, henceforth RMRW) the formulation of space-group theory for quasiperiodic structures in Fourier space is reviewed and applied to a unified computation of the space groups for materials with point groups containing a unique n-fold axis of maximum rotational symmetry. The analysis of RMRW applies to the hexagonal, tetragonal, and trigonal crystal systems, and to all their quasicrystallographic

[1]But see J. W. Jeffrey, 1963, who a mere year later cites Bienenstock and Ewald as "a landmark in the theoretical development of crystallography."

generalizations for n less than 23.[2] These three crystal systems are simply special cases of five general quasicrystal types, and the space-group scheme can be developed in a unified way for each type, for general values of the rotational symmetry n.[3] In the present paper I complete the program of RMRW by examining the remaining "special cases" where the point group has no unique axis of highest symmetry, namely the icosahedral quasicrystals and the cubic, orthorhombic, monoclinic,[4] and triclinic crystals.

I have tried to write an essay that is independent of RMRW, so that the two can be read in either order. Although there is therefore some duplication between Sec. II and the corresponding section of RMRW, I here set forth the foundations of the approach from a somewhat different and, I hope, more intuitive perspective, basing the formulation on a fundamental distinction between "indistinguishable" as opposed to "identical" densities.[5]

Section II offers a formulation of crystallography that the giants of the field—Frankenheim, Bravais, Fedorov, Schönflies, *et al.*—could have arrived at over a hundred years ago, had they only realized that the restriction of their scheme to periodic materials was entirely artificial. While they might more readily have come upon this insight had x-ray diffraction been discovered before, rather than after, their investigations, there is no reason why their bad luck should continue to plague future students of the subject. As in RMRW, the focus here will be primarily on the concept of space group, so as not to be distracted by the problem of classifying the lattices. While a lattice is easy enough to define in Fourier space, the issue of how many there are with a given point-group symmetry—answered a century and a half ago by Frankenheim and Bravais for three-dimensional crystals—is subtle in the crystallographic case and for noncrystallographic point groups leads rapidly into number-theoretic questions that even mathematicians have not fully explored. I therefore limit myself to defining the lattices and specifying the properties on which the formulation of space-group theory relies. To avoid obscuring the structure of space-group theory, however, I shall then regard the particular lattices of interest as given and focus on the question of how to enumerate the categories of materials with those lattices.[6]

The rest of this paper puts flesh on the dry bones of Sec. II. In Sec. III, to emphasize that icosahedral quasicrystallographic space groups do not require an excursion into six-dimensional crystallography, and to demonstrate the unity of the Fourier-space approach, whether applied to crystals or to quasicrystals, I give a single unified computation of the 11 icosahedral and 36 cubic space groups.[7]

In Sec. IV, I apply the Fourier-space method to a computation of all 59 of the orthorhombic space groups, and in Sec. V, for completeness, I give the uninteresting computation of the 13 monoclinic and 2 triclinic space groups. I have deliberately worked from the richest and most subtle case down to the simplest, not out of a perverse taste for inverse pedagogy, but because a certain artistry is employed in the icosahedral-cubic and (to a lesser extent) the orthorhombic cases, which I fear the reader might never get to enjoy, if forced first to traverse the tedium of more routine applications.

Section VI shows how to extract from the results of Secs. III–V the extinctions (or "systematic absences") associated with each space group, probably the single most important application of the space-group formalism.

In Sec. VII, a brief Conclusion, I comment on the relevance of the Fourier-space approach to earlier computations of lattices and space groups for incommensurately modulated structures and make a final plea on behalf of reformulating the foundations of crystallography without relying on periodicity.

Appendix A describes the scale invariance of the primitive icosahedral lattice. (The more straightforward scale invariances of the two centered icosahedral lattices are established in Sec. III.E.)

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[2]When n exceeds 22 the possibility of "nonstandard lattices" arises and a complete classification scheme takes one into still unplumbed depths of number theory, as noted by Mermin, Rokhsar, and Wright (1987). The analysis of RMRW is valid for arbitrary n when the lattices are standard.

[3]For standard lattices.

[4]Monoclinic crystals do have a unique twofold axis of highest symmetry, but twofold crystals are pathological from the n-fold point of view, since the n-fold rotations of a single vector perpendicular to an axis fail to produce enough vectors to span the orthogonal plane only when $n=2$. RMRW therefore did not consider them.

[5]Much of this general formulation, and a preliminary version of its application to the icosahedral and cubic space groups, have appeared in Mermin, 1991a, 1991b.

[6]We have examined elsewhere the question of what lattices must be considered in extending crystallography to quasicrystallography. See Rokhsar, Mermin, and Wright, 1987; Mermin, Rokhsar, and Wright, 1987; and Mermin, Rabson, Rokhsar, and Wright, 1990. The lattices for incommensurately modulated structures are discussed by de Wolff, Janssen, and Janner, 1981; Janner, Janssen, and de Wolff, 1983a, 1983b, and 1983c. A Fourier-space treatment, which suggests a simpler formulation of their conclusions, has been given by Mermin and Lifshitz, 1992.

[7]Bertaut, 1970, has derived the 10 cubic space groups with point group O_h using the original Bienenstock-Ewald method, with some of the complicating features (4×4 matrices, nonprimitive generating vectors for the centered lattices) that our formulation avoids. The application of the Fourier-space approach to the icosahedral case has been given by Rokhsar, Wright, and Mermin, 1988. Their paper focused on a single issue (scale invariance) and passed lightly over the details of the rest of the computation, which I present here in a new and simpler form.

Appendix B gives the bases in six-dimensional "real" space dual to the threefold symmetric bases we use here to generate the icosahedral lattices, which can be useful in *constructing* real-space structures, but are not needed for *classifying* them.

Appendix C is intended as a convenience for those who, like me, are nonalgorithmic readers. It contains a brief index, citing the place (or places) where the major technical terms are first defined.

II. GENERALIZED CRYSTALLOGRAPHY

Crystals, quasicrystals, and amorphous solids share the property of being mesoscopically homogeneous although microscopically inhomogeneous. The microscopic inhomogeneity is on the atomic scale: the time-averaged atomic positions are not uniformly distributed (as they are in liquids and perhaps, on sufficiently long time scales, in glasses). The mesoscopic homogeneity is a consequence of the fact that detailed microscopic features of regions large on the atomic scale, but small on the scale of a given macroscopic specimen, recur throughout, so that any given mesoscopic subregion is indistinguishable from similar subregions scattered, with the same statistical distribution, throughout the macroscopic sample.

Crystals achieve this mesoscopic homogeneity in an extreme way, by being microscopically periodic. Amorphous solids are mesoscopically homogeneous because the properties of a collection of enormously many randomly structured subregions do not vary if the subregions are randomly rearranged. Quasicrystals and incommensurately modulated crystals accomplish the trick with the most subtlety, having the property, familiar in Penrose tilings, that the microscopic structure of any region of a given size D can be found perfectly reproduced in other regions whose distance from the first is of order D.

This property of mesoscopic homogeneity lies at the heart of a unified classification scheme that encompasses all quasiperiodic structures: crystals, quasicrystals, and incommensurately modulated crystals or quasicrystals. Unfortunately, when the scheme used today was developed in the late 19th century, quasicrystals and incommensurately modulated crystals were unknown and the classification focused narrowly on spatial periodicity rather than the broader mesoscopic homogeneity of which periodicity is only a special case. Thus crystals were classified by their space group—the subgroup of the full Euclidean group that brings the density into coincidence with itself.

Viewed from the broader perspective, however, *identity* of densities is far too restrictive a way to define the structural indistinguishability of two mesoscopically homogeneous materials. All one can sensibly require is the identity of the distribution of structures of all mesoscopic subregions. In a mesoscopically homogeneous material the mathematical statement of this condition is the identity for arbitrary n of the nth-order positionally averaged correlation functions c_n given by

$$c_n(r_1,\ldots,r_n)=(1/V)\int d^3r\,\rho(\mathbf{r}_1-\mathbf{r})\cdots\rho(\mathbf{r}_n-\mathbf{r})\ . \tag{2.1}$$

We shall say that two densities ρ and ρ' are *indistinguishable* if all their correlation functions c_n and c_n' are identical.

Evidently two densities that differ only by a translation are indistinguishable. The converse—that two densities are indistinguishable only if they are identical to within a translation—holds if a material is periodic in three independent directions. So for crystals the shift in emphasis from identity to indistinguishability is a trivial one. Notice, though, that even for crystals it changes the way one thinks about space groups:

If the space group is the subgroup of the Euclidean group that leaves the density *identical,* then it contains elements from the subgroup $O(3)$ of rotations (proper and improper), elements from the translation subgroup $T(3)$ that express the (incidental, from our broader perspective) periodicity of the density, and elements whose presence defines the *nonsymmorphic* space groups, called *screw axes* or *glide planes,* that combine a rotation and a translation neither of which individually leaves the density invariant.

If, however, we inquire into the subgroup of the Euclidean group that leaves the density of a crystal *indistinguishable* from what it was, then that subgroup contains all translations. The subtle interplay between translations and rotations leading to the rich catalogue of nonsymmorphic space groups seems to have disappeared. Nothing seems to remain to characterize particular materials but the point group. We appear to have achieved a greater generality at a cost of losing something important. We shall see below how nonsymmorphic space groups (for both periodic and quasiperiodic materials) reemerge from this new perspective.

In contrast to crystals, densities of indistinguishable quasiperiodic structures (quasicrystals or incommensurately modulated crystals) can differ by more than just a translation. If one insists on classifying the symmetries of such materials by a subgroup of a Euclidean group, one is forced to the clumsy expedient of introducing the Euclidean group in unphysically many dimensions. There is, however, no reason to insist; it is far easier to follow the path that would have been taken for crystals as well, had the superiority of indistinguishability to identity not been masked in the periodic case by their trivial connection. Quasicrystals, incommensurately modulated crystals, and ordinary crystals can all be classified by a point group and something else. In the case of crystals, both the point group and the something else are familiar. In the case of quasicrystals and incommensurately modulated crystals, as well as in the case of ordinary crystals, when the emphasis is on indistinguishability rather than on identity, these concepts have

to be reformulated. That reformulation is carried out in Secs. II.A–II.J.

A. Indistinguishable densities in Fourier space

The condition (2.1) that two densities are indistinguishable assumes a useful form when expressed in terms of the density Fourier coefficients. If

$$\rho(\mathbf{r})=\sum_{\mathbf{k}}\rho(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}\ , \tag{2.2}$$

then two densities ρ and ρ' will have identical correlation functions (2.1) if and only if their Fourier coefficients always satisfy

$$\rho(\mathbf{k}_1)\cdots\rho(\mathbf{k}_n)=\rho'(\mathbf{k}_1)\cdots\rho'(\mathbf{k}_n) \tag{2.3}$$

whenever

$$\mathbf{k}_1+\cdots+\mathbf{k}_n=0\ . \tag{2.4}$$

Since real-space densities are real, the Fourier coefficients satisfy

$$\rho(-\mathbf{k})=\rho^*(\mathbf{k})\ , \tag{2.5}$$

and therefore Eq. (2.3), applied to $\mathbf{k}+(-\mathbf{k})=0$, tells us that the Fourier coefficients of indistinguishable densities have the same magnitude—i.e., that the Fourier coefficients themselves differ only by a (real) phase:[8]

$$\rho'(\mathbf{k})=e^{2\pi i\chi(\mathbf{k})}\rho(\mathbf{k})\ . \tag{2.6}$$

We call $\chi(\mathbf{k})$ a *gauge function* in analogy to the gauge functions of electrodynamics, which can alter the phase of a wave function without changing any observable properties.

Equations (2.5) and (2.6) together require that

$$\chi(-\mathbf{k})\equiv-\chi(\mathbf{k})\ , \tag{2.7}$$

where we use the symbol "$\equiv$" to specify equality to within an additive integer. This, together with the indistinguishability condition (2.3) for three vectors summing to zero, leads to the stronger condition that χ be linear to within an additive integer:

$$\chi(\mathbf{k}_1+\mathbf{k}_2)\equiv\chi(\mathbf{k}_1)+\chi(\mathbf{k}_2)\ . \tag{2.8}$$

With χ satisfying Eq. (2.8), the indistinguishability condition (2.3) is automatically satisfied for all higher values of n.[9]

Thus two densities are indistinguishable if and only if their Fourier coefficients are related by a linear[10] gauge function as in Eq. (2.6).

B. The point group and the phase functions

We define the point group G of a material to be the set of all proper and improper rotations g under which its density is indistinguishably altered. Thus the real-space condition for g to be in the point group of the material is that all correlation functions (2.1) constructed out of $\rho(g\mathbf{r})$ and $\rho(\mathbf{r})$ be the same. I stress the difference between this definition and the conventional crystallographic one, which requires $\rho(g\mathbf{r})$ and $\rho(\mathbf{r})$ to be *identical* to within a microscopic translation rather than merely *indistinguishable.*

The equivalent Fourier-space condition is that for each g in the point group G there should be a linear gauge function $\Phi_g(\mathbf{k})$ relating $\rho(g\mathbf{k})$ and $\rho(\mathbf{k})$ as in Eq. (2.6):

$$\rho(g\mathbf{k})=e^{2\pi i\Phi_g(\mathbf{k})}\rho(\mathbf{k})\ . \tag{2.9}$$

We call the gauge functions associated with the point-group operations *phase functions.* From the broader point of view we are developing here, a space group is specified by the point group taken together with its phase functions.

C. Gauge-equivalent phase functions

Two sets of phase functions $\Phi'_g(k)$ and $\Phi_g(k)$ that can characterize indistinguishable densities ρ' and ρ should clearly be regarded as equivalent. The Fourier-space condition (2.6) for indistinguishability of the densities combined with the definition (2.9) of the phase functions leads directly to the relation

$$\Phi'_g(\mathbf{k})\equiv\Phi_g(\mathbf{k})+\chi(g\mathbf{k})-\chi(\mathbf{k})=\Phi_g(\mathbf{k})+\chi([g-1]\mathbf{k})\ . \tag{2.10}$$

Two sets of phase functions related in this way through a linear gauge function are said to be *gauge equivalent,* and the relationship holding between them is called a *gauge transformation.* Note that Eq. (2.10) must hold with the same gauge function χ for every g in the point group G. If two crystals have gauge-equivalent phase functions, then they have the same space group. The space-group classification scheme is basically a classification into classes of gauge-equivalent phase functions. (The cir-

[8]By explicitly introducing the factor of 2π in the definition of χ, we eliminate it from most subsequent results.

[9]I find it remarkable that merely by taking Fourier transforms one produces an elementary proof that the identity of the two- and three-point correlation functions is enough to insure the identity of all higher-order correlation functions, since the geometrical basis for this theorem in real space is considerably less obvious.

[10]When referring to gauge functions, which are defined only to within an additive integer, we shall always understand terms like "linear," "equal," or "vanishing" to mean linear, equal, or vanishing to within an additive integer. Note also that χ is defined only on the restricted set of $\mathbf{k}$ at which $\rho(\mathbf{k})\neq0$, so it is not possible, in general, to extend it to a function that is linear for all $\mathbf{k}$.

cumstances under which distinct gauge equivalence classes are associated with the same space group are described below in Sec. II.G.)

D. Extinctions

If $g\mathbf{k}=\mathbf{k}$, then it follows from Eq. (2.10) that $\Phi_g(\mathbf{k})$ is invariant under arbitrary gauge transformations. These gauge-invariant parts of the phase functions are directly related to the phenomenon of *extinctions,* for it follows directly from the definition (2.9) of the phase function that whenever $g\mathbf{k}=\mathbf{k}$, the Fourier coefficient $\rho(\mathbf{k})$ must vanish unless the (gauge-invariant) phase function $\Phi_g(\mathbf{k})$ vanishes (modulo an integer). Thus the nonintegral gauge-invariant parts of the phase functions determine sets of wave vectors at which the density Fourier coefficients necessarily vanish.[11]

E. Group compatibility condition on the phase functions

Since $\rho([gh]\mathbf{k})=\rho(g[h\mathbf{k}])$, it follows from the definition (2.9) that the phase function belonging to the product of two point-group elements can be constructed out of those belonging to the individual elements by the rule

$$\Phi_{gh}(\mathbf{k})\equiv\Phi_g(h\mathbf{k})+\Phi_h(\mathbf{k}) \ . \tag{2.11}$$

This rule, which we shall call the *group compatibility condition,* plays a central role in determining the crystallographic and quasicrystallographic space groups, in specifying the extinctions, and in constructing real-space structures associated with a given space group.

Since every element in the point group G can be expressed as a product built from a small number of elements that generate G (never more than three, and except for the orthorhombic point group *mmm* never more than two in any of the cases considered here), the phase function for any element can be found from those for the point-group generators, by repeated applications of the group compatibility condition. There are, however, many different ways to express an element of G as a product of generators. In building the group from its generators one imposes a set of *generating relations* that guarantee all such expressions to be identical. These generating relations specify, through the group compatibility condition, constraints on the phase functions associated with the group generators. The constraints insure that the phase functions for the generators yield unique phase functions for arbitrary elements of G, independent of how those elements are expressed in terms of the generators. Applying these group compatibility conditions to the phase functions restricts them to a small number of forms, which are closely related to the space groups.

F. The lattice of wave vectors

Crystals, quasicrystals, and incommensurately modulated crystals share the property that their diffraction patterns consist of sharp Bragg peaks. Each peak determines a wave vector $\mathbf{k}$, according to the usual Laue rules, at which the density has a nonvanishing Fourier coefficient. In general, one expects that if the diffraction pattern has peaks at wave vectors $\mathbf{k}_1$ and $\mathbf{k}_2$, it may also have peaks at $\mathbf{k}_1\pm\mathbf{k}_2$. The Fourier components of the density are thus to be found within the set L of all integral linear combinations of wave vectors determined by the diffraction pattern.

We restrict ourselves to sets L that can be finitely indexed, by which we mean that any wave vector in L can be expressed as an integral linear combination of just D integrally independent wave vectors $\mathbf{b}^{(1)},\ldots,\mathbf{b}^{(D)}$:

$$\mathbf{k}=\sum_{i=1}^{D} n_i\mathbf{b}^{(i)} \ . \tag{2.12}$$

The vectors $\mathbf{b}^{(i)}$ are called generating vectors of L, and if L consists of *all* integral linear combinations, the $\mathbf{b}^{(i)}$ are called primitive generating vectors.

We call such a set L of wave vectors a *lattice*[12] and refer to D as the *indexing dimension* (or *rank*) of the lattice. If the indexing dimension D is equal to the dimension d of physical space, then the lattice is an ordinary crystallographic reciprocal lattice and is related, in the familiar way, to a lattice of translations in ordinary d-dimensional space.[13] Allowing D to exceed d admits incommensurately modulated crystals, quasicrystals, and incommensurately modulated quasicrystals, none of which have the translational symmetry of a d-dimensional crystal. We shall not deal here with the complexities of sets of wave vectors that cannot be finitely indexed.

We are thus developing crystallography not as a scheme to classify the exact symmetries of periodic real-space structures, but as a scheme to classify the symmetries, to within indistinguishable differences, of struc-

[11]Other aspects of the Fourier-space perspective on extinctions are discussed in Sec. VI and illustrated by application to the space groups computed in Secs. III–V.

[12]The practice has arisen in the field of incommensurately modulated crystals of calling this set a Z module, reserving the term "lattice" for ordinary three-dimensional Bravais lattices. We do not adopt this nomenclature (a) because in the Fourier-space formulation both kinds of sets play identical roles, (b) because in the case of quasicrystals the intensities of the Bragg peaks do not identify a unique underlying three-dimensional Bravais lattice, and (c) because the habit of singling out on the basis of peak intensities a subset of the "Z module" for special treatment as the "lattice" runs counter to the spirit of a classification scheme based entirely on symmetry, and can lead one into trouble, as noted in Sec. VII.

[13]See Sec. II.H, below.

tures that give rise to diffraction patterns consisting of sharp Bragg peaks. For us the term "lattice" always refers only to the lattice (in the mathematical sense of a set closed under addition and subtraction) of wave vectors determined by the diffraction pattern—i.e., what crystallographers call the reciprocal lattice. The lattice can be viewed as the set of all integral linear combinations of wave vectors in the diffraction pattern or, equivalently, as the smallest set of vectors, closed under addition and subtraction, that contains all those vectors. Only in the special crystallographic case can "lattice" also refer to a real-space "direct" lattice dual to the lattice of wave vectors.

I shall not explore the subtleties of enumerating the distinct lattices that can exist with a given point-group symmetry. It is important, however, to note a few general points.

(a) The theorem that a three-dimensional lattice can have only n-fold symmetry axes for the crystallographic values $n=2$, 3, 4, or 6 relies critically on the assumption that there is a minimum distance between points of the lattice (and proceeds by demonstrating that, if an n-fold axis with any other n is present, then it can be used to construct from any pair of points another pair that is closer together.) Now a shortest distance between points is a *sine qua non* for a lattice in real space, viewed as a template for a periodic structure, for the structure itself is realized by putting down an appropriate atomic unit at each site of the real space lattice, and such units have a nonzero size. Our lattices, however, are in Fourier space, inferred from diffraction patterns consisting of Bragg peaks. Real diffraction experiments measure only a finite number of peaks. But it takes only a finite number (at least D, but, if properly chosen, not enormously more than D) to determine the mathematical lattice. Each vector of that lattice is associated with a possible density Fourier coefficient and therefore with a possible Bragg peak. However, in any real experiment the resolution will be less than perfect, and all but a finite number of the peaks will be unobservable. That lattices with $D>d$ have points that are arbitrarily close together—"dense" in the mathematical sense—has its physical counterpart in the fact that their diffraction patterns reveal more and more Bragg peaks between existing ones, as the resolution of the apparatus is made better and better.

(b) A *quasicrystal,* as opposed to an *incommensurately modulated crystal* (or an *incommensurately modulated quasicrystal),* is a material with a noncrystallographic point group and a lattice with the smallest possible rank D compatible with that point group.[14] Thus icosahedral lattices have rank 6. Lattices with lower rank cannot have icosahedral symmetry, and lattices of higher rank with icosahedral symmetry are better viewed as describing incommensurately modulated icosahedral quasicrystals, just as lattices of rank higher than 3 with crystallographic point groups are associated with incommensurately modulated crystals.

(c) There are just three distinct varieties of icosahedral lattice,[15] a fact that was conjectured immediately after the discovery of icosahedral quasicrystals but proved only with some effort (Rokhsar, Mermin, and Wright, 1987). The icosahedral lattices bear a close relation to the three three-dimensional cubic lattices and are described in detail in Sec. III.

(d) Aside from the icosahedral group, all other noncrystallographic point groups in three dimensions are axial—they have a unique n-fold axis of highest symmetry with $n=5$ or $n>6$. Space groups for materials with axial lattices are described in RMRW, and will not concern us here, but I briefly describe their lattices, to convey a sense of the issues we neglect here by taking the lattices for granted (Mermin, Rabson, Rokhsar, and Wright, 1990.)

When n is less than 23 the situation is uncomplicated. The lattices are periodic stackings of a unique plane lattice perpendicular to the n-fold lattice, consisting of all integral linear combinations of an n-fold star of vectors of equal length, separated in angle by $2\pi/n$. If successive layers of the stacking have no displacement perpendicular to the n-fold axis ("vertical stackings"), then n is necessarily even, and this state of affairs continues to hold for all even n less than 46. A single stacking with an additional horizontal shift[16] ("staggered stacking") is possible only when n is a power of a single prime number p (i.e., $n=5,7,8,9,11,13,16,17,19$), and this stacking repeats every p layers. Crystallographic examples of staggered stackings are the rhombohedral ($n=3$) and centered tetragonal ($n=4=2^2$) lattices.

These lattices continue to exist for larger values of n, but when n is 23 or larger (staggered stackings) or 46 or larger (vertical stackings) then it is one of the great discoveries of number theory (made, coincidentally and in an entirely unrelated context, in the same decade of the 19th century that Bravais completed the classification scheme for crystallographic lattices) that there can be additional "nonstandard" two-dimensional sublattices of great complexity. Although the existence of nonstandard lattices is of great conceptual importance, demonstrating as it does that the sufficiency of standard lattices for smaller values of n is a highly nontrivial matter, practical quasicrystallographers would be well advised to ignore them until the day when a homogeneous material is discovered with a 46-fold diffraction pattern. (Recent

[14]This is the point of view of Rokhsar, Mermin, and Wright, 1987. There is still not complete agreement on how these distinctions ought to be made.

[15]The overwhelming majority of icosahedral quasicrystals have P lattices, but an I^* (F) lattice has been reported in the Al-Cu-Fe system by Ebalard and Spaepen, 1989.

[16]There might appear to be more than one possible shift, but it has been shown that all of them differ by no more than a rotation and a rescaling.

work by Renn and Lubensky suggests that the day may be coming. For a review see Lubensky, 1991).

G. The space-group classification scheme

Suppose two materials have the same lattice and the same point group acting in the same way on their lattices. If their phase functions differ only by a gauge transformation, then we say the materials belong to the same space group. This generalization of the space-group concept makes it a classification scheme based on phase relations between Fourier coefficients at symmetry-related points (rather than a group of transformations in real space).[17]

From the reciprocal-space point of view, the space groups are just the distinct classes of gauge-equivalent phase functions, with one additional proviso:

There is a set of conditions under which one should assign gauge-inequivalent phase functions to the same space group. This may happen if there are proper operations h not in the point group of the material, that leave the lattice of wave vectors invariant and for which the group hGh^{-1} (i.e., the group of all operations hgh^{-1} with g in G) acts on the lattice in the same way as G itself. Under these circumstances, phase functions defined by

$$\Psi_g(\mathbf{k})=\Phi_{hgh^{-1}}(h\mathbf{k}) \tag{2.13}$$

should clearly not be associated with a different space group from the $\Phi_g(\mathbf{k})$, since they merely describe the same point group, operating in a different, but entirely equivalent, manner with respect to the lattice. Indeed, when h does belong to the point group G, then the Ψ_g and Φ_g are easily seen to be gauge equivalent, for repeated application of the group compatibility condition (2.11) to the definition (2.13) of Ψ_g gives

$$\Psi_g(\mathbf{k})\equiv\Phi_h(g\mathbf{k})+\Phi_g(\mathbf{k})+\Phi_{h^{-1}}(h\mathbf{k}) . \tag{2.14}$$

But application of Eq. (2.11) to $e=h^{-1}h$ gives

$$0\equiv\Phi_e(\mathbf{k})\equiv\Phi_{h^{-1}}(h\mathbf{k})+\Phi_h(\mathbf{k}) , \tag{2.15}$$

and therefore Ψ_g and Φ_g are indeed gauge equivalent, with Φ_h playing the role of the gauge function χ in Eq. (2.10):

$$\Psi_g(\mathbf{k})\equiv\Phi_g(\mathbf{k})+\Phi_h([g-1]\mathbf{k}) . \tag{2.16}$$

When h is not in the point group G, however, Φ_h is not defined, and Ψ_g and Φ_g need not in general be gauge equivalent, even though the two space-group categories they specify should not be viewed as distinct. As we shall see below (Sec. III.H), this situation occurs in a single instance in the cubic case, when the point group G is only tetrahedral and h is a fourfold rotation. It also occurs in the quasicrystallographic icosahedral case when h is a rescaling of the lattice by an appropriate factor λ, a lattice symmetry forbidden in the crystallographic case that clearly leaves each individual element of G invariant: $\lambda g(\mathbf{k}/\lambda)=g\mathbf{k}$. It occurs routinely in the orthorhombic case, where h combines a point-group operation with independent rescalings along two or more orthogonal directions. And in certain axial quasicrystals it occurs with h a combination of a rescaling and an element not in the point group, as described in RMRW.

If the point group G lacks the inversion i, then this situation also arises with $h=i$, since all lattices have inversion symmetry, and clearly $igi\mathbf{k}=g\mathbf{k}$. If we applied the rule here too we would identify enantiamorphic pairs of space groups, arriving at 219 distinct three-dimensional space groups instead of the conventional 230. There is, however, a sound argument for not making such an identification when the operation h is improper. When h is a proper point-group operation and/or a rescaling, one can devise a continuous family of rotations and/or rescalings that take a structure with one set of phase functions into another one with the gauge-inequivalent set. There is thus genuinely no basis for distinguishing the space group of one from the other. When h is improper, however, there is no way continuously to deform a structure from one space group to the other, and the two sets of phase functions can unambiguously be distinguished, though which is which depends on an arbitrary convention.[18]

H. Special features of the crystallographic case

When the indexing dimension D is equal to the dimension d of physical space, then the lattice of wave vectors *is* dual to a lattice of real-space translations, and the relation between the concepts developed above and conventional crystallography is recovered. The crucial point is that it is then possible to define a real-space basis dual to the $\mathbf{b}^{(i)}$ satisfying

$$\mathbf{a}^{(i)}\cdot\mathbf{b}^{(j)}=2\pi\delta_{ij} , \quad i,j=1,\ldots,d . \tag{2.17}$$

Since any wave vector in the lattice is of the form

[17]We nevertheless retain the term "space group" since the scheme does have a natural group-theoretic interpretation in the crystallographic case. It can be given such an interpretation in the quasicrystallographic case by going to an unphysically large number of dimensions ("superspace"—see Sec. II.I below), an excursion which from our point of view serves no purpose beyond justifying the nomenclature (Rabson, Ho, and Mermin, 1988). More than one person has told me that what I am calculating here are cohomology groups. I have found this information less valuable than M. Jourdain found the news that he was speaking prose, but am too ignorant to state with confidence that this is not a useful point of view.

[18]Which I hope, but am reluctant to guarantee, is honored in Table IX for cubic space groups Nos. 212 and 213.

$\mathbf{k}=\sum_i n_i\mathbf{b}^{(i)}$, any gauge function χ, by linearity, can be expressed in the form

$$2\pi\chi(\mathbf{k})=2\pi\sum_i n_i\chi(\mathbf{b}^{(i)})\equiv\mathbf{k}\cdot\sum_i\chi(\mathbf{b}^{(i)})\mathbf{a}^{(i)} . \tag{2.18}$$

As a result, if ρ' and ρ are indistinguishable densities whose Fourier coefficients (2.2) differ only by a phase as in (2.6), then in real space they will be related by

$$\rho'(\mathbf{r})=\rho(\mathbf{r}+\sum_i\chi(\mathbf{b}^{(i)})\mathbf{a}^{(i)}) . \tag{2.19}$$

Thus indistinguishable densities can differ at most by a real-space translation, and we are back to ordinary crystallography. If the gauge function χ is the phase function Φ_g associated with a point-group operation g, then we have

$$\rho(g\mathbf{r})=\rho(\mathbf{r}+\sum_i\mathbf{a}^{(i)}\Phi_g(\mathbf{b}^{(i)})) , \tag{2.20}$$

which specifies the real-space translation that combines with g to leave the density invariant. A gauge transformation on the phase function corresponds to the effect on that real-space translation of a change of the origin through which g acts.

I. The superspace approach

If one is used to developing crystallography in real space, the facts in Sec. II.H above are so comfortably familiar that it is tempting to try to cast the case $D>d$ into the same mold. To do this one extends the D vectors $\mathbf{b}^{(i)}$ into an independent set $\mathbf{B}^{(i)}$ in D dimensions,[19] whose first d components agree with those of the $\mathbf{b}^{(i)}$. One then introduces a dual basis $\mathbf{A}^{(i)}$ in "real" D-dimensional space satisfying

$$\mathbf{A}^{(i)}\cdot\mathbf{B}^{(j)}=2\pi\delta_{ij} , \quad i,j=1,\ldots,D . \tag{2.21}$$

One introduces a D-dimensional position vector $\mathbf{R}$ whose first d components lie in ordinary real space, and one extends each d-dimensional wave vector $\mathbf{k}=\sum n_i\mathbf{b}^{(i)}$ determined by the diffraction pattern into a D vector $\mathbf{K}=\sum_i n_i\mathbf{B}^{(i)}$. The physical density $\rho(\mathbf{r})$ is then a "slice" in the first d dimensions of the (periodic) superspace density $\rho(\mathbf{R})=(1/V)\sum\rho(\mathbf{k})e^{i\mathbf{K}\cdot\mathbf{R}}$, and a gauge-equivalent density satisfies $\rho'(\mathbf{R})=\rho(\mathbf{R}+\sum\chi(\mathbf{b}^{(i)})\mathbf{A}^{(i)})$. As in the crystallographic case, gauge-equivalent densities then differ by translations, which in general have components outside of the physical subspace. The real-space distortion corresponding to the component of the translation outside the physical subspace is described as a *phason*.

[19]In general there is no uniquely natural way to do this. In the icosahedral case there is. Although we make no use of it here, it is useful in building real-space structures and is therefore given explicitly for each of the three icosahedral lattices in Appendix B.

This is a useful and important trick for many purposes—notably to help in building real-space structures with the observed diffraction patterns. It is not, however, to be recommended for extracting the space-group classification scheme unless one is so wedded to doing crystallography for periodic structures in real space that one would prefer to squeeze the results of D-dimensional crystallography down into d dimensions rather than directly developing them in d-dimensional Fourier space for quasiperiodic structures. Since developing the d-dimensional crystallography of ordinary periodic structures in d-dimensional Fourier space is a much simpler exercise than developing it in d-dimensional real space, there is no advantage and considerable disadvantage to be had from exploring higher-dimensional crystallography for this particular purpose.

J. Real-space structures with a given space group

Given a point group G, a lattice of wave vectors primitively generated by $\mathbf{b}^{(i)}$, and the phase functions $\Phi_g(\mathbf{k})$ appropriate to a given space group, it is easy to construct a real-space specimen of a structure with that space group. The key is to define a set of density Fourier coefficients by

$$\rho(\mathbf{k})=\sum_h f(h\mathbf{k})e^{-2\pi i\Phi_h(\mathbf{k})} , \tag{2.22}$$

where the sum is over all elements h of the point group G, and where f is any function on the lattice of wave vectors that satisfies $f^*(-\mathbf{k})=f(\mathbf{k})$ (to ensure that $\rho(\mathbf{r})$ is real).

We then have

$$\rho(g\mathbf{k})=\sum_h f(hg\mathbf{k})e^{-2\pi i\Phi_h(g\mathbf{k})} . \tag{2.23}$$

The group compatibility condition (2.11) tells us that

$$\Phi_{hg}(\mathbf{k})\equiv\Phi_h(g\mathbf{k})+\Phi_g(\mathbf{k}) , \tag{2.24}$$

so that

$$\rho(g\mathbf{k})=e^{2\pi i\Phi_g(\mathbf{k})}\sum_h f(hg\mathbf{k})e^{-2\pi i\Phi_{hg}(\mathbf{k})} . \tag{2.25}$$

But for fixed g in G, as h runs through all the elements of G so does hg. The sum on the right side of Eq. (2.25) is therefore identical to the sum on the right side of Eq. (2.22), which establishes that the Fourier coefficients $\rho(\mathbf{k})$ satisfy Eq. (2.9). Thus $\rho(\mathbf{k})$ as defined in Eq. (2.22) will indeed be the Fourier transform of a density characterized by a space group with the given phase functions, provided only that it does not vanish systematically on a set of wave vectors so large that the lattice is thinned out to a sublattice for which the space group has a different character. We can avoid this pitfall by taking the function $f(\mathbf{k})$ to lack any symmetry under the operation of the point group G. One such choice is

$$f(\mathbf{k})=e^{i\mathbf{k}\cdot\mathbf{r}_0}f_0(\mathbf{k}) , \tag{2.26}$$

where f_0 is invariant under the operations of G, but $\mathbf{r}_0$ is a generic vector, left invariant under none of them.

In the crystallographic case this choice (with $f_0=1$) has a direct geometrical interpretation in real space, since the phase function appearing in Eq. (2.22) can be expressed [using (2.18)] as

$$2\pi\Phi_h(\mathbf{k})\equiv\mathbf{k}\cdot\sum_i\Phi_h(\mathbf{b}^{(i)})\mathbf{a}^{(i)}\ , \tag{2.27}$$

where the $\mathbf{a}^{(i)}$ are the basis for the real-space direct lattice dual to the $\mathbf{b}^{(i)}$ satisfying the orthogonality relations (2.17). Consequently Eq. (2.22) reduces to

$$\rho(\mathbf{k})=\sum_h\exp(ih\mathbf{k}\cdot\mathbf{r}_0)\exp[-i\mathbf{k}\cdot\sum_i\Phi_h(\mathbf{b}^{(i)})\mathbf{a}^{(i)}]\ . \tag{2.28}$$

Since we are summing over the whole group G, we can replace h in the summand by h^{-1} and note that $h^{-1}\mathbf{k}\cdot\mathbf{r}_0=\mathbf{k}\cdot h\mathbf{r}_0$. Using Eq. (2.15) to reexpress $\Phi_{h^{-1}}(\mathbf{b}^{(i)})$ as $-\Phi_h(h^{-1}\mathbf{b}^{(i)})$, we have

$$\rho(\mathbf{k})=\sum_h\exp\{i\mathbf{k}\cdot[h\mathbf{r}_0+\sum_i\Phi_h(h^{-1}\mathbf{b}^{(i)})a^{(i)}]\}\ , \tag{2.29}$$

But this is precisely the "geometrical structure factor" that describes a set of points given by displacing through all the vectors of the real-space lattice a basis consisting of a collection of points—one for each member h of the point group G—at the positions ("general Wyckoff positions")

$$\mathbf{r}_h=h\mathbf{r}_0+\sum_i\Phi_h(h^{-1}\mathbf{b}^{(i)})\mathbf{a}^{(i)}\ . \tag{2.30}$$

K. Computing space groups: an overview

To compute the space groups for a specified lattice and point group, we must find the classes of gauge-equivalent phase functions; i.e., we must find the general solutions to the group compatibility condition (2.11) and classify them by gauge equivalence class. We must then check to see whether any of those classes should be associated with the same space group, because of operations that leave the lattice invariant but are not in the point group, as described in Sec. II.G above, but this is a simple and straightforward procedure.[20]

In carrying out the determination of the gauge equivalence classes it is important to use a set of vectors $\mathbf{b}^{(i)}$ that generate the lattice primitively. The advantage of primitive lattice generators is that the generating vectors $\mathbf{b}^{(i)}$ are themselves in the lattice, and must therefore themselves satisfy the group compatibility condition (2.11). Because the phase functions are linear, if they satisfy the group compatibility condition at the lattice-generating vectors, they will satisfy it everywhere. It is thus enough to impose the group compatibility condition on the lattice-generating vectors themselves.[21]

The group compatibility conditions need only be applied to the phase functions associated with each point-group generator.[22] Since these phase functions in turn need only be determined at the lattice-generating vectors, the problem reduces to the computation of a small number of phases, $\Phi_g(\mathbf{b}^{(i)})$. The number of these phases is just the number of point-group generators (at most 3) times the number of primitive lattice-generating vectors (6 in the icosahedral case and 3 in the crystallographic cases).

The sought-for phases are determined by the point-group generating relations which impose linear relations on those phases through the group compatibility condition (2.11). The gauge degrees of freedom[23] (6 in the icosahedral case and 3 in the crystallographic case) play a central role in solving these linear relations. To specify a given gauge equivalence class it is enough to specify a single member of that class (the entire class then being given by applying an arbitrary gauge transformation to that given member). By using the gauge freedom to eliminate some of the unknown phases at the start of the calculation, and carefully using at subsequent stages whatever gauge freedom remains to reduce the possible forms of the remaining phases, we can always arrive at a unique representative of each gauge equivalence class. The problem of classifying the general solutions by gauge equivalence class is thus solved by the same procedure that produces the general solutions.[24]

The cubic and icosahedral space groups offer the most spectacular examples of the procedure, since every point group is generated by only two of its elements, and the phase function for one of the point-group generators can always be made to vanish at all lattice-generating vectors by an initial choice of gauge. One is therefore computing only three (cubic) or six (icosahedral) numbers.

The weary reader should bear in mind that although what follows, when we descend to particular cases, may

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[20]Except that it has sometimes been overlooked.

[21]The analysis is more intricate if the lattice is represented in terms of a set of nonprimitive generating vectors with restrictions on the indexing, as in Bienenstock and Ewald, 1962.

[22]They then insure that the phase function for any other point-group element can be computed from the point group generating relations, with a result that does not depend on how one chooses to express that element as a product of generators.

[23]In the crystallographic case the choice of gauge is equivalent to the choice of real-space origin; in the icosahedral case it can be viewed as the choice of origin in superspace, or the choice of real space origin combined with the choice of "local isomorphism class." From the point of view of Fourier space this is of little interest.

[24]One can always confirm at the end of the calculation that two gauge equivalence classes arrived at in this way are indeed distinct, by finding gauge-invariant linear combinations of phase functions that have different values in the two classes. The real burden of the calculation is to make sure one gets a representative of *every* class.

look dense and elaborate, this is only because we are calculating the space groups in every possible case. We shall be examining seven icosahedral or cubic point groups each of which can be associated with three different lattices, leading to 21 cases, three orthorhombic point groups each of which can be associated with four different lattices, leading to 13 cases,[25] three monoclinic point groups associated with two lattices, and two triclinic point groups with a single lattice. The method can be applied directly to any one of these 42 cases, where the ensuing calculation is extremely brief. The reader is strongly urged not to plow through all 42 cases, but to read selectively at the level of individual cases, to see how easily the space groups for any particular point group and lattice emerge.

III. THE CUBIC AND ICOSAHEDRAL SPACE GROUPS

A. Generators for the cubic and icosahedral point groups

The computation of the space groups associated with a given lattice and point group can be made quite easy by a judicious choice of the point-group generators and the vectors that primitively generate the lattice. (Conversely, an injudicious choice can make it significantly more cumbersome.) The trick is to try to have among the point-group generators one or more operations whose phase functions can be made simple in an appropriate gauge, and to select as lattice-generating vectors sets that behave in an especially transparent way under those operations.

For each of the two icosahedral and five cubic groups, the most efficacious choice of point group generators and lattice-generating vectors exploits the presence of a threefold axis and the existence of primitive lattice-generating vectors that are symmetrically disposed about that axis. Each of the seven points groups can be generated by an operation associated with the threefold axis and a second operation of order 2 (see Figs. 1–3):

(i) One generator, g_3, is either a threefold rotation r_3 or a threefold rotoinversion $\bar{r}_3 = ir_3$ (where i is the inversion, $i:\mathbf{k}\rightarrow -\mathbf{k}$):

(ii) The other generator, g_2, is either a twofold rotation r_2 or a mirror m, which can also be viewed as a twofold rotoinversion about an axis normal to the invariant plane of the mirror: $m=\bar{r}_2=ir_2$.

These choices for the generators are summarized in Table I, which also lists the generating relations. Note that the groups[26] Y_h, O_h, and T_h are all generated by a threefold rotoinversion and a mirror, and Y, O, and T by a threefold and twofold rotation. The three point groups in each of these two sets differ only in the order (fivefold, fourfold, or threefold) of the rotation given by the product of the two generators. T_d is in a class by itself, being generated by a threefold rotation and a mirror.

B. Vanishing of the phase functions for the threefold generators

Since there are only two generators, we require only two phase functions. The analysis is enormously simplified by the fact that *we can always work in a gauge in which the phase function associated with the threefold rotation (or rotoinversion) is zero,* thereby reducing the problem to a determination of the single phase function Φ_{g_2}.

1. The vanishing of the rotoinversion phase function

Note that, acting on any vector,

$$(\bar{r}_3-1)(1+\bar{r}_3+\bar{r}_3^{\,2})=\bar{r}_3^{\,3}-1=-2\ , \tag{3.1}$$

since $\bar{r}_3^{\,3}$ is the inversion. Consequently if we define a linear gauge function by

$$\chi(\mathbf{k})=\tfrac{1}{2}\Phi_{\bar{r}_3}([1+\bar{r}_3+\bar{r}_3^{\,2}]\mathbf{k})\ , \tag{3.2}$$

then the general definition (2.10) of a gauge transformation gives

$$\Delta\Phi_{\bar{r}_3}(\mathbf{k})=\chi([\bar{r}_3-1]\mathbf{k})=-\Phi_{\bar{r}_3}(\mathbf{k})\ , \tag{3.3}$$

which sets $\Phi_{\bar{r}_3}$ to zero.

2. The vanishing of the rotation phase function

Here the vanishing depends critically on the fact that each cubic lattice can be primitively generated by a set of three vectors that is invariant under r_3, and the fact that each icosahedral lattice can be primitively generated by six vectors consisting of two such sets. Call the cubic

[25] One of the point groups can be associated with one of the lattices in two distinct ways.

[26] Although I adhere to the international point-group notation at solemn moments (in tables and important equations), I freely use the old Schönflies names in the text when they are easier on the eye and ear. Though less informative, Y is more attractive and euphonious than 532. In the orthorhombic case the Schönflies names are not much more humane than their international counterparts, and I use them less.

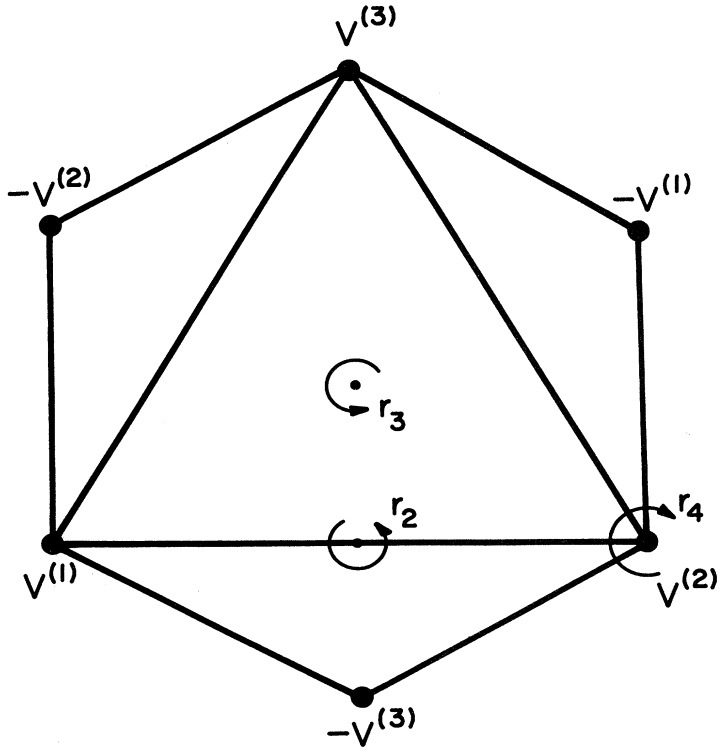

FIG. 1. An octahedron, viewed along an axis of threefold symmetry. The vectors $\mathbf{v}^{(1)}$, $\mathbf{v}^{(2)}$, and $\mathbf{v}^{(3)}$ are along the fourfold axes and generate the cubic P lattice. Primitive generating vectors $\mathbf{b}^{(1)}$, $\mathbf{b}^{(2)}$, and $\mathbf{b}^{(3)}$ for the three cubic lattices that are symmetrically situated about the threefold axis are defined in terms of the $\mathbf{v}^{(i)}$ in Eqs. (3.17), (3.18), and (3.19). The generating vectors for the F^* (I) lattice point toward the centers of the three octahedral edges surrounding the central face. Those for the I^* (F) lattice point towards the centers of the three octahedral faces surrounding the central one. The senses of the twofold, threefold and fourfold rotations r_2, r_3, and $r_4=r_3r_2$ are as indicated. The axis of $r_2'=r_4^2$ is the same as the axis of r_4; the axis of $r_3'=r_3r_2'$ passes through the center of the triangular face with vertices $-\mathbf{v}^{(1)},\mathbf{v}^{(2)},\mathbf{v}^{(3)}$. The mirrors m and m' are in planes perpendicular to the axes of r_2 and r_2'.

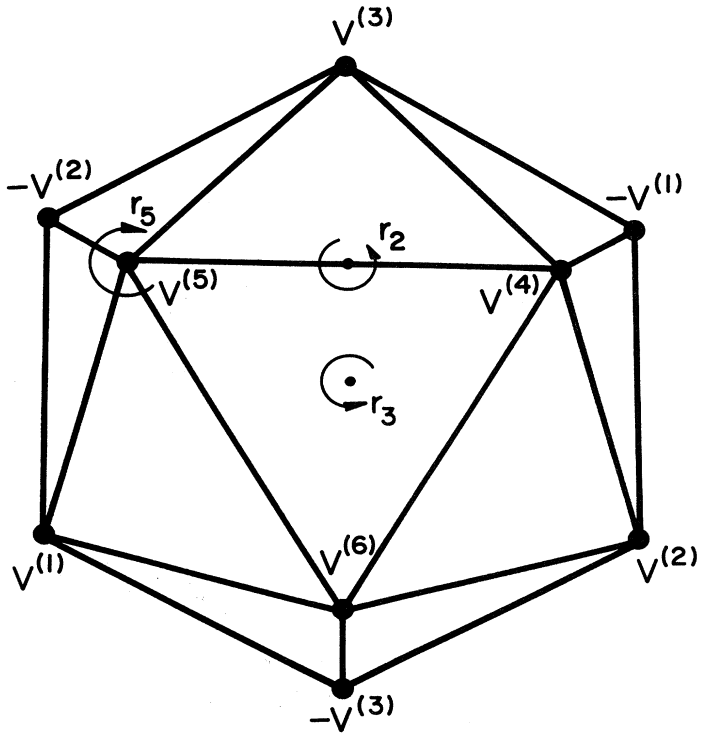

FIG. 2. An icosahedron, viewed along an axis of threefold symmetry. The threefold-symmetric set of vectors $\mathbf{v}^{(1)},\ldots,\mathbf{v}^{(6)}$ are along the fivefold axes and generate the icosahedral P lattice. Threefold-symmetric sets of six primitive generating vectors for the icosahedral F^* (I) and I^* (F) lattice are given in Eqs. (3.21) and (3.22). The senses of the twofold, threefold, and fivefold rotations r_2, r_3, and $r_5=r_3r_2$ are as indicated. The mirror m is in the plane perpendicular to the axis of r_2.

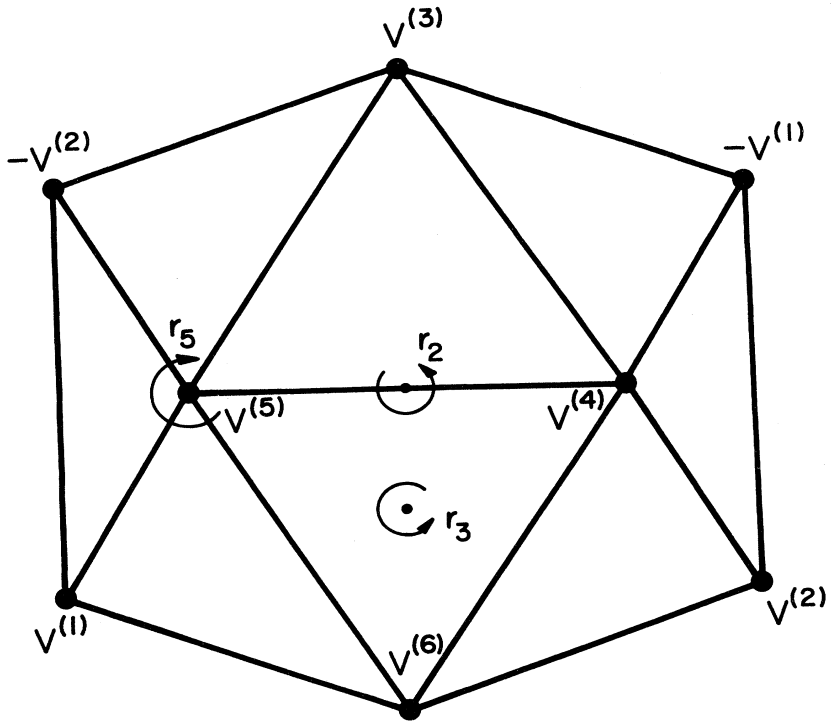

FIG. 3. The icosahedron of Fig. 2, viewed straight down the twofold axis of r_2, to emphasize that under the twofold rotation r_2, $\mathbf{v}^{(1)}\to-\mathbf{v}^{(1)}$, $\mathbf{v}^{(2)}\to-\mathbf{v}^{(2)}$, $\mathbf{v}^{(3)}\to\mathbf{v}^{(6)}$, $\mathbf{v}^{(4)}\to\mathbf{v}^{(5)}$. Note that the vectors $\mathbf{v}^{(1)}$, $\mathbf{v}^{(2)}$, $\mathbf{v}^{(6)}-\mathbf{v}^{(3)}$, and $\mathbf{v}^{(5)}-\mathbf{v}^{(4)}$ all lie in the plane of the mirror $m=ir_2$.

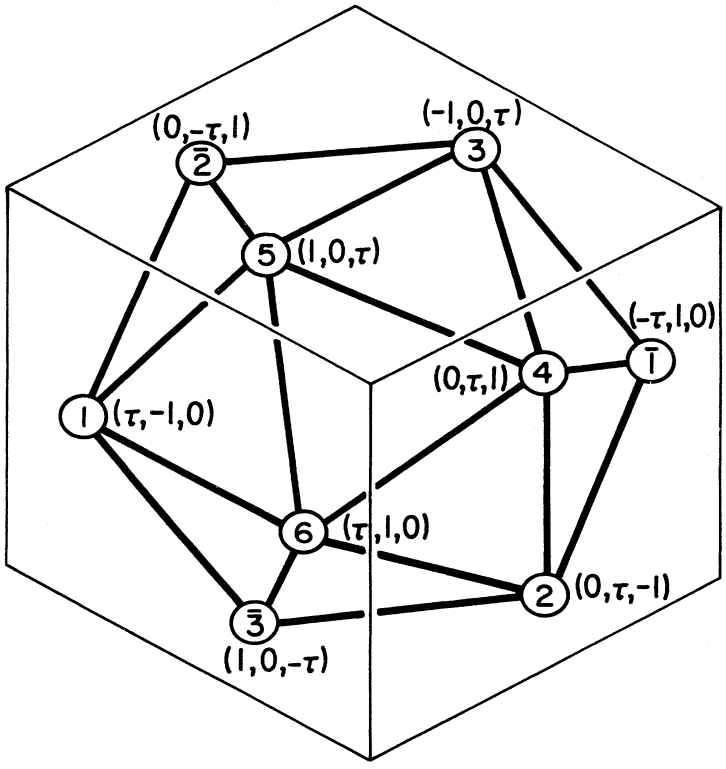

FIG. 4. The icosahedron of Figs. 2 and 3, inscribed in a cube of side 2τ. Each edge of the icosahedron has length 2. The vertices are numbered to correspond to the vectors $\mathbf{v}^{(i)}$ in Figs. 2 and 3. For edges in the cube faces to have the same length as the edges connecting points in different faces, we must have $\tau^2=1+\tau$, which fixes τ at the golden mean. The F^* generating vectors $\mathbf{b}^{(4)}=\mathbf{v}^{(4)}-\mathbf{v}^{(1)}$ and $\mathbf{b}^{(1)}=\mathbf{v}^{(2)}+\mathbf{v}^{(3)}$ are $(-\tau,\tau+1,1)$ and $(-1,\tau,\tau-1)$. Because τ is the golden mean, it follows that $\mathbf{b}^{(4)}=\tau\mathbf{b}^{(1)}$. The I^* generating vector $\mathbf{b}^{(4)}=\mathbf{v}^{(1)}-\mathbf{v}^{(2)}-\mathbf{v}^{(3)}-\mathbf{v}^{(4)}+\mathbf{v}^{(5)}+\mathbf{v}^{(6)}$ is $2(\tau+1,-\tau,0)$ which is $2\tau\mathbf{v}^{(1)}=\tau\mathbf{b}^{(1)}$. Note finally that the sum $\mathbf{v}^{(1)}-\mathbf{v}^{(2)}+\mathbf{v}^{(3)}+\mathbf{v}^{(4)}+\mathbf{v}^{(6)}$ of the 5-vectors surrounding $\mathbf{v}^{(5)}$ is $(2\tau-1,0,2+\tau)$, which is $(2\tau-1)\mathbf{v}^{(5)}=(\tau^3-2)\mathbf{v}^{(5)}$.

generators and one of the threefold symmetric subsets of icosahedral generators $\mathbf{b}^{(1)}$, $\mathbf{b}^{(2)}$, and $\mathbf{b}^{(3)}$; call the second symmetric icosahedral set $\mathbf{b}^{(4)}$, $\mathbf{b}^{(5)}$, and $\mathbf{b}^{(6)}$. We shall always work with such primitive generating vectors, transforming under r_3 by the cyclic permutations

$$\begin{aligned} r_3:\ & \mathbf{b}^{(1)}\to\mathbf{b}^{(2)}\ ,\ \mathbf{b}^{(2)}\to\mathbf{b}^{(3)}\ ,\ \mathbf{b}^{(3)}\to\mathbf{b}^{(1)}\ , \\ & \mathbf{b}^{(4)}\to\mathbf{b}^{(5)}\ ,\ \mathbf{b}^{(5)}\to\mathbf{b}^{(6)}\ ,\ \mathbf{b}^{(6)}\to\mathbf{b}^{(4)}\ . \end{aligned} \tag{3.4}$$

Explicit forms for these vectors are given below in Sec. III.D.

In the cubic case, a gauge function χ will give a gauge transformation (2.10) that reduces Φ_{r_3} to zero, if it reduces it to zero at the three lattice-generating vectors:

$$\begin{aligned} \Delta\Phi_{r_3}(\mathbf{b}^{(1)}) &\equiv -\Phi_{r_3}(\mathbf{b}^{(1)}) \equiv \chi(\mathbf{b}^{(2)})-\chi(\mathbf{b}^{(1)})\ , \\ \Delta\Phi_{r_3}(\mathbf{b}^{(2)}) &\equiv -\Phi_{r_3}(\mathbf{b}^{(2)}) \equiv \chi(\mathbf{b}^{(3)})-\chi(\mathbf{b}^{(2)})\ , \\ \Delta\Phi_{r_3}(\mathbf{b}^{(3)}) &\equiv -\Phi_{r_3}(\mathbf{b}^{(3)}) \equiv \chi(\mathbf{b}^{(1)})-\chi(\mathbf{b}^{(3)})\ . \end{aligned} \tag{3.5}$$

These three equations have a solution for the three $\chi(\mathbf{b}^{(i)})$ if and only if

$$\Phi_{r_3}(\mathbf{b}^{(1)})+\Phi_{r_3}(\mathbf{b}^{(2)})+\Phi_{r_3}(\mathbf{b}^{(3)}\equiv 0\ . \tag{3.6}$$

But Eq. (3.6) is precisely the constraint imposed on Φ_{r_3} by the group compatibility condition (2.11) applied twice to the generating relation $r_3^3=e$:

$$\begin{aligned} 0\equiv\Phi_{r_3^3}(\mathbf{b}^{(i)}) &\equiv \Phi_{r_3}(r_3^2\mathbf{b}^{(i)})+\Phi_{r_3^2}(\mathbf{b}^{(i)}) \\ &\equiv \Phi_{r_3}(r_3^2\mathbf{b}^{(i)})+\Phi_{r_3}(r_3\mathbf{b}^{(i)})+\Phi_{r_3}(\mathbf{b}^{(i)})\ . \end{aligned} \tag{3.7}$$

Therefore the required gauge function exists.

The above analysis holds in the icosahedral case for the lattice-generating vectors $\mathbf{b}^{(1)}$, $\mathbf{b}^{(2)}$, and $\mathbf{b}^{(3)}$, and independently for $\mathbf{b}^{(4)}$, $\mathbf{b}^{(5)}$, and $\mathbf{b}^{(6)}$. Thus a gauge can again be found in which Φ_{r_3} vanishes at all the lattice-generating vectors and hence everywhere (by linearity).

3. Remaining gauge freedom

It is important to note that, whether the threefold generator is $\bar{r}_3$ or r_3, there remains an additional freedom of choice of gauge consistent with keeping the associated phase functions $\Phi_{\bar{r}_3}$ or Φ_{r_3} zero.

If the rotoinversion $\bar{r}_3$ is a generator, a further gauge function χ_1 will yield a gauge transformation (3.3) that does not alter $\Phi_{\bar{r}_3}$ if and only if it satisfies

$$\chi_1(\bar{r}_3\mathbf{b}^{(i)})\equiv\chi_1(\mathbf{b}^{(i)}) \tag{3.8}$$

for all the lattice-generating vectors. The condition (3.8) requires $\chi_1(\mathbf{b}^{(i)})$ to have the same value (modulo an integer) on $\mathbf{b}^{(i)}$ and all the images of $\mathbf{b}^{(i)}$ under repeated applications of $\bar{r}_3$. Since one of those images is $\bar{r}_3^{\,3}\mathbf{b}^{(i)}=i\mathbf{b}^{(i)}=-\mathbf{b}^{(i)}$, that value can be only 0 or $\frac{1}{2}$. So for the point groups with $\bar{r}_3$ as a generator, within the gauge in which $\Phi_{\bar{r}_3}$ vanishes, two sets of phase functions will be gauge equivalent if they are related by a gauge transformation given by

$$\begin{aligned} &\chi_1(\mathbf{b}^{(1)})\equiv\chi_1(\mathbf{b}^{(2)})\equiv\chi_1(\mathbf{b}^{(3)})\equiv\alpha\ , \\ &\chi_1(\mathbf{b}^{(4)})\equiv\chi_1(\mathbf{b}^{(5)})\equiv\chi_1(\mathbf{b}^{6})\equiv\beta\ , \end{aligned} \tag{3.9}$$

where α and β can be independently 0 or $\frac{1}{2}$. (The second equation applies only in the icosahedral case.)

If the rotation r_3 is a generator, the remaining degree of gauge freedom is less restricted. A gauge transformation (3.5) does not alter Φ_{r_3} if and only if

$$\chi_1(r_3\mathbf{b}^{(i)})\equiv\chi_1(\mathbf{b}^{(i)})\ , \tag{3.10}$$

so $\chi_1(\mathbf{b}^{(i)})$ satisfying Eq. (3.9) for arbitrary α and (in the icosahedral case) β gives a gauge transformation (3.5) that does not alter Φ_{r_3}.

TABLE I. Generators for the icosahedral and cubic point groups. The actions of the generators r_3 and r_2 are shown in Figs. 1 (cubic) and 2 (icosahedral), and the generator r_2' is a twofold rotation about the indicated fourfold axis in Fig. 1. The rotoinversion $\bar{r}_3$ is ir_3 where i is the inversion, and the mirrors m and m' are ir_2 and ir_2'. The first three sets of generating relations differ from the last four because it is $\bar{r}_3^{\,6}$ that is the identity, since $\bar{r}_3^{\,3}=i$, and because it is necessary to express the additional fact that i commutes with the twofold operation.

Schönflies	International	Generators	Point-Group Generating Relations
Y_h	$\bar{5}\bar{3}\frac{2}{m}$ $(53m)$	$\bar{r}_3$, m	$\bar{r}_3^6=m^2=(\bar{r}_3m)^5=e$, $\bar{r}_3^3m=m\bar{r}_3^3$
O_h	$\frac{4}{m}\bar{3}\frac{2}{m}$ $(m3m)$	$\bar{r}_3$, m	$\bar{r}_3^6=m^2=(\bar{r}_3m)^4=e$, $\bar{r}_3^3m=m\bar{r}_3^3$
T_h	$\frac{2}{m}\bar{3}$ $(m3)$	$\bar{r}_3$, m'	$\bar{r}_3^6=m'^2=(\bar{r}_3m')^3=e$, $\bar{r}_3^3m'=m'\bar{r}_3^3$
Y	532	r_3, r_2	$r_3^3=r_2^2=(r_3r_2)^5=e$
O	432	r_3, r_2	$r_3^3=r_2^2=(r_3r_2)^4=e$
T	23	r_3, r_2'	$r_3^3=r_2'^2=(r_3r_2')^3=e$
T_d	$\bar{4}3m$	r_3, m	$r_3^3=m^2=(r_3m)^4=e$

C. Conditions imposed on the phase functions by the generating relations

Since we work in a gauge in which the phase function Φ_{g_3} associated with the threefold generator vanishes, the

problem of determining the space groups reduces to finding the single phase function Φ_{g_2} associated with the twofold generator. This is accomplished by imposing the group compatibility condition (2.11) on all the generating relations listed in Table I.

All but three of those generating relations are of the form $g^n=e$ (with $n=2$, 3, 4, 5, or 6), leading [as in (3.7)] through repeated applications of (2.11) to

$$0\equiv\Phi_{g^n}(\mathbf{k})\equiv\Phi_g([1+g+\cdots+g^{n-1}]\mathbf{k}) . \tag{3.11}$$

Since Φ_{g_3} vanishes, this holds automatically when $g=g_3$. For the twofold operations g_2 it leads to the condition

$$0\equiv\Phi_{g_2}([1+g_2]\mathbf{k})\equiv\Phi_{g_2}(2P_{g_2}\mathbf{k}) , \tag{3.12}$$

which requires Φ_{g_2} to vanish at twice the projection of any vector in the invariant space of g_2 (either the twofold axis or the plane of the mirror).[27] For the n-fold operations of the form g_3g_2, our choice of gauge leads with Eq. (2.11) to

$$\Phi_{g_3g_2}(\mathbf{k})\equiv\Phi_{g_2}(\mathbf{k}) , \tag{3.13}$$

so that Eq. (3.11) applied to $g=g_3g_2$ reduces to a second condition on Φ_{g_2}:

$$0\equiv\Phi_{g_2}([1+g_3g_2+\cdots+(g_3g_2)^{n-1}]\mathbf{k})\equiv\Phi_{g_2}(nP_{g_n}\mathbf{k}) . \tag{3.14}$$

When g_3g_2 is a proper n-fold rotation, this requires Φ_{g_2} to vanish at n times the projection of any vector on the axis of that rotation. This is the only case we must consider, since when g_3g_2 is improper (which happens only for the point group T_d) $[1+g_3g_2+\cdots+(g_3g_2)^{n-1}]\mathbf{k}$ vanishes and the condition (3.14) is guaranteed to hold.

The three remaining generating relations (applicable only to the point groups Y_h, O_h, and T_h with $\bar{r}_3$ as a generator) assert that the inversion i commutes with the twofold generator g_2. Since $i=\bar{r}_3^3$, it follows from Eq. (3.11) that Φ_i vanishes in the gauge in which $\Phi_{\bar{r}_3}=0$. Applying Eq. (2.11) to $ig_2=g_2i$ and noting that $i\mathbf{k}=-\mathbf{k}$ we conclude that

$$\Phi_{g_2}(2\mathbf{k})\equiv 0 , \quad G=Y_h,O_h,T_h . \tag{3.15}$$

This restricts the values of Φ_{g_2} to 0 or $\frac{1}{2}$ for the groups having $\bar{r}_3$ as a generator.

[27]Quite generally, for any point-group operation g, we shall denote by P_g the operator that replaces $\mathbf{k}$ by its projection on the invariant subspace of g.

Because Φ_{g_2} can be taken to be the only nonvanishing phase function, to determine the cubic (icosahedral) space groups it is enough to determine the three (six) phases

$$\Theta_i=\Phi_{g_2}(\mathbf{b}^{(i)}) . \tag{3.16}$$

These phases are easily found by imposing on each of the primitive lattice-generating vectors $\mathbf{b}^{(i)}$ the two conditions (3.12) and (3.14) [and, when $\bar{r}_3$ is a generator, the further restriction (3.15)].

For the point groups Y_h, O_h, and T_h with $\bar{r}_3$ as a generator, the procedure is substantially simplified by the fact that the only allowed values for the phases Θ_i are 0 or $\frac{1}{2}$. On the other hand, the ability to simplify the analysis for these point groups by an appropriate further choice of gauge is subject to the restriction that the parameters α and β in Eq. (3.9) are also restricted to the values 0 or $\frac{1}{2}$. For the other four point groups Y, O, T, and T_d one cannot take advantage of an initial restriction on the phases Θ_i, but the corresponding lack of any restriction on α or β allows for a greater simplification by a judicious further choice of gauge.

D. The cubic and icosahedral lattices

To find their projections on the symmetry axes or in the mirror planes, we must explicitly specify the threefold-symmetric sets of lattice-generating vectors.

We first list the familiar threefold-symmetric sets of primitive generating vectors for the cubic lattices in terms of the orthonormal vectors $\mathbf{v}^{(1)}$, $\mathbf{v}^{(2)}$, and $\mathbf{v}^{(3)}$ along the fourfold axes of the octahedron in Fig. 1. For the simple cubic (P) lattice we have

Cubic P lattice:

$$\begin{aligned}\mathbf{b}^{(1)}&=\mathbf{v}^{(1)} ,\\ \mathbf{b}^{(2)}&=\mathbf{v}^{(2)} ,\\ \mathbf{b}^{(3)}&=\mathbf{v}^{(3)} .\end{aligned} \tag{3.17}$$

The lattice that is face centered in Fourier space [but indelibly labeled as the I lattice (body centered) because of the unfortunate emphasis on real space—we prefer to refer to it as the F^* lattice since it is face centered in the space of primary importance to us], consists of all integral linear combinations $n_1\mathbf{v}^{(1)}+n_2\mathbf{v}^{(2)}+n_3\mathbf{v}^{(3)}$ with $n_1+n_2+n_3$ even. It is therefore given by all integral linear combinations of the following set:

Cubic F^* (I) lattice:

$$\begin{aligned}\mathbf{b}^{(1)}&=\mathbf{v}^{(2)}+\mathbf{v}^{(3)} ,\\ \mathbf{b}^{(2)}&=\mathbf{v}^{(3)}+\mathbf{v}^{(1)} ,\\ \mathbf{b}^{(3)}&=\mathbf{v}^{(1)}+\mathbf{v}^{(2)} .\end{aligned} \tag{3.18}$$

The I^* or F lattice, body centered in Fourier space, has n_1, n_2, and n_3 either all odd or all even, and is therefore generated primitively by the following set:

Cubic I^* (F) lattice:

$$\begin{aligned}&\mathbf{b}^{(1)}=\mathbf{v}^{(2)}+\mathbf{v}^{3}-\mathbf{v}^{(1)}\ ,\\ &\mathbf{b}^{(2)}=\mathbf{v}^{(3)}+\mathbf{v}^{(1)}-\mathbf{v}^{(2)}\ ,\\ &\mathbf{b}^{(3)}=\mathbf{v}^{(1)}+\mathbf{v}^{(2)}-\mathbf{v}^{(3)}\ .\end{aligned}\tag{3.19}$$

We next specify the two sets of threefold-symmetric vectors that primitively generate each of the three icosahedral lattices, in terms of the threefold-symmetric set of vectors $\mathbf{v}^{(1)},\ldots,\mathbf{v}^{(6)}$ along the distinct fivefold axes of the icosahedron in Figs. 2 or 3.

For the primitive icosahedral lattice (P) lattice we have

Icosahedral P lattice:

$$\begin{aligned}&\mathbf{b}^{(1)}=\mathbf{v}^{(1)}\ ,\quad \mathbf{b}^{(4)}=\mathbf{v}^{(4)}\ ,\\ &\mathbf{b}^{(2)}=\mathbf{v}^{(2)}\ ,\quad \mathbf{b}^{(5)}=\mathbf{v}^{(5)}\ ,\\ &\mathbf{b}^{(3)}=\mathbf{v}^{(3)}\ ,\quad \mathbf{b}^{(6)}=\mathbf{v}^{(6)}\ .\end{aligned}\tag{3.20}$$

The F^* lattice, consisting of all integral linear combinations $n_1\mathbf{v}^{(1)}+\cdots+n_6\mathbf{v}^{(6)}$ with $n_1+\cdots+n_6$ even, can be generated primitively by the following set:

Icosahedral F^* (I) lattice:

$$\begin{aligned}&\mathbf{b}^{(1)}=\mathbf{v}^{(2)}+\mathbf{v}^{(3)}\ ,\quad \mathbf{b}^{(4)}=\mathbf{v}^{(4)}-\mathbf{v}^{(1)}=\tau\mathbf{b}^{(1)}\ ,\\ &\mathbf{b}^{(2)}=\mathbf{v}^{(3)}+\mathbf{v}^{(1)}\ ,\quad \mathbf{b}^{(5)}=\mathbf{v}^{(5)}-\mathbf{v}^{(2)}=\tau\mathbf{b}^{(2)}\ ,\\ &\mathbf{b}^{(3)}=\mathbf{v}^{(1)}+\mathbf{v}^{(2)}\ ,\quad \mathbf{b}^{(6)}=\mathbf{v}^{(6)}-\mathbf{v}^{(3)}=\tau\mathbf{b}^{(3)}\ .\end{aligned}\tag{3.21}$$

One easily verifies that all integral linear combinations of these yield the desired integral linear combinations of the $\mathbf{v}^{(i)}$. That $\mathbf{b}^{(4)}$ is parallel to $\mathbf{b}^{(1)}$ is evident from an inspection of Figs. 2 or 3. That the proportionality constant is just the golden mean τ follows directly from the coordinates given in Fig. 4 and the fact that $\tau^2=1+\tau$. (The corresponding relations on the next two lines of Eq. (3.21) follow from the threefold symmetry.)

The I^* lattice has $n_1,\ldots,n_6$ either all odd or all even and can be generated primitively by the following set:

Icosahedral I^* (F) lattice:

$$\begin{aligned}&\mathbf{b}^{(1)}=2\mathbf{v}^{(1)}\ ,\quad \mathbf{b}^{(4)}=\mathbf{v}^{(1)}-\mathbf{v}^{(2)}-\mathbf{v}^{(3)}-\mathbf{v}^{(4)}+\mathbf{v}^{(5)}+\mathbf{v}^{(6)}=\tau\mathbf{b}^{(1)}\ ,\\ &\mathbf{b}^{(2)}=2\mathbf{v}^{(2)}\ ,\quad \mathbf{b}^{(5)}=\mathbf{v}^{(2)}-\mathbf{v}^{(3)}-\mathbf{v}^{(1)}-\mathbf{v}^{(5)}+\mathbf{v}^{(6)}+\mathbf{v}^{(4)}=\tau\mathbf{b}^{(2)}\ ,\\ &\mathbf{b}^{(3)}=2\mathbf{v}^{(3)}\ ,\quad \mathbf{b}^{(6)}=\mathbf{v}^{(3)}-\mathbf{v}^{(1)}-\mathbf{v}^{(2)}-\mathbf{v}^{(6)}+\mathbf{v}^{(4)}+\mathbf{v}^{(5)}=\tau\mathbf{b}^{(3)}\ .\end{aligned}\tag{3.22}$$

That these produce all the required linear combinations of the $\mathbf{v}^{(i)}$ follows from the fact that $2\mathbf{v}^{(4)}$, $2\mathbf{v}^{(5)}$, $2\mathbf{v}^{(6)}$, and $\mathbf{v}^{(1)}+\mathbf{v}^{(2)}+\cdots+\mathbf{v}^{(6)}$ are all readily extracted as integral linear combinations. That $\mathbf{b}^{(4)}$ is parallel to $\mathbf{b}^{(1)}=2\mathbf{v}^{(1)}$ can be confirmed by noting from Fig. 2 that $\mathbf{b}^{(4)}$ is just the sum of $\mathbf{v}^{(1)}$ and vectors $\pm\mathbf{v}^{(i)}$ that point to the five vertices surrounding $\mathbf{v}^{(1)}$. That the proportionality constant between two such sets is τ can be verified from the coordinates given in Fig. 4.

E. Scale invariance of the icosahedral lattices

In contrast to crystallographic lattices, the icosahedral lattices are invariant under certain changes of scale. As noted in general in Sec. II.G, and as described in particular in Sec. III.H below, this can lead to the further identification of certain space groups associated with distinct gauge equivalence classes.

The scale invariance of the F^* and I^* lattices follows from the fact that each can be expressed [see Eqs. (3.21) and (3.22)] as the set of all integral linear combinations of a triad of vectors $\mathbf{b}^{(i)}$ and the same triad scaled by τ, $\tau\mathbf{b}^{(i)}$, $i=1,2,3$. When scaled by the factor τ such a lattice becomes the set of all integral linear combinations of $\tau\mathbf{b}^{(i)}$ and $\tau^2\mathbf{b}^{(i)}$. But since $\tau^2=1+\tau$ the original lattice contains every vector in the rescaled lattice. The rescaled lattice, in turn, contains both $\tau\mathbf{b}^{(i)}$ and $\mathbf{b}^{(i)}=\tau^2\mathbf{b}^{(i)}-\tau\mathbf{b}^{(i)}$, and therefore contains every vector in the original lattice. Hence the F^* and I^* lattices are indeed invariant under an operation h which rescales every lattice vector by τ.

The icosahedral P lattice is not invariant under a scaling by τ, but is invariant when rescaled by τ^3. Establishing this is a slightly more intricate matter, relegated to Appendix A.

F. Projections of lattice generators on rotation axes or mirror planes

To determine the space groups we impose the conditions (3.12), (3.14), and (3.15) demanded by the point-group generating relations on each primitive generating vector of the lattice. To apply Eqs. (3.12) and (3.14) we must have at hand the projections of the lattice-generating vectors on the n-fold axis and on either the twofold axis or the mirror plane perpendicular to that axis. These are given in Tables II–VII for each of the icosahedral and cubic lattices. We abbreviate

$$P_{g_n}\rightarrow P_n \text{ or } P_n'\ ,\tag{3.23}$$

depending on whether the n-fold operation g_n is r_n or r_n' (i.e., depending on whether or not the twofold operation is associated with the 2 or the 2′ axis), and

$$P_{g_2}\rightarrow P_2\ ,\ P_2'\ ,\ P_m\ ,\text{ or } P_m'\ ,\tag{3.24}$$

depending on whether the twofold operation g_2 is a rotation about the 2 or 2′ axis or a mirror normal to the 2 or 2′ axis. (The various axes are specified in the captions of Figs. 1 and 2. The primed operations occur only for the tetrahedral groups T and T_h.)

Although an entirely elementary exercise, the construction of these Tables II–VII is undoubtedly the most elaborate step in the entire analysis. The entries for the primitive lattices can be read directly from Figs. 1 and 2 of the octahedron and icosahedron; those for the centered lattices then follow directly from the expressions (3.18), (3.19), (3.21), and (3.22) for their primitive generating vectors in terms of those for the P lattices.

The table entries for the projections P_{g_2} serve as a double purpose. Because $r_2 = im$, the action of this projection on any vector can be expressed in two different ways:

$$2P_2 = 1 + r_2 \text{ or } 1 - m \tag{3.25}$$

and

$$2P_m = 1 + m \text{ or } 1 - r_2 \ . \tag{3.26}$$

As a result we can read directly from the expression for the projection of $\mathbf{b}^{(i)}$ on the twofold axis of r_2 not only the constraint (3.12) on the phase function Φ_{r_2}, but also the form (2.10) for the possible simplification of Φ_m by an additional gauge transformation given by Eq. (3.9):

$$\Delta\Theta_i \equiv \Delta\Phi_m(\mathbf{b}^{(i)}) \equiv \chi_1([m-1]\mathbf{b}^{(i)}) \equiv -\chi_1(2P_2\mathbf{b}^{(i)}) \ . \tag{3.27}$$

A similar secondary purpose is served by the table entries for the projections in the mirror planes:

$$\Delta\Theta_i \equiv \Delta\Phi_{r_2}(\mathbf{b}^{(i)}) \equiv \chi_1([r_2-1]\mathbf{b}^{(i)}) \equiv -\chi_1(2P_m\mathbf{b}^{(i)}) \ . \tag{3.28}$$

(The same relations hold, of course, for the primed twofold axes or mirrors.)

We are now ready to compute the icosahedral and cu-

TABLE II. Icosahedral P-lattice projections. The primitive generating vectors $\mathbf{b}^{(i)}$ for the P lattice are identical to the vectors $\mathbf{v}^{(i)}$ specified in Figs. 2 or 3 (as indicated at the top of the table). The projections P_2 on the twofold axis can immediately be confirmed by a glance at Fig. 3 (which views the icosahedron along that twofold axis). The projections P_m follow directly from the projections P_2, since $P_2 + P_m$ is the identity. The projections P_5 can immediately be confirmed by a glance at either Fig. 2 or Fig. 3.

$\mathbf{b}^{(1)} = \mathbf{v}^{(1)}$,	$\mathbf{b}^{(2)} = \mathbf{v}^{(2)}$,	$\mathbf{b}^{(3)} = \mathbf{v}^{(3)}$,
$\mathbf{b}^{(4)} = \mathbf{v}^{(4)}$,	$\mathbf{b}^{(5)} = \mathbf{v}^{(5)}$,	$\mathbf{b}^{(6)} = \mathbf{v}^{(6)}$.

	$2P_2 = 1 + r_2 = 1 - m$
$\mathbf{b}^{(1)}, \mathbf{b}^{(2)} \rightarrow$	$\mathbf{0}$
$\mathbf{b}^{(3)}, \mathbf{b}^{(6)} \rightarrow$	$\mathbf{b}^{(3)} + \mathbf{b}^{(6)}$
$\mathbf{b}^{(4)}, \mathbf{b}^{(5)} \rightarrow$	$\mathbf{b}^{(4)} + \mathbf{b}^{(5)}$
	$2P_m = 1 + m = 1 - r_2$
$\mathbf{b}^{(1)} \rightarrow$	$2\mathbf{b}^{(1)}$
$\mathbf{b}^{(2)} \rightarrow$	$2\mathbf{b}^{(2)}$
$\mathbf{b}^{(3)}, -\mathbf{b}^{(6)} \rightarrow$	$\mathbf{b}^{(3)} - \mathbf{b}^{(6)}$
$\mathbf{b}^{(4)}, -\mathbf{b}^{(5)} \rightarrow$	$\mathbf{b}^{(4)} - \mathbf{b}^{(5)}$
	$5P_5$
$\mathbf{b}^{(1)}, -\mathbf{b}^{(2)},$ $\mathbf{b}^{(3)}, \mathbf{b}^{(4)}, \mathbf{b}^{(6)} \rightarrow$	$\mathbf{b}^{(1)} - \mathbf{b}^{(2)} + \mathbf{b}^{(3)} + \mathbf{b}^{(4)} + \mathbf{b}^{(6)}$
$\mathbf{b}^{(5)} \rightarrow$	$5\mathbf{b}^{(5)}$

TABLE III. Icosahedral F^* (I)-lattice projections. The projections can be verified from the expressions for the generating vectors $\mathbf{b}^{(i)}$ in terms of the P-lattice generating vectors $\mathbf{v}^{(i)}$ (given at the top of the table), and the projections of the $\mathbf{v}^{(i)}$ given in Table II (for the P-lattice $\mathbf{b}^{(i)} = \mathbf{v}^{(i)}$). The projections for $\mathbf{b}^{(4)}, \mathbf{b}^{(5)}$, and $\mathbf{b}^{(6)}$ can also be confirmed from those for $\mathbf{b}^{(1)}, \mathbf{b}^{(2)}$, and $\mathbf{b}^{(3)}$ using the fact that $\mathbf{b}^{(4)} = \tau\mathbf{b}^{(1)}, \mathbf{b}^{(5)} = \tau\mathbf{b}^{(2)}$, $\mathbf{b}^{(6)} = \tau\mathbf{b}^{(3)}$, and the fact that $\tau^2 = 1 + \tau$. Since, for example $2P_2\mathbf{b}^{(1)} = \mathbf{b}^{(1)} + \mathbf{b}^{(2)} - \mathbf{b}^{(3)} + \mathbf{b}^{(6)} = \mathbf{b}^{(1)} + \mathbf{b}^{(2)} + (\tau - 1)\mathbf{b}^{(3)}$, it follows that $2P_2\mathbf{b}^{(4)} = \tau 2P_2\mathbf{b}^{(1)} = \tau\mathbf{b}^{(1)} + \tau\mathbf{b}^{(2)} + (\tau^2 - \tau)\mathbf{b}^{(3)} = \mathbf{b}^{(3)} + \mathbf{b}^{(4)} + \mathbf{b}^{(5)}$.

$\mathbf{b}^{(1)} = \mathbf{v}^{(2)} + \mathbf{v}^{(3)}$,	$\mathbf{b}^{(4)} = \mathbf{v}^{(4)} - \mathbf{v}^{(1)} = \tau\mathbf{b}^{(1)}$,
$\mathbf{b}^{(2)} = \mathbf{v}^{(3)} + \mathbf{v}^{(1)}$,	$\mathbf{b}^{(5)} = \mathbf{v}^{(5)} - \mathbf{v}^{(2)} = \tau\mathbf{b}^{(2)}$,
$\mathbf{b}^{(3)} = \mathbf{v}^{(1)} + \mathbf{v}^{(2)}$,	$\mathbf{b}^{(6)} = \mathbf{v}^{(6)} - \mathbf{v}^{(3)} = \tau\mathbf{b}^{(3)}$.

	$2P_2 = 1 + r_2 = 1 - m$
$\mathbf{b}^{(1)}, \mathbf{b}^{(2)} \rightarrow$	$\mathbf{b}^{(1)} + \mathbf{b}^{(2)} - \mathbf{b}^{(3)} + \mathbf{b}^{(6)}$
$\mathbf{b}^{(3)}, \mathbf{b}^{(6)} \rightarrow$	$\mathbf{0}$
$\mathbf{b}^{(4)}, \mathbf{b}^{(5)} \rightarrow$	$\mathbf{b}^{(3)} + \mathbf{b}^{(4)} + \mathbf{b}^{(5)}$
	$2P_m = 1 + m = 1 - r_2$
$\mathbf{b}^{(1)} \rightarrow$	$\mathbf{b}^{(1)} - \mathbf{b}^{(2)} + \mathbf{b}^{(3)} - \mathbf{b}^{(6)}$
$\mathbf{b}^{(2)} \rightarrow$	$-\mathbf{b}^{(1)} + \mathbf{b}^{(2)} + \mathbf{b}^{(3)} - \mathbf{b}^{(6)}$
$\mathbf{b}^{(3)} \rightarrow$	$2\mathbf{b}^{(3)}$
$\mathbf{b}^{(4)} \rightarrow$	$-\mathbf{b}^{(3)} + \mathbf{b}^{(4)} - \mathbf{b}^{(5)}$
$\mathbf{b}^{(5)} \rightarrow$	$-\mathbf{b}^{(3)} - \mathbf{b}^{(4)} + \mathbf{b}^{(5)}$
$\mathbf{b}^{(6)} \rightarrow$	$2\mathbf{b}^{(6)}$
	$5P_5$
$\mathbf{b}^{(1)}, \mathbf{b}^{(3)},$ $\mathbf{b}^{(4)}, \mathbf{b}^{(6)} \rightarrow$	$\mathbf{0}$
$\mathbf{b}^{(2)} \rightarrow$	$-\mathbf{b}^{(1)} + 5\mathbf{b}^{(2)} - \mathbf{b}^{(3)} + 2\mathbf{b}^{(4)} + 2\mathbf{b}^{(6)}$
$\mathbf{b}^{(5)} \rightarrow$	$2\mathbf{b}^{(1)} + 2\mathbf{b}^{(3)} + \mathbf{b}^{(4)} + 5\mathbf{b}^{(5)} + \mathbf{b}^{(6)}$

bic space groups. We first find the classes of gauge-equivalent phase functions, and then check to see whether any distinct classes should be associated with the same space groups as a consequence of the existence of lattice symmetries not in the point group (as discussed in Sec. II.G).

G. The classes of gauge-equivalent phase functions

In determining the gauge equivalence classes we first exploit the remaining gauge freedom (3.9) to reduce some of the unknown phases to zero. Because of the relations (3.27) and (3.28), the allowed shifts $\Delta\Theta_i$ can be read directly from the table of projections for the appropriate lattice. Since χ_1 has the common value α for the first three $\mathbf{b}^{(i)}$ and the value β for the next three, if the table entry for the relevant projection is $n_1\mathbf{b}^{(1)}+\cdots+n_6\mathbf{b}^{(6)}$ then we have

$$\Delta\Theta_i \equiv -(n_1+n_2+n_3)\alpha-(n_4+n_5+n_6)\beta\ , \qquad (3.29)$$

so a glance at the table informs us which values of $\Theta_i=\Phi_{g_2}(\mathbf{b}^{(i)})$ (if any) can be made zero by a further choice of gauge.

In the case of Y_h, O_h, and T_h, the possible phase shifts (3.29) are severely limited because α and β can only be 0 or $\frac{1}{2}$. But since the Θ_i are also restricted to be 0 or $\frac{1}{2}$, as noted in Eq. (3.15), it is sometimes still possible to reduce one or even two of them to zero in this way. Note also, in treating Y_h, O_h, and T_h, that because Θ_i, α, and β can only be 0 or $\frac{1}{2}$, we can replace the coefficients of each

TABLE IV. Icosahedral I^* (F)-lattice projections. The projections can be verified from the expressions for the generating vectors $\mathbf{b}^{(i)}$ in terms of the P-lattice generating vectors $\mathbf{v}^{(i)}$ (given at the top of the table), and the projections of the $\mathbf{v}^{(i)}$, given in Table II (for the P-lattice $\mathbf{b}^{(i)}=\mathbf{v}^{(i)}$. The projections for $\mathbf{b}^{(4)}$, $\mathbf{b}^{(5)}$, and $\mathbf{b}^{(6)}$ can also be confirmed from those for $\mathbf{b}^{(1)}$, $\mathbf{b}^{(2)}$, and $\mathbf{b}^{(3)}$ using the fact that $\mathbf{b}^{(4)}=\tau\mathbf{b}^{(1)},\mathbf{b}^{(5)}=\tau\mathbf{b}^{(2)},\mathbf{b}^{(6)}=\tau\mathbf{b}^{(3)}$, and the fact that $\tau^2=1+\tau$. Since, for example, $2P_2\mathbf{b}^{(3)}=2\mathbf{b}^{(3)}+\mathbf{b}^{(4)}+\mathbf{b}^{(5)}=2\mathbf{b}^{(3)}+\tau\mathbf{b}^{(1)}+\tau\mathbf{b}^{(2)}$, it follows that $2P_2\mathbf{b}^{(6)}=\tau 2P_2\mathbf{b}^{(3)}=2\tau\mathbf{b}^{(3)}+(1+\tau)\mathbf{b}^{(1)}+(1+\tau)\mathbf{b}^{(2)}=\mathbf{b}^{(1)}+\mathbf{b}^{(2)}+\mathbf{b}^{(4)}+\mathbf{b}^{(5)}+2\mathbf{b}^{(6)}$.

$\mathbf{b}^{(1)}=2\mathbf{v}^{(1)}$,	$\mathbf{b}^{(4)}=\mathbf{v}^{(1)}-\mathbf{v}^{(2)}-\mathbf{v}^{(3)}-\mathbf{v}^{(4)}+\mathbf{v}^{(5)}+\mathbf{v}^{(6)}=\tau\mathbf{b}^{(1)}$,
$\mathbf{b}^{(2)}=2\mathbf{v}^{(2)}$,	$\mathbf{b}^{(4)}=\mathbf{v}^{(2)}-\mathbf{v}^{(3)}-\mathbf{v}^{(1)}-\mathbf{v}^{(5)}+\mathbf{v}^{(6)}+\mathbf{v}^{(4)}=\tau\mathbf{b}^{(2)}$,
$\mathbf{b}^{(3)}=2\mathbf{v}^{(3)}$,	$\mathbf{b}^{(4)}=\mathbf{v}^{(3)}-\mathbf{v}^{(1)}-\mathbf{v}^{(2)}-\mathbf{v}^{(6)}+\mathbf{v}^{(4)}+\mathbf{v}^{(5)}=\tau\mathbf{b}^{(3)}$.

	$2P_2=1+r_2=1-m$
$\mathbf{b}^{(1)}$, $\mathbf{b}^{(2)}$	
$\mathbf{b}^{(4)}$, $\mathbf{b}^{(5)}\rightarrow$	0
$\mathbf{b}^{(3)}\rightarrow$	$2\mathbf{b}^{(3)}+\mathbf{b}^{(4)}+\mathbf{b}^{(5)}$
$\mathbf{b}^{(6)}\rightarrow$	$\mathbf{b}^{(1)}+\mathbf{b}^{(2)}+\mathbf{b}^{(4)}+\mathbf{b}^{(5)}+2\mathbf{b}^{(6)}$
	$2P_m=1+m=1-r_2$
$\mathbf{b}^{(1)}\rightarrow$	$2\mathbf{b}^{(1)}$
$\mathbf{b}^{(2)}\rightarrow$	$2\mathbf{b}^{(2)}$
$\mathbf{b}^{(3)}\rightarrow$	$-\mathbf{b}^{(4)}-\mathbf{b}^{(5)}$
$\mathbf{b}^{(4)}\rightarrow$	$2\mathbf{b}^{(4)}$
$\mathbf{b}^{(5)}\rightarrow$	$2\mathbf{b}^{(5)}$
$\mathbf{b}^{(6)}\rightarrow$	$-\mathbf{b}^{(1)}-\mathbf{b}^{(2)}-\mathbf{b}^{(4)}-\mathbf{b}^{(5)}$
	$5P_5$
$\mathbf{b}^{(1)}$, $-\mathbf{b}^{(2)}$, $\mathbf{b}^{(3)}\rightarrow$	$2\mathbf{b}^{(1)}-\mathbf{b}^{(2)}+2\mathbf{b}^{(3)}+\mathbf{b}^{(4)}+2\mathbf{b}^{(5)}+\mathbf{b}^{(6)}$
$\mathbf{b}^{(4)}$, $-\mathbf{b}^{(5)}$, $\mathbf{b}^{(6)}\rightarrow$	$\mathbf{b}^{(1)}+2\mathbf{b}^{(2)}+\mathbf{b}^{(3)}+3\mathbf{b}^{(4)}+\mathbf{b}^{(5)}+3\mathbf{b}^{(6)}$

TABLE V. Cubic P-lattice projections. The primitive generating vectors $\mathbf{b}^{(i)}$ for the P lattice are identical to the vectors $\mathbf{v}^{(i)}$ specified in Fig. 1 (as indicated at the top of the table). The projections P_2, P_4, P_2', P_3' can all be confirmed by a glance at Fig. 1, where the axes of r_2 and r_4 are explicitly indicated. The 2′ axis is along the axis $\mathbf{v}^{(2)}$ of r_4. (Consequently the action of $2P_2'$ is identical to that of $4P_4$ except for a factor of 2.) The 3′ axis ($r_3' = r_3 r_2'$) is through the center of the triangle in Fig. 1 whose vertices are $-\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \mathbf{v}^{(3)}$. The projections P_m and P_m' follow directly from the projections P_2 and P_2', since $P_2 + P_m$ or $P_2' + P_m'$ are the identity.

	$\mathbf{b}^{(1)} = \mathbf{v}^{(1)}$,	$\mathbf{b}^{(2)} = \mathbf{v}^{(2)}$,	$\mathbf{b}^{(3)} = \mathbf{v}^{(3)}$.
	$2P_2 = 1 + r_2 = 1 - m$	$4P_4$	$2P_2' = 1 + r_2' = 1 - m'$
$\mathbf{b}^{(1)} \rightarrow$	$\mathbf{b}^{(1)} + \mathbf{b}^{(2)}$	0	0
$\mathbf{b}^{(2)} \rightarrow$	$\mathbf{b}^{(1)} + \mathbf{b}^{(2)}$	$4\mathbf{b}^{(2)}$	$2\mathbf{b}^{(2)}$
$\mathbf{b}^{(3)} \rightarrow$	0	0	0
	$2P_m = 1 + m = 1 - r_2$	$3P_3'$	$2P_m' = 1 + m' = 1 - r_2'$
$\mathbf{b}^{(1)} \rightarrow$	$\mathbf{b}^{(1)} - \mathbf{b}^{(2)}$	$-\mathbf{b}^{(1)} + \mathbf{b}^{(2)} + \mathbf{b}^{(3)}$	$2\mathbf{b}^{(1)}$
$\mathbf{b}^{(2)} \rightarrow$	$-\mathbf{b}^{(1)} + \mathbf{b}^{(2)}$	$\mathbf{b}^{(1)} - \mathbf{b}^{(2)} - \mathbf{b}^{(3)}$	0
$\mathbf{b}^{(3)} \rightarrow$	$2\mathbf{b}^{(3)}$	0	$2\mathbf{b}^{(3)}$

lattice-generating vector in the projections by their values modulo 2: i.e., we can ignore terms with even coefficients and replace all odd coefficients by ± 1 (choosing the sign at our convenience).

We compute the gauge equivalence classes point group by point group, collecting the resulting information in Tables VIII–X. In each case we begin by listing the particular form of the constraints (3.12) and (3.14) for the point group, and the general form for an additional gauge transformation that preserves the vanishing of Φ_{g_3}. We first consider the three point groups Y_h, O_h, and T_h for which all the Θ_i and the values of α (and β) in the gauge function (3.9) can only be 0 or $\frac{1}{2}$. In every case the text refers to the table of projections for the lattice under consideration. For a given projection P, I explicitly mention all relevant values of $P(\mathbf{b}^{(i)})$; there are generally fewer than six (icosahedral) or three (cubic) of these because more than one generating vector can have the same projection (to within an irrelevant sign), or because a given projection contributes no constraints beyond those already noted (including the overall constraint that all phases are 0 or $\frac{1}{2}$ for Y_h, O_h, and T_h).

TABLE VI. Cubic F^* (I)-lattice projections. The projections can be verified from the expressions for the generating vectors $\mathbf{b}^{(i)}$ in terms of the P-lattice generating vectors $\mathbf{v}^{(i)}$ (given at the top of the table), and the projections of the $\mathbf{v}^{(i)}$ given in Table V (for the P-lattice $\mathbf{b}^{(i)} = \mathbf{v}^{(i)}$). The axes r_2, r_4, r_2', and r_3' are as shown in Fig. 1 and described in the caption of Table V.

	$\mathbf{b}^{(1)} = \mathbf{v}^{(2)} + \mathbf{v}^{(3)}$,	$\mathbf{b}^{(2)} = \mathbf{v}^{(3)} + \mathbf{v}^{(1)}$,	$\mathbf{b}^{(3)} = \mathbf{v}^{(1)} + \mathbf{v}^{(2)}$.
	$2P_2 = 1 + r_2 = 1 - m$	$4P_4$	$2P_2' = 1 + r_2' = 1 - m'$
$\mathbf{b}^{(1)} \rightarrow$	$\mathbf{b}^{(3)}$	$2\mathbf{b}^{(1)} - 2\mathbf{b}^{(2)} + 2\mathbf{b}^{(3)}$	$\mathbf{b}^{(1)} - \mathbf{b}^{(2)} + \mathbf{b}^{(3)}$
$\mathbf{b}^{(2)} \rightarrow$	$\mathbf{b}^{(3)}$	0	0
$\mathbf{b}^{(3)} \rightarrow$	$2\mathbf{b}^{(3)}$	$2\mathbf{b}^{(1)} - 2\mathbf{b}^{(2)} + 2\mathbf{b}^{(3)}$	$\mathbf{b}^{(1)} - \mathbf{b}^{(2)} + \mathbf{b}^{(3)}$
	$2P_m = 1 + m = 1 - r_2$	$3P_3'$	$2P_m' = 1 + m' = 1 - r_2'$
$\mathbf{b}^{(1)} \rightarrow$	$2\mathbf{b}^{(1)} - \mathbf{b}^{(3)}$	$3\mathbf{b}^{(1)} - \mathbf{b}^{(2)} - \mathbf{b}^{(3)}$	$\mathbf{b}^{(1)} + \mathbf{b}^{(2)} - \mathbf{b}^{(3)}$
$\mathbf{b}^{(2)} \rightarrow$	$2\mathbf{b}^{(2)} - \mathbf{b}^{(3)}$	0	$2\mathbf{b}^{(2)}$
$\mathbf{b}^{(3)} \rightarrow$	0	0	$-\mathbf{b}^{(1)} + \mathbf{b}^{(2)} + \mathbf{b}^{(3)}$

TABLE VII. Cubic I^* (F)-lattice projections. The projections can be verified from the expressions for the generating vectors $\mathbf{b}^{(i)}$ in terms of the P-lattice generating vectors $\mathbf{v}^{(i)}$ (given at the top of the table), and the projections of the $\mathbf{v}^{(i)}$ given in Table V (for the P-lattice $\mathbf{b}^{(i)}=\mathbf{v}^{(i)}$). The axes r^2, r^4, r_2', and r_3' are as shown in Fig. 1 and described in the caption of Table V.

$\mathbf{b}^{(1)}=\mathbf{v}^{(2)}+\mathbf{v}^{(3)}-\mathbf{v}^{(1)}$, $\mathbf{b}^{(2)}=\mathbf{v}^{(3)}+\mathbf{v}^{(1)}-\mathbf{v}^{(2)}$, $\mathbf{b}^{(3)}=\mathbf{v}^{(1)}+\mathbf{v}^{(2)}-\mathbf{v}^{(3)}$.

	$2P_2=1+r_2=1-m$	$4P_4$	$2P_2'=1+r_2'=1-m'$
$\mathbf{b}^{(1)}\rightarrow$	0	$2\mathbf{b}^{(1)}+2\mathbf{b}^{(3)}$	$\mathbf{b}^{(1)}+\mathbf{b}^{(3)}$
$\mathbf{b}^{(2)}\rightarrow$	0	$-2\mathbf{b}^{(1)}-2\mathbf{b}^{(3)}$	$-\mathbf{b}^{(1)}-\mathbf{b}^{(3)}$
$\mathbf{b}^{(3)}\rightarrow$	$\mathbf{b}^{(1)}+\mathbf{b}^{(2)}+2\mathbf{b}^{(3)}$	$2\mathbf{b}^{(1)}+2\mathbf{b}^{(3)}$	$\mathbf{b}^{(1)}+\mathbf{b}^{(3)}$
	$2P_m=1+m=1-r_2$	$3P_3'$	$2P_m'=1+m'=1-r_2'$
$\mathbf{b}^{(1)}\rightarrow$	$2\mathbf{b}^{(1)}$	$3\mathbf{b}^{(1)}$	$\mathbf{b}^{(1)}-\mathbf{b}^{(3)}$
$\mathbf{b}^{(2)}\rightarrow$	$2\mathbf{b}^{(2)}$	$-\mathbf{b}^{(1)}$	$\mathbf{b}^{(1)}+2\mathbf{b}^{(2)}+\mathbf{b}^{(3)}$
$\mathbf{b}^{(3)}\rightarrow$	$-\mathbf{b}^{(1)}-\mathbf{b}^{(2)}$	$-\mathbf{b}^{(1)}$	$-\mathbf{b}^{(1)}+\mathbf{b}^{(3)}$

1. Point group Y_h

Constraints and remaining gauge freedom:

$$0\equiv\Phi_m(2P_m\mathbf{b}^{(i)})\ ,\quad 0\equiv\Phi_m(5P_5\mathbf{b}^{(i)})\ ,$$
$$\Delta\Theta_i\equiv-\chi_1(2P_2(\mathbf{b}^{(i)}))\ . \tag{3.30}$$

P lattice (Y_h). From the entries in Table II for $2P_2$ we see that $\Delta\Theta_3\equiv-\alpha-\beta$, so we can always pick a gauge in which Θ_3 vanishes. The table shows that the remaining gauge freedom (shifting both α and β by $\frac{1}{2}$) can alter no additional phases. With this choice of gauge, we then learn from $2P_m(b^{(3)})$ that Θ_6 must also vanish, and from $2P_m(\mathbf{b}^{(4)})$ that Θ_4 and Θ_5 must have the same value. We learn from $5P_5(\mathbf{b}^{(5)})$ that Θ_5 must vanish and $5P_5(\mathbf{b}^{(3)})$ then tells us that $\Theta_1\equiv\Theta_2$. There are thus two classes:[28]

$$P\text{ lattice, }53m\text{: }\Phi_m(\mathbf{b}^{(i)})\equiv 000\,000\text{ or }\tfrac{1}{2}\tfrac{1}{2}0\,000\ . \tag{3.31}$$

F^* (I) lattice (Y_h). From the entries in Table III for $2P_2$ we find that $\Delta\Theta_4\equiv\alpha+2\beta\equiv\alpha$, and $\Delta\Theta_1\equiv\alpha+\beta$. We can thus choose α to make Θ_4 vanish and, whatever that value of α, we can then choose β to make Θ_1 vanish:

$$0\equiv\Theta_1\ \text{ and }\ 0\equiv\Theta_4\ . \tag{3.32}$$

With this choice of gauge, we learn from $5P_5(\mathbf{b}^{(2)})$ and $5P_5(\mathbf{b}^{(5)})$ that

$$0\equiv\Theta_2+\Theta_3\ \text{ and }\ 0\equiv\Theta_5+\Theta_6\ , \tag{3.33}$$

and from $2P_m$ that

$$0\equiv\Theta_2+\Theta_3+\Theta_6\ \text{ and }\ 0\equiv\Theta_3+\Theta_5\ . \tag{3.34}$$

Equations (3.32)–(3.34) imply that all the Θ_i vanish, so all classes are gauge equivalent to the one with phases

$$F^*\ (I)\text{ lattice, }53m\text{: }\Phi_m(\mathbf{b}^{(i)})\equiv 000\,000\ . \tag{3.35}$$

I^* (F) lattice (Y_h). From the entries in Table IV for $2P_2$, we find no remaining freedom to alter any phases with a gauge transformation. From $2P_m$ we get

$$0\equiv\Theta_4+\Theta_5\ \text{ and }\ 0\equiv\Theta_1+\Theta_2\ . \tag{3.36}$$

In view of these, $5P_5$ gives

$$0\equiv\Theta_2+\Theta_4+\Theta_6\ \text{ and }\ 0\equiv\Theta_1+\Theta_3+\Theta_6\ . \tag{3.37}$$

Thus Θ_1 and Θ_4 can independently be taken to be 0 or $\frac{1}{2}$, and the values of the other four phases are then determined, giving four gauge equivalence classes:

I^* (F) lattice, $53m$:

$$\Phi_m(\mathbf{b}^{(i)})\equiv 000\,000\ ,\ \tfrac{1}{2}\tfrac{1}{2}0\,00\tfrac{1}{2}\ ,$$
$$00\tfrac{1}{2}\ \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\ ,\text{ or }\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\ \tfrac{1}{2}\tfrac{1}{2}0\ . \tag{3.38}$$

2. Point group O_h

Constraints and remaining gauge freedom:

$$0\equiv\Phi_m(2P_m\mathbf{b}^{(i)})\ ,\quad 0\equiv\Phi_m(4P_4\mathbf{b}^{(i)})\ ,$$
$$\Delta\Theta_i\equiv-\chi_1(2P_2(\mathbf{b}^{(i)}))\ . \tag{3.39}$$

[28] We list the values of $\Theta_i=\Phi_m(\mathbf{b}^{(i)})$, $i=1,\ldots,6$, by simply listing the six numbers: $\Theta_1\Theta_2\Theta_3\Theta_4\Theta_5\Theta_6$.

P lattice (O_h). The entries in Table V for $2P_2$ show that no phases can be changed by the remaining gauge freedom. We learn that $\Theta_1=\Theta_2$ from $2P_m$, and nothing new from $4P_4$, so there are four gauge equivalence classes:

$$P \text{ lattice, } m3m\text{: } \Phi_m(\mathbf{b}^{(i)})\equiv 000\ ,\ 00\tfrac{1}{2}\ ,\ \tfrac{1}{2}\tfrac{1}{2}0\ ,\ \text{or } \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\ . \tag{3.40}$$

F^* (I) lattice, (O_h). The entries in Table VI for $2P_2$ show that we can pick a gauge in which $\Theta_2\equiv 0$. In this gauge we learn from $2P_m$ that $\Theta_3\equiv 0$. We learn nothing new from $4P_4$, so there are two gauge equivalence classes:

$$F^*\ (I) \text{ lattice, } m3m\text{: } \Phi_m(\mathbf{b}^{(i)})\equiv 000 \text{ or } \tfrac{1}{2}00\ . \tag{3.41}$$

I^* (F) lattice, (O_h). The entries in Table VII for $2P_2$ show that no phases can be changed by the remaining gauge freedom. We learn that $\Theta_1\equiv\Theta_2$ from $2P_m$, and nothing new from $4P_4$, so there are four gauge equivalence classes:

$$I^*\ (F) \text{ lattice, } m3m\text{: } \Phi_m(\mathbf{b}^{(i)})\equiv 000\ ,\ 00\tfrac{1}{2}\ ,\ \tfrac{1}{2}\tfrac{1}{2}0\ ,\ \text{or } \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\ . \tag{3.42}$$

3. Point group T_h

Constraints and remaining gauge freedom:

$$0=\Phi_m(2P'_m\mathbf{b}^{(i)})\ ,\quad 0\equiv\Phi_m(3P'_3\mathbf{b}^{(i)})\ ,\qquad \Delta\Theta_i\equiv-\chi_1(2P'_2(\mathbf{b}^{(i)}))\ . \tag{3.43}$$

P lattice (T_h). The entries in Table V for $2P'_2$ show that no phases can be changed by the remaining gauge freedom. We learn nothing new from $2P'_m$, and $3P'_3$ simply requires an even number of those phases to be $\frac{1}{2}$, so there are four classes:

$$P \text{ lattice, } m3\text{: } \Phi_m(\mathbf{b}^{(i)})\equiv 000\ ,\ \tfrac{1}{2}0\tfrac{1}{2}\ ,\ \tfrac{1}{2}\tfrac{1}{2}0\ ,\ \text{or } 0\tfrac{1}{2}\tfrac{1}{2}\ . \tag{3.44}$$

F^* (I) lattice (T_h). The entries in Table VI for $2P'_2$ show that we can pick a gauge in which $\Theta_3\equiv 0$. In this gauge we learn from $2P'_m$ that $\Theta_1\equiv\Theta_2$, and nothing more from $3P'_3$, so there are two classes:

$$F^*\ (I) \text{ lattice, } m3\text{: } \Phi_m(\mathbf{b}^{(i)})\equiv 000 \text{ or } \tfrac{1}{2}\tfrac{1}{2}0\ . \tag{3.45}$$

I^* (F) lattice (T_h). The entries in Table VII for $2P'_2$ show that no phases can be changed by the remaining gauge freedom. We learn from $2P'_m$ that $\Theta_1\equiv\Theta_3$, and from $3P'_3$ that $\Theta_1\equiv 0$, so there are two classes:

TABLE VIII. The space groups with point groups Y_h, O_h, or T_h. All phase functions are gauge equivalent to one of the (gauge-inequivalent) sets listed for each lattice and point group. The phase functions are specified by giving the phases $\Theta_i=\Phi_m(\mathbf{b}^{(i)})$ in the form $\Theta_1\Theta_2\Theta_3,\Theta_4\Theta_5\Theta_6$ (for Y_h) or $\Theta_1\Theta_2\Theta_3$ (for O_h and T_h). (The phase function associated with the other point group generator, $\Phi_{\bar{r}_3}$, is zero in all cases, because of our choice of gauge.) The international name (long form) and number (in italics) for the space group associated with each gauge equivalence class is listed alongside its phases. The three sets of phases in braces specify distinct gauge equivalence classes, but give the same space group as the entries directly above them, for the reasons discussed in general in Sec. II.G and in particular in Sec. III.H. There being no obvious way to generalize the international glide-plane notation to the two nonsymmorphic icosahedral groups, I follow the notation of Rokhsar, Wright, and Mermin, 1988, replacing m by the noncommital q (for "quasi").

	$\bar{5}\bar{3}\frac{2}{m}$ (Y_h)	Φ_m	$\frac{4}{m}\bar{3}\frac{2}{m}$ (O_h)	Φ_m	$\frac{2}{m}\bar{3}$ (T_h)	$\Phi_{m'}$
	$P\bar{5}\bar{3}\frac{2}{m}$	000 000	$P\frac{4}{m}\bar{3}\frac{2}{m}$ *221*	000	$P\frac{2}{m}\bar{3}$ *200*	000
	$P\bar{5}\bar{3}\frac{2}{q}$	$\frac{1}{2}\frac{1}{2}0$ 000	$P\frac{4}{n}\bar{3}\frac{2}{n}$ *222*	$00\frac{1}{2}$	$P\frac{2}{n}\bar{3}$ *201*	$\frac{1}{2}0\frac{1}{2}$
P			$P\frac{4_2}{n}\bar{3}\frac{2}{m}$ *224*	$\frac{1}{2}\frac{1}{2}0$	$P\frac{2_1}{a}\bar{3}$ *205*	$\frac{1}{2}\frac{1}{2}0$
			$P\frac{4_2}{m}\bar{3}\frac{2}{n}$ *223*	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$		$\{0\frac{1}{2}\frac{1}{2}\}$
F^*	$F^*\bar{5}\bar{3}\frac{2}{m}$	000 000	$I\frac{4}{m}\bar{3}\frac{2}{m}$ *229*	000	$I\frac{2}{m}\bar{3}$ *204*	000
(I)			$I\frac{4_1}{a}\bar{3}\frac{2}{d}$ *230*	$\frac{1}{2}00$	$I\frac{2_1}{a}\bar{3}$ *206*	$\frac{1}{2}\frac{1}{2}0$
	$I^*\bar{5}\bar{3}\frac{2}{m}$	000 000	$F\frac{4}{m}\bar{3}\frac{2}{m}$ *225*	000	$F\frac{2}{m}\bar{3}$ *202*	000
I^*	$I^*\bar{5}\bar{3}\frac{2}{q}$	$\frac{1}{2}\frac{1}{2}0$ $00\frac{1}{2}$	$F\frac{4_1}{d}\bar{3}\frac{2}{m}$ *227*	$00\frac{1}{2}$	$F\frac{2}{d}\bar{3}$ *203*	$0\frac{1}{2}0$
(F)		$\{00\frac{1}{2}\ \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$	$F\frac{4_1}{d}\bar{3}\frac{2}{n}$ *228*	$\frac{1}{2}\frac{1}{2}0$		
		$\{\frac{1}{2}\frac{1}{2}\frac{1}{2}\ \frac{1}{2}\frac{1}{2}0\}$	$F\frac{4}{m}\bar{3}\frac{2}{c}$ *226*	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$		

I^* (F) lattice, $m3$: $\Phi_m(\mathbf{b}^{(i)}) \equiv 000$ or $0\frac{1}{2}0$. (3.46)

These exhaust the point groups for which Θ_i, α, and β, are required to be 0 or $\frac{1}{2}$. For the remaining four point groups they can have arbitrary values (modulo 1).

4. Point group Y

Constraints and remaining gauge freedom:

$$0 \equiv \Phi_{r_2}(2P_2\mathbf{b}^{(i)}) \ , \quad 0 \equiv \Phi_{r_2}(5P_5\mathbf{b}^{(i)}) \ , \quad \Delta\Theta_i \equiv -\chi_1(2P_m(\mathbf{b}^{(i)})) \ . \tag{3.47}$$

P lattice (Y). The entries in Table II for $2P_m$ show that $\Delta\Theta_2 \equiv 2\alpha$ and $\Delta\Theta_6 \equiv \alpha - \beta$, so we can choose α and β to make

$$0 \equiv \Theta_2 \equiv \Theta_6 \ . \tag{3.48}$$

In this gauge $2P_2(\mathbf{b}^{(3)})$ and $2P_2(\mathbf{b}^{(4)})$ then give

$$0 \equiv \Theta_3 \quad \text{and} \quad 0 = \Theta_4 + \Theta_5 \ , \tag{3.49}$$

and $5P_5(\mathbf{b}^{(1)})$ and $5P_5(\mathbf{b}^{(5)})$ give

$$0 \equiv \Theta_1 + \Theta_4 \quad \text{and} \quad 0 \equiv 5\Theta_5 \ . \tag{3.50}$$

The complete set of solutions to Eqs. (3.48)–(3.50) is

TABLE IX. The space groups with point groups Y or O. All phase functions are gauge equivalent to one of the (gauge-inequivalent) sets listed for each lattice and point group. The phase functions are specified by giving $\Theta_i = \Phi_{r_2}(\mathbf{b}^{(i)})$ in the form $\Theta_1\Theta_2\Theta_3, \Theta_4\Theta_5\Theta_6$ (for Y) or $\Theta_1\Theta_2\Theta_3$ (for O). (The phase function associated with the other point group generator, $\Phi_{\bar{r}_3}$, is zero in all cases, because of our choice of gauge.) The International name (long form) and number (in italics) for the space group associated with each gauge equivalence class is listed alongside its phases. Although they are gauge inequivalent, the three sets of phases in braces for each icosahedral point group specify the same space group as the entries directly above them, for the reasons discussed in general in Sec. II.G and in particular in Sec. III.H.

	532 (Y)	Φ_{r_2}	432 (O)	Φ_{r_2}
P	$P532$	$000\ 000$	$P432$ *207*	000
	$P5_132$	$\frac{1}{5}00\ \frac{4}{5}\frac{1}{5}0$	$P4_132$ *213*	$\frac{1}{4}\frac{3}{4}0$
		$\{2[\frac{1}{5}00\ \frac{4}{5}\frac{1}{5}0]\}$	$P4_232$ *208*	$2[\frac{1}{4}\frac{3}{4}0]$
		$\{4[\frac{1}{5}00\ \frac{4}{5}\frac{1}{5}0]\}$	$P4_332$ *212*	$3[\frac{1}{4}\frac{3}{4}0]$
		$\{3[\frac{1}{5}00\ \frac{4}{5}\frac{1}{5}0]\}$		
F^* (I)	F^*532	$000\ 000$	$I432$ *211*	000
	F^*5_132	$0\frac{1}{5}\frac{2}{5}\ 0\frac{3}{5}\frac{1}{5}$	$I4_132$ *214*	$\frac{1}{2}00$
		$\{3[0\frac{1}{5}\frac{2}{5}\ 0\frac{3}{5}\frac{1}{5}]\}$		
		$\{4[0\frac{1}{5}\frac{2}{5}\ 0\frac{3}{5}\frac{1}{5}]\}$		
		$\{2[0\frac{1}{5}\frac{2}{5}\ 0\frac{3}{5}\frac{1}{5}]\}$		
I^* (F)	I^*532	$000\ 000$	$F432$ *209*	000
	I^*5_132	$\frac{1}{5}0\frac{1}{5}\ \frac{3}{5}0\frac{3}{5}$	$F4_132$ *210*	$\frac{1}{2}\frac{1}{2}0$
		$\{3[\frac{1}{5}0\frac{1}{5}\ \frac{3}{5}0\frac{3}{5}]\}$		
		$\{4[\frac{1}{5}0\frac{1}{5}\ \frac{3}{5}0\frac{3}{5}]\}$		
		$\{2[\frac{1}{5}0\frac{1}{5}\ \frac{3}{5}0\frac{3}{5}]\}$		

TABLE X. The space groups with point groups T or T_d. All phases functions are gauge equivalent to one of the (gauge-inequivalent) sets listed for each lattice and point group. The phase functions are specified by giving $\Theta_i=\Phi_{g_2}(\mathbf{b}^{(i)})$ in the form $\Theta_1\Theta_2\Theta_3$, where $g=r_2'$ for T and m for T_d. (The phase function associated with the other point-group generator, Φ_{r_3}, is zero in all cases, because of our choice of gauge.) The International name (long form) and number (in italics) for the space group associated with each gauge equivalence class is listed alongside its phases.

	23 (T)	$\Phi_{r_2'}$	$\bar{4}3m$ (T_d)	Φ_m
P	$P23$ *195*	000	$P\bar{4}3m$ *215*	000
	$P2_13$ *198*	$0\frac{1}{2}\frac{1}{2}$	$P\bar{4}3n$ *218*	$00\frac{1}{2}$
F^*	$I23$ *197*	000	$I\bar{4}3m$ *217*	000
(I)	$I2_13$ *199*	$0\frac{1}{2}\frac{1}{2}$	$I\bar{4}3d$ *220*	$0\frac{1}{2}0$
I^*	$F23$ *196*	000	$F\bar{4}3m$ *216*	000
(F)			$F\bar{4}3c$ *219*	$\frac{1}{2}\frac{1}{2}0$

readily seen to be[29]

$$P \text{ lattice, } 532: \quad \Phi_{r_2}(\mathbf{b}^{(i)})\equiv\frac{n}{5}(100,\bar{1}10),\ n=0,1,2,3,4\ . \tag{3.51}$$

F^* (I) lattice (Y). The entries in Table III for $2P_m$ show that $\Delta\Theta_1\equiv-\alpha+\beta$ and $\Delta\Theta_4\equiv\alpha$, so we can choose α and β so that

$$\Theta_1\equiv\Theta_4\equiv0\ . \tag{3.52}$$

In this gauge, $2P_2(\mathbf{b}^{(1)})$ and $2P_2(\mathbf{b}^{(4)})$ give

$$0=\Theta_2-\Theta_3+\Theta_6 \text{ and } 0\equiv\Theta_3+\Theta_5\ , \tag{3.53}$$

while $5P_5(\mathbf{b}^{(2)})$ and $5P_5(\mathbf{b}^{(5)})$ give

$$0\equiv5\Theta_2-\Theta_3+2\Theta_6 \text{ and } 0\equiv2\Theta_3+5\Theta_5+\Theta_6\ . \tag{3.54}$$

The complete set of solutions to Eqs. (3.52)–(3.54) is

$F^*(I)$ lattice ,532:

$$\Phi_{r_2}(\mathbf{b}^{(i)})\equiv\frac{n}{5}(012,0\bar{2}1)\ ,\ n=0,1,2,3,4\ . \tag{3.55}$$

I^* (F) lattice (Y). The entries in Table IV for $2P_m$ give $\Delta\Theta_2\equiv2\alpha$ and $\Delta\Theta_5\equiv2\beta$, so we can choose α and β so that

$$\Theta_2\equiv\Theta_5\equiv0\ . \tag{3.56}$$

In this gauge $2P_2(\mathbf{b}^{(3)})$ and $2P_2(\mathbf{b}^{(6)})$ give

$$0\equiv2\Theta_3+\Theta_4 \text{ and } 0\equiv\Theta_1+\Theta_4+2\Theta_6\ , \tag{3.57}$$

while $5P_5(\mathbf{b}^{(1)})$ and $5P_5(\mathbf{b}^{(4)})$ give

$$0\equiv2\Theta_1+2\Theta_3+\Theta_4+\Theta_6\ ,$$
$$0\equiv\Theta_1+\Theta_3+3\Theta_4+3\Theta_6\ . \tag{3.58}$$

The complete set of solutions to Eqs. (3.57) and (3.58) is

I^* (F) lattice, 532:

$$\Phi_{r_2}(\mathbf{b}^{(i)})\equiv\frac{n}{5}(101,\bar{2}0\bar{2})\ ,\ n=0,1,2,3,4\ . \tag{3.59}$$

5. Point group O

Constraints and remaining gauge freedom:

$$0\equiv\Phi_{r_2}(2P_2\mathbf{b}^{(i)})\ ,\quad 0\equiv\Phi_{r_2}(4P_4\mathbf{b}^{(i)})\ ,$$
$$\Delta\Theta_i\equiv-\chi_1(2P_m(\mathbf{b}^{(i)}))\ . \tag{3.60}$$

P lattice (O). The entries in Table V for $2P_m$ enable us to pick a gauge in which $\Theta_3\equiv0$. We learn from $2P_2$ that $\Theta_1\equiv-\Theta_2$ and from $4P_4$ that their common value must be an integral multiple of $\frac{1}{4}$, so there are four classes:

$$P \text{ lattice, } 432: \quad \Phi_{r_2}(\mathbf{b}^{(i)})\equiv\tfrac{n}{4}(1\bar{1}0)\ ,\ n=0,1,2,3\ . \tag{3.61}$$

F^* (I) lattice (O). The entries in Table VI for $2P_m$ enables us to pick a gauge in which $\Theta_2\equiv0$. In this gauge we learn from $2P_2$ that $\Theta_3\equiv0$ and from $4P_4$ that $2\Theta_1\equiv0$, so there are two classes:

$$F^* \ (I) \text{ lattice, } 432: \quad \Phi_{r_2}(\mathbf{b}^{(i)})\equiv000 \text{ or } \tfrac{1}{2}00\ . \tag{3.62}$$

I^* (F) lattice (O). The entries in Table VII for $2P_m$ enable us to pick a gauge in which $\Theta_3\equiv0$. In this gauge we learn from $2P_2$ that $\Theta_1\equiv-\Theta_2$ and from $4P_4$ that $\Theta_1\equiv0,\frac{1}{2}$, so there are two classes:

$$I^* \ (F) \text{ lattice, } 432: \quad \Phi_{r_2}(\mathbf{b}^{(i)})\equiv000 \text{ or } \tfrac{1}{2}\tfrac{1}{2}0\ . \tag{3.63}$$

6. Point group T

Constraints and remaining gauge freedom:

$$0\equiv\Phi_{r_2'}(2P_2'\mathbf{b}^{(i)})\ ,\quad 0\equiv\Phi_{r_2'}(3P_3'\mathbf{b}^{(i)})\ ,$$
$$\Delta\Theta_i\equiv-\chi_1(2P_m'(\mathbf{b}^{(i)}))\ . \tag{3.64}$$

P lattice (T). The entries in Table V for $2P_m'$ enable us to pick a gauge in which $\Theta_1\equiv0$. We learn from $2P_2'$ that $2\Theta_2\equiv0$ and $3P_3'$ requires $\Theta_3+\Theta_2\equiv0$, so there are two classes:

$$P \ (I) \text{ lattice, } 23: \quad \Phi_{r_2'}(\mathbf{b}^{(i)})\equiv000 \text{ or } 0\tfrac{1}{2}\tfrac{1}{2}\ . \tag{3.65}$$

F^* (I) lattice (T). The entries in Table VI for $2P_m'$ en-

[29]It is convenient to write -1 as $\bar{1}$, etc.

able us to pick a gauge in which $\Theta_1 \equiv 0$. In this gauge we learn from $2P_2'$ that $\Theta_2 \equiv \Theta_3$, and from $3P_3'$ that $\Theta_2 \equiv -\Theta_3$, so there are two classes:

$$F^*\ (I)\ \text{lattice, } 23\text{: } \Phi_{r_2'}(\mathbf{b}^{(i)}) \equiv 000 \text{ or } 0\tfrac{1}{2}\tfrac{1}{2}\ . \quad (3.66)$$

Since, as we shall see in Sec. VI, the second possibility gives one of the only two examples[30] of a nonsymmorphic space group without extinctions, it is worth confirming directly that it is not gauge equivalent to a set of vanishing phase functions. To see this note from Table VI and Eq. (3.5) that

$$\Phi_{r_2'}(\mathbf{b}^{(3)}) - \Phi_{r_2'}(\mathbf{b}^{(1)}) + 2\Phi_{r_3}(\mathbf{b}^{(3)}) \quad (3.67)$$

is gauge invariant. But in the gauge in which $\Phi_{r_3} \equiv 0$, this combination of phases is equal to $\frac{1}{2}$ when $\Phi_{r_2'}(\mathbf{b}^{(i)}) = 0\frac{1}{2}\frac{1}{2}$. We therefore cannot reduce $\Phi_{r_2'}(\mathbf{b}^{(i)})$ to 000, without making Φ_{r_3} nonzero [as is also evident from the detailed calculation leading to (3.66)].

I^* (F) lattice (T). The entries in Table VII for $2P_m'$ enable us to pick a gauge in which $\Theta_2 \equiv 0$. We learn from $2P_2'$ that $\Theta_1 \equiv -\Theta_3$, and from $3P_3'$ that $\Theta_1 \equiv 0$, so there is only the single class

$$I^*\ (F)\ \text{lattice, } 23\text{: } \Phi_{r_2}(\mathbf{b}^{(i)}) \equiv 000\ . \quad (3.68)$$

7. Point group T_d

Constraints and remaining gauge freedom:

$$0 \equiv \Phi_m(2P_m\mathbf{b}^{(i)})\ , \quad \Delta\Theta_i \equiv -\chi_1(2P_2(\mathbf{b}^{(i)}))\ . \quad (3.69)$$

P lattice (T_d). The entries in Table V for $2P_2$ enable us to pick a gauge in which $\Theta_1 \equiv 0$. We then learn from $2P_m$ that $\Theta_2 \equiv 0$ and $2\Theta_3 \equiv 0$, so there are two classes:

$$P\ \text{lattice, } \bar{4}3m\text{: } \Phi_m(\mathbf{b}^{(i)}) \equiv 000 \text{ or } 00\tfrac{1}{2}\ . \quad (3.70)$$

F^* (I) lattice (T_d). The entries in Table VI for $2P_2$ enable us to pick a gauge in which $\Theta_1 \equiv 0$. In this gauge we learn from $2P_m$ that $\Theta_3 \equiv 0$ and $2\Theta_2 \equiv 0$, so there are two classes:

$$F^*\ (I)\ \text{lattice, } \bar{4}3m\text{: } \Phi_m(\mathbf{b}^{(i)}) \equiv 000 \text{ or } 0\tfrac{1}{2}0\ . \quad (3.71)$$

I^* (F) lattice (T_d). The entries in Table VII for $2P_2$ enable us to pick a gauge in which $\Theta_3 \equiv 0$. We learn from $2P_m$ that $\Theta_1 \equiv \Theta_2 \equiv 0, \frac{1}{2}$, so there are two classes:

$$I^*\ (F)\ \text{lattice, } \bar{4}3m\text{: } \Phi_m(\mathbf{b}^{(i)}) \equiv 000 \text{ or } \tfrac{1}{2}\tfrac{1}{2}0\ . \quad (3.72)$$

[30]The other is $I2_12_12_1$ (No. 24) in the orthorhombic system, as noted in Sec. IV.C.2.

This completes the calculation of the gauge equivalence classes of phase functions for all point groups on all cubic and icosahedral lattices. The results are tabulated in Tables VIII, IX, and X.

H. The cubic and icosahedral space groups

Before associating each of these gauge equivalence classes with a distinct space group, we must check for further identification of distinct classes described in Sec. II.G. This cannot happen for O_h, which is the full point group of the lattice, or for O, which differs from it only by improper operations. Among the tetrahedral point groups, only T_h on the P lattice has more than a single class of nonzero phase functions, and there we find two classes [the last two listed in Eq. (3.44)] which differ only by the interchange of the values of $\Phi_m(\mathbf{b}^{(1)})$ and $\Phi_m(\mathbf{b}^{(3)})$. Since this interchange can be accomplished by the operation $h = r_4$ (see Fig. 1), which is a proper lattice symmetry not in the point group, the two gauge-inequivalent sets of phase functions do not specify distinct space groups. For that reason the second choice is enclosed in braces in Table VIII.

For the icosahedral groups such an identification of the space groups associated with distinct gauge equivalence classes can only arise from the scale invariance of the icosahedral lattices, since Y_h is the full symmetry group of the lattice and Y differs from it only by improper operations. When the point group is Y_h, only the I^* lattice has more than a single nontrivial gauge equivalence class, but the invariance of the I^* lattice under a scaling by τ leads to the identification of the space groups associated with all three of the nontrivial classes. This is because the invariance of the I^* lattice under a scaling by τ means that there is no way to distinguish between the phases $\Phi_m(\mathbf{b}^{(i)})$ and $\Psi_m(\mathbf{b}^{(i)}) = \Phi_m(\tau\mathbf{b}^{(i)})$. Since $\tau\mathbf{b}^{(i)} = \mathbf{b}^{(i+3)}$ and $\tau\mathbf{b}^{(i+3)} = \mathbf{b}^{(i)} + \mathbf{b}^{(i+3)}$, $i = 1,2,3$, we have

$$\Psi_m(\mathbf{b}^{(i)}) = \Phi_m(\mathbf{b}^{(i+3)})\ ,$$
$$\Psi_m(\mathbf{b}^{(i+3)}) \equiv \Phi_m(\mathbf{b}^{(i)}) + \Phi_m(\mathbf{b}^{(i+3)})\ ,$$
$$i = 1,2,3\ . \quad (3.73)$$

Thus if two sets of phases differ by the alteration

$$\Theta_1\Theta_2\Theta_3\ ,\ \Theta_4\Theta_5\Theta_6$$
$$\rightarrow \Theta_4\Theta_5\Theta_6\ ,(\Theta_1+\Theta_4)(\Theta_2+\Theta_5)(\Theta_3+\Theta_6)\ , \quad (3.74)$$

the second structure will have exactly the same phase relations as the first does with respect to the rescaled primitive set. But this is precisely how each of the last two sets of phases in Table VIII for Y_h on the I^* lattice is related to the set above it. Therefore all three specify the same space group.

When the point group is Y, scale invariance leads to the identification of the space groups associated with four nonzero gauge equivalence classes on all three lattices.

This is most easily verified for the F^* and I^* lattices, since both are invariant under a rescaling by τ and one easily verifies that each of the four nonzero entries for the F^* and I^* lattices is indeed obtained from the one above (modulo 1) by precisely the transformation (3.74).

The corresponding identification of space groups is slightly more subtle for the P lattice, which is invariant under a scaling by τ^3 (see Appendix A.) It follows from Eq. (A7) that if $\Phi(\mathbf{b}^{(i)})$ is given by $\frac{n}{5}(100,\bar{1}10)$ then $\Phi(\tau^3\mathbf{b}^{(i)})\equiv\frac{n}{5}(\bar{1}2\bar{1},\bar{2}21)$. But this is gauge equivalent to $\frac{2n}{5}(100,\bar{1}10)$ the shift in phases being $\frac{n}{5}(\bar{2}\,\bar{2}1,00\bar{1})$, which Table II shows follows from the gauge transformation given by

$$\chi(\mathbf{b}^{(1)})\equiv\chi(\mathbf{b}^{(2)})\equiv\chi(\mathbf{b}^{(3)})\equiv\tfrac{n}{5}\ ,\qquad \chi(\mathbf{b}^{(4)})\equiv\chi(\mathbf{b}^{(5)})\equiv\chi(\mathbf{b}^{(6)})\equiv\tfrac{2n}{5}\ . \tag{3.75}$$

Thus each of the four nonzero entries in Table IX for the icosahedral P lattice is gauge equivalent (modulo 1) to one obtained from the one above it (modulo 1) by changing primitive vectors from $\mathbf{b}^{(i)}$ to $\tau^3\mathbf{b}^{(i)}$.

IV. THE ORTHORHOMBIC SPACE GROUPS

A. Generators for the orthorhombic point groups

Given an axis **a**, let r_a be the twofold rotation about **a** and let m_a be the mirroring ir_a in the plane perpendicular to **a** (i is the inversion). The orthorhombic point groups contain either r or m or both for each of three mutually perpendicular axes, **a**, **b**, **c**. Since $r_a r_b = r_c$, there are just three possibilities: 222 (D_2), which has only rotations; $mm2$ (C_{2v}), which has a rotation associated with one axis and mirrors associated with the other two; and mmm (D_{2h}), which has mirrors and rotations associated with all three. The group 222 is generated by any two of the rotations; a symmetric set of generators for $mm2$ consists of the two mirrors; and mmm has all three mirrors as its generators. The generating relations simply express the fact that all the generators are of order two and all commute with each other. This information is summarized in Table XI.

B. The orthorhombic lattices

There are four orthorhombic lattices, which we specify in terms of their primitive generating vectors, expressed, in turn, as integral linear combinations of three mutually orthogonal vectors **a**, **b**, and **c** of unequal lengths. For the simple orthorhombic lattice we have

P lattice:

$$\mathbf{b}^{(1)}=\mathbf{a}\ ,\quad \mathbf{b}^{(2)}=\mathbf{b}\ ,\quad \mathbf{b}^{(3)}=\mathbf{c}\ . \tag{4.1}$$

The lattice that is face centered in Fourier space is called body-centered orthorhombic and is given by all integral linear combinations of the following set:

F^* (I) lattice:

$$\mathbf{b}^{(1)}=\mathbf{b}+\mathbf{c}\ ,\quad \mathbf{b}^{(2)}=\mathbf{c}+\mathbf{a}\ ,\quad \mathbf{b}^{(3)}=\mathbf{a}+\mathbf{b}\ . \tag{4.2}$$

The lattice that is body centered in Fourier space is called face-centered orthorhombic and is given by all integral linear combinations of

I^* (F) lattice:

$$\mathbf{b}^{(1)}=\mathbf{b}+\mathbf{c}-\mathbf{a}\ ,\quad \mathbf{b}^{(2)}=\mathbf{c}+\mathbf{a}-\mathbf{b}\ ,\quad \mathbf{b}^{(3)}=\mathbf{a}+\mathbf{b}-\mathbf{c}\ . \tag{4.3}$$

The fourth orthorhombic lattice is called centered orthorhombic and consists of centered rectangular planar lattices stacked directly above one another. We take it to be given by all integral linear combinations of

TABLE XI. Generators for the orthorhombic point groups. The subscripts a, b, and c refer to the three orthogonal axes. The twofold rotation r_a is about the axis **a**, and the mirror m_a is in the plane through the origin perpendicular to **a**, etc. The two are related by $m_a=ir_a$, where i is the inversion. Note that the product of rotations about any two of the axes is the rotation about the third: $r_a r_b = m_a m_b = r_c$, etc. The generating relations simply assert that the squares of all generators are the identity and that all generators commute.

Schönflies	International	Generators	Point-Group Generating Relations
D_2	222	r_a, r_b	$r_a^2 = r_b^2 = e,\ r_a r_b = r_b r_a$
C_{2v}	$mm2$	m_a, m_b	$m_a^2 = m_b^2 = e,\ m_a m_b = m_b m_a$
D_{2h}	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$ (mmm)	m_a, m_b, m_c	$m_i^2 = e,\ m_i m_j = m_j m_i,\ i,j = a,b,c$

C lattice:

$$\mathbf{b}^{(1)}=\mathbf{b}+\mathbf{a}\ ,\quad \mathbf{b}^{(2)}=\mathbf{b}-\mathbf{a}\ ,\quad \mathbf{b}^{(3)}=\mathbf{c}\ . \tag{4.4}$$

Note that the a, b, and c axes are on an equal footing in the first three lattices, but the c axis is distinguishable from the other two (which remain on an equal footing) in the C lattice.

C. The orthorhombic space groups

We again determine the space groups by applying the group compatibility condition (2.11) to the generating relations, always selecting a gauge to make the analysis simple. The two types of generating relation with their associated conditions on the phase functions, and the general form (2.10) of a gauge transformation are

$$\begin{aligned} &g^2=e\text{:}\quad \Phi_g([1+g]\mathbf{b}^{(i)})\equiv 0\ ;\\ &gg'=g'g\text{:}\quad \Phi_{g'}([1-g]\mathbf{b}^{(i)})\equiv\Phi_g([1-g']\mathbf{b}^{(i)})\ ;\\ &\text{gauge transformation:}\quad \chi([1-g]\mathbf{b}^{(i)})\equiv-\Delta\Phi_g(\mathbf{b}^{(i)})\ . \end{aligned} \tag{4.5}$$

The first two lines of Eq. (4.5) yield linear equations for the values of the phase functions for the point-group generators at the lattice-generating vectors, and a judicious choice of the three numbers $\chi(\mathbf{b}^{(i)})$ in the third leads to a unique representative of each class of gauge-equivalent solutions to those equations.

The point groups 222 and $mm2$ have two generators (see Table XI), so there are just three constraints on their phase functions; mmm has three generators and its phase functions are therefore subject to six constraints.

Since all of the conditions (4.5) used to compute the space groups are on the values of phase functions at vectors of the form $[1\pm g]\mathbf{b}^{(i)}$, it is helpful to have at hand explicit tables of the values of $[1+g]\mathbf{b}^{(i)}$ and $[1-g]\mathbf{b}^{(i)}$, for each of the four lattice types (Tables XII-XV). A mirror m differs from the corresponding rotation r only by the inversion i, so we have

$$\begin{aligned} &[1+m]\mathbf{b}^{(i)}=[1-r]\mathbf{b}^{(i)}\ ,\\ &[1-m]\mathbf{b}^{(i)}=[1+r]\mathbf{b}^{(i)}\ . \end{aligned} \tag{4.6}$$

Since $1+r$ is twice the projection on the axis of the rotation and $1+m$ is twice the projection in the plane of the mirror, the table for each of the four types of lattice can be read directly from the expressions (4.1)–(4.4) for their primitive vectors in terms of the rotation axes (mirror normals) **a**, **b**, and **c** association with the point-group generators. Although the content of these tables is trivial, examining them leads directly to the classes of phase functions.

The choice of gauge is specified by three independent parameters, $\chi(\mathbf{b}^{(1)})$, $\chi(\mathbf{b}^{(2)})$, and $\chi(\mathbf{b}^{(3)})$. We shall choose those parameters to make $\Phi_g(\mathbf{b}^{(i)})$ zero for three pairs of point-group elements g and primitive lattice-generating vectors $\mathbf{b}^{(i)}$. Since $\Delta\Phi_g(\mathbf{b}^{(i)})\equiv\chi([g-1]\mathbf{b}^{(i)})$, to establish that this can be done one need only confirm from the table for the lattice under consideration that the three values of $[1-g]\mathbf{b}^{(i)}$ give three linearly independent vectors. In each case that we consider, I shall simply state which phases we choose to vanish, leaving it to the reader to confirm, by a glance at the appropriate table, that such a choice can indeed be made.

While I have tried to organize the computation that follows to parallel as much as possible the treatment of the icosahedral and cubic space groups in Sec. III, there are two main differences:

(1) In Sec. III we examined each of the seven icosahedral and cubic point groups, computing for each point group the gauge equivalence classes for the three icosahedral or cubic lattices. It was convenient to treat

TABLE XII. Orthorhombic I^* (F)-lattice projections. The primitive generating vectors $\mathbf{b}^{(i)}$ are expressed in terms of the orthoronormal vectors **a**, **b**, and **c** at the top of the table. Since r_a takes **a** into itself and **b** and **c** into their negatives, the entries for $1+r_a$ are easily confirmed, and the entries for $1-r_a$ follow immediately [most directly from the fact that $(1+r_a)+(1-r_a)=2$]. The entries associated with r_b and r_c are found in the same way.

$\mathbf{b}^{(1)}=\mathbf{b}+\mathbf{c}-\mathbf{a}$,	$\mathbf{b}^{(2)}=\mathbf{c}+\mathbf{a}-\mathbf{b}$,	$\mathbf{b}^{(3)}=\mathbf{a}+\mathbf{b}-\mathbf{c}$.	
	$1+r_a=1-m_a$	$1+r_b=1-m_b$	$1+r_c=1-m_c$
$\mathbf{b}^{(1)}\rightarrow$	$-\mathbf{b}^{(2)}-\mathbf{b}^{(3)}$	$\mathbf{b}^{(3)}+\mathbf{b}^{(1)}$	$\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$
$\mathbf{b}^{(2)}\rightarrow$	$\mathbf{b}^{(2)}+\mathbf{b}^{(3)}$	$-\mathbf{b}^{(3)}-\mathbf{b}^{(1)}$	$\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$
$\mathbf{b}^{(3)}\rightarrow$	$\mathbf{b}^{(2)}+\mathbf{b}^{(3)}$	$\mathbf{b}^{(3)}+\mathbf{b}^{(1)}$	$-\mathbf{b}^{(1)}-\mathbf{b}^{(2)}$
	$1-r_a=1+m_a$	$1-r_b=1+m_b$	$1-r_c=1+m_c$
$\mathbf{b}^{(1)}\rightarrow$	$2\mathbf{b}^{(1)}+\mathbf{b}^{(2)}+\mathbf{b}^{(3)}$	$-\mathbf{b}^{(3)}+\mathbf{b}^{(1)}$	$\mathbf{b}^{(1)}-\mathbf{b}^{(2)}$
$\mathbf{b}^{(2)}\rightarrow$	$\mathbf{b}^{(2)}-\mathbf{b}^{(3)}$	$2\mathbf{b}^{(2)}+\mathbf{b}^{(3)}+\mathbf{b}^{(1)}$	$-\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$
$\mathbf{b}^{(3)}\rightarrow$	$-\mathbf{b}^{(2)}+\mathbf{b}^{(3)}$	$\mathbf{b}^{(3)}-\mathbf{b}^{(1)}$	$2\mathbf{b}^{(3)}+\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$

TABLE XIII. Orthorhombic F^* (I)-lattice projections. The primitive generating vectors $\mathbf{b}^{(i)}$ are expressed in terms of the orthoronormal vectors **a**, **b**, and **c** at the top of the table. Since r_a takes **a** into itself and **b** and **c** into their negatives, the entries for $1+r_a$ are easily confirmed, and the entries for $1-r_a$ follow immediately [most directly from the fact that $(1+r_a)+(1-r_a)=2$]. The entries associated with r_b and r_c are found in the same way.

$\mathbf{b}^{(1)}=\mathbf{b}+\mathbf{c}$,	$\mathbf{b}^{(2)}=\mathbf{c}+\mathbf{a}$,	$\mathbf{b}^{(3)}=\mathbf{a}+\mathbf{b}$.	
	$1+r_a=1-m_a$	$1+r_b=1-m_b$	$1+r_c=1-m_c$
$\mathbf{b}^{(1)}\rightarrow$	0	$-\mathbf{b}^{(2)}+\mathbf{b}^{(3)}+\mathbf{b}^{(1)}$	$-\mathbf{b}^{(3)}+\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$
$\mathbf{b}^{(2)}\rightarrow$	$-\mathbf{b}^{(1)}+\mathbf{b}^{(2)}+\mathbf{b}^{(3)}$	0	$-\mathbf{b}^{(3)}+\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$
$\mathbf{b}^{(3)}\rightarrow$	$-\mathbf{b}^{(1)}+\mathbf{b}^{(2)}+\mathbf{b}^{(3)}$	$-\mathbf{b}^{(2)}+\mathbf{b}^{(3)}+\mathbf{b}^{(1)}$	0
	$1-r_a=1+m_a$	$1-r_b=1+m_b$	$1-r_c=1+m_c$
$\mathbf{b}^{(1)}\rightarrow$	$2\mathbf{b}^{(1)}$	$\mathbf{b}^{(2)}-\mathbf{b}^{(3)}+\mathbf{b}^{(1)}$	$\mathbf{b}^{(3)}+\mathbf{b}^{(1)}-\mathbf{b}^{(2)}$
$\mathbf{b}^{(2)}\rightarrow$	$\mathbf{b}^{(1)}+\mathbf{b}^{(2)}-\mathbf{b}^{(3)}$	$2\mathbf{b}^{(2)}$	$\mathbf{b}^{(3)}-\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$
$\mathbf{b}^{(3)}\rightarrow$	$\mathbf{b}^{(1)}-\mathbf{b}^{(2)}+\mathbf{b}^{(3)}$	$\mathbf{b}^{(2)}+\mathbf{b}^{(3)}-\mathbf{b}^{(1)}$	$2\mathbf{b}^{(3)}$

together all the cases for a given point group, because for each point group a different set of projections had to be examined. Here, however, essentially the same set of projections is relevant for each of the three point groups, and for each lattice the analysis for *mmm* is simply an extension of the analysis for *mm*2. It is therefore now more convenient to examine each of the four orthorhombic lattices, computing for each lattice the gauge equivalence classes for the three orthorhombic point groups.

(2) In the icosahedral and cubic cases we separated out the computation of the gauge equivalence classes from the further association of distinct classes with the same space group, as a result of the existence of lattice symmetries h not in the point group. The orthorhombic case is rife with such identifications, but they are all of a rather trivial sort, associated with the arbitrary choice made in labeling the three orthogonal directions **a**, **b**, and **c**. Formally this leads to an identification of distinct gauge equivalence classes associated with an operation h that simultaneously permutes the directions of **a**, **b**, and **c**, while rescaling independently along those three directions in such a way as to leave the resulting lattice unchanged. Such a combination of rotations and rescalings is clearly not an operation in the point group of the material, though it is a symmetry of the lattice, so the gen-

TABLE XIV. Orthorhombic C-lattice projections. The primitive generating vectors $\mathbf{b}^{(i)}$ are expressed in terms of the orthonormal vectors **a**, **b**, and **c** at the top of the table. Since r_a takes **a** into itself and **b** and **c** into their negatives, r_a takes $\mathbf{b}^{(1)}$ into $-\mathbf{b}^{(2)}$, $\mathbf{b}^{(2)}$ into $-\mathbf{b}^{(1)}$, and **c** into $-\mathbf{c}$. Similarly, $\mathbf{r}_b$ interchanges $\mathbf{b}^{(1)}$ and $\mathbf{b}^{(2)}$ and takes **c** into $-\mathbf{c}$. Finally, r_c takes $\mathbf{b}^{(1)}$ and $\mathbf{b}^{(2)}$ into their negatives and **c** into itself. The entries are easily constructed from this.

$\mathbf{b}^{(1)}=\mathbf{a}+\mathbf{b}$,	$\mathbf{b}^{(2)}=-\mathbf{a}+\mathbf{b}$,	$\mathbf{b}^{(3)}=\mathbf{c}$.	
	$1+r_a=1-m_a$	$1+r_b=1-m_b$	$1+r_c=1-m_c$
$\mathbf{b}^{(1)}\rightarrow$	$\mathbf{b}^{(1)}-\mathbf{b}^{(2)}$	$\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$	0
$\mathbf{b}^{(2)}\rightarrow$	$-\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$	$\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$	0
$\mathbf{b}^{(3)}\rightarrow$	0	0	$2\mathbf{b}^{(3)}$
	$1-r_a=1+m_a$	$1-r_b=1+m_b$	$1-r_c=1+m_c$
$\mathbf{b}^{(1)}\rightarrow$	$\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$	$\mathbf{b}^{(1)}-\mathbf{b}^{(2)}$	$2\mathbf{b}^{(1)}$
$\mathbf{b}^{(2)}\rightarrow$	$\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$	$-\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$	$2\mathbf{b}^{(2)}$
$\mathbf{b}^{(3)}\rightarrow$	$2\mathbf{b}^{(3)}$	$2\mathbf{b}^{(3)}$	0

TABLE XV. Orthorhombic P-lattice projections. The primitive generating vectors $\mathbf{b}^{(i)}$ are identified with the orthonormal vectors **a**, **b**, and **c** at the top of the table. The entries for $1+r_a$ and $1-r_a$ follow immediately from the fact that r_a takes **a** into itself and **b** and **c** into their negatives. The entries associated with r_b and r_c follow in the same way.

$\mathbf{b}^{(1)}=\mathbf{a}$,	$\mathbf{b}^{(2)}=\mathbf{b}$,	$\mathbf{b}^{(3)}=\mathbf{c}$.	
	$1+r_a=1-m_a$	$1+r_b=1-m_b$	$1+r_c=1-m_c$
$\mathbf{b}^{(1)}\rightarrow$	$2\mathbf{b}^{(1)}$	0	0
$\mathbf{b}^{(2)}\rightarrow$	0	$2\mathbf{b}^{(2)}$	0
$\mathbf{b}^{(3)}\rightarrow$	0	0	$2\mathbf{b}^{(3)}$
	$1-r_a=1+m_a$	$1-r_b=1+m_b$	$1-r_c=1+m_c$
$\mathbf{b}^{(1)}\rightarrow$	0	$2\mathbf{b}^{(1)}$	$2\mathbf{b}^{(1)}$
$\mathbf{b}^{(2)}\rightarrow$	$2\mathbf{b}^{(2)}$	0	$2\mathbf{b}^{(2)}$
$\mathbf{b}^{(3)}\rightarrow$	$2\mathbf{b}^{(3)}$	$2\mathbf{b}^{(3)}$	0

TABLE XVI. The space groups on the orthohombic I^* (F) lattice. One can verify from the group compatibility condition [Eq. (2.11)] that the phase functions for the unlisted rotations associated with the two nonsymmorphic groups are given by $\Phi_{r_c}(\mathbf{b}^{(i)})\equiv\Phi_{m_a}(\mathbf{b}^{(i)})+\Phi_{m_b}(\mathbf{b}^{(i)})+\frac{1}{2}\frac{1}{2}\frac{1}{2}$ and (in the case of *mmm*) the two additional relations given by cyclically permuting a, b, and c.

222 (D_2)	Φ_{r_a}	Φ_{r_b}	*mmm* (D_{2h})	Φ_{m_a}	Φ_{m_b}	Φ_{m_c}
*F*222 *22*	000	000	$F\frac{2}{m}\frac{2}{m}\frac{2}{m}$ *69*	000	000	000
mm2 (C_{2v})	Φ_{m_a}	Φ_{m_b}	$F\frac{2}{d}\frac{2}{d}\frac{2}{d}$ *70*	$\frac{1}{2}00$	$0\frac{1}{2}0$	$00\frac{1}{2}$
Fmm2 *42*	000	000				
Fdd2 *43*	$\frac{1}{2}00$	$0\frac{1}{2}0$				

TABLE XVII. The space groups on the orthorhombic F^* (I) lattice. One can verify from the group compatibility condition (2.11) that the phase functions for the unlisted rotations associated with the nonsymmorphic groups are given by $\Phi_{r_c}(\mathbf{b}^{(i)})\equiv\Phi_{m_a}(\mathbf{b}^{(i)})+\Phi_{m_b}(\mathbf{b}^{(i)})$ and (in the case of *mmm*) the two additional relations given by cyclically permuting a, b, and c.

222 (D_2)	Φ_{r_a}	Φ_{r_b}	*mmm* (D_{2h})	Φ_{m_a}	Φ_{m_b}	Φ_{m_c}
*I*222 *23*	000	000	$I\frac{2}{m}\frac{2}{m}\frac{2}{m}$ *71*	000	000	000
$I2_12_12_1$ *24*	$\frac{1}{2}\frac{1}{2}0$	$0\frac{1}{2}\frac{1}{2}$	$I\frac{2_1}{m}\frac{2_1}{m}\frac{2_1}{a}$ *74*	000	000	$\frac{1}{2}0\frac{1}{2}$
mm2 (C_{2v})	Φ_{m_a}	Φ_{m_b}	$I\frac{2}{b}\frac{2}{a}\frac{2}{m}$ *72*	$\frac{1}{2}\frac{1}{2}0$	$0\frac{1}{2}\frac{1}{2}$	000
Imm2 *44*	000	000	$I\frac{2_1}{b}\frac{2_1}{c}\frac{2_1}{a}$ *73*	$\frac{1}{2}\frac{1}{2}0$	$0\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}0\frac{1}{2}$
Ibm2 *46*	$\frac{1}{2}\frac{1}{2}0$	000				
Iba2 *45*	$\frac{1}{2}\frac{1}{2}0$	$\frac{1}{2}\frac{1}{2}0$				

eral argument of Sec. II.G applies. In practice, however, the need for identifying the space groups associated with gauge equivalence classes related in this way is so obvious that we do not make a special point of it.

The results derived in the four subsections that follow are collected together in Tables XVI–XIX.

1. I^* (F) lattice

Everything follows from an examination of Table XII:

Point group 222 (I^* (F) lattice). We can pick a gauge in which

$$\Phi_{r_a}(\mathbf{b}^{(1)})\equiv\Phi_{r_a}(\mathbf{b}^{(3)})\equiv\Phi_{r_b}(\mathbf{b}^{(3)})\equiv 0\ . \tag{4.7}$$

In this gauge the conditions (4.5) associated with the generating relations $r_a^2\equiv e$ and $r_b^2=e$ reduce to

$$\Phi_{r_a}(\mathbf{b}^{(2)})\equiv 0\ ,\quad \Phi_{r_b}(\mathbf{b}^{(1)})\equiv 0\ , \tag{4.8}$$

and the condition (4.5) associated with $r_a r_b=r_b r_a$ then requires the only remaining nonzero phase to vanish:

$$\Phi_{r_b}(\mathbf{b}^{(2)})\equiv 0\ . \tag{4.9}$$

We have thus established that any set of phase functions is gauge equivalent to 0, so there is only the symmorphic space group

I^* (F) lattice, 222:

$$\begin{matrix}\Phi_{r_a}(\mathbf{b}^{(i)}) \\ \Phi_{r_b}(\mathbf{b}^{(i)})\end{matrix}\equiv\begin{matrix}000 \\ 000\end{matrix}\ . \tag{4.10}$$

Point Group mm2 (I^* (F) lattice). We pick a gauge in which

$$\Phi_{m_a}(\mathbf{b}^{(3)})\equiv\Phi_{m_b}(\mathbf{b}^{(3)})\equiv 0\ . \tag{4.11}$$

[Note that we are still left with enough gauge freedom to make $\Phi_{m_c}(\mathbf{b}^{(i)})\equiv 0$ for any given $\mathbf{b}^{(i)}$, when we come to the case of *mmm*.]

In the gauge (4.11) the conditions (4.5) associated with the generating relations $m_a^2\equiv e$ and $m_b^2=e$ reduce to

$$\begin{aligned}&\Phi_{m_a}(\mathbf{b}^{(2)})\equiv 0\ ,\quad 2\Phi_{m_a}(\mathbf{b}^{(1)})\equiv 0\ ,\\ &\Phi_{m_b}(\mathbf{b}^{(1)})\equiv 0\ ,\quad 2\Phi_{m_b}(\mathbf{b}^{(2)})\equiv 0\ ,\end{aligned} \tag{4.12}$$

and the conditions (4.5) associated with $m_a m_b=m_b m_a$ all reduce to

TABLE XVIII. The space groups on the orthorhombic C lattice. The space groups for $m2m$ on the centered lattice are more commonly denoted by $Amm2$ $Abm2$, $Ama2$, and $Aba2$, a nomenclature based on taking the twofold axis of G along **c** (instead of **b**) and the preferred direction of the lattice along **a** (instead of **c**). One can verify from the group compatibility condition (2.11) that the phase functions for the unlisted rotations associated with the nonsymmorphic groups are given by $\Phi_{r_c}(\mathbf{b}^{(i)})\equiv\Phi_{m_a}(\mathbf{b}^{(i)})+\Phi_{m_b}(\mathbf{b}^{(i)})$ and (when relevant) the two additional relations given by cyclically permuting a, b, and c.

222 (D_2)	Φ_{r_a}	Φ_{r_b}	
$C222$ 21	000	000	
$C222_1$ 20	000	$00\frac{1}{2}$	
$mm2$ (C_{2v})	Φ_{m_a}	Φ_{m_b}	Φ_{m_c}
$Cmm2$ 35	000	000	
$Cmc2_1$ 36	000	$00\frac{1}{2}$	
$Ccc2$ 37	$00\frac{1}{2}$	$00\frac{1}{2}$	
$m2m$ (D_{2d})	Φ_{m_a}	Φ_{m_b}	Φ_{m_c}
$Cm2m$ 38	000		000
$Cm2a$ 39	000		$\frac{1}{2}\frac{1}{2}0$
$Cc2m$ 40	$00\frac{1}{2}$		000
$Cc2a$ 41	$00\frac{1}{2}$		$\frac{1}{2}\frac{1}{2}0$

mmm (D_{2h})	Φ_{m_a}	Φ_{m_b}	Φ_{m_c}
$C\frac{2}{m}\frac{2}{m}\frac{2}{m}$ 65	000	000	000
$C\frac{2}{m}\frac{2}{c}\frac{2_1}{m}$ 63	000	$00\frac{1}{2}$	000
$C\frac{2}{c}\frac{2}{c}\frac{2}{m}$ 66	$00\frac{1}{2}$	$00\frac{1}{2}$	000
$C\frac{2}{m}\frac{2}{m}\frac{2}{a}$ 67	000	000	$\frac{1}{2}\frac{1}{2}0$
$C\frac{2}{m}\frac{2}{c}\frac{2_1}{a}$ 64	000	$00\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}0$
$C\frac{2}{c}\frac{2}{c}\frac{2}{a}$ 68	$00\frac{1}{2}$	$00\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}0$

$$\Phi_{m_a}(\mathbf{b}^{(1)}) \equiv \Phi_{m_b}(\mathbf{b}^{(2)}) \ . \tag{4.13}$$

In addition to the symmorphic space group there is thus a single additional one in which the only nonvanishing phases can be taken to be

$$\Phi_{m_a}(\mathbf{b}^{(1)}) \equiv \Phi_{m_b}(\mathbf{b}^{(2)}) \equiv \tfrac{1}{2} \ . \tag{4.14}$$

The unused remaining gauge freedom cannot reduce this to the symmorphic space group, since $\Phi_{m_a}(\mathbf{b}^{(1)}) + \Phi_{m_a}(\mathbf{b}^{(2)})$ is gauge invariant and nonzero.

I^* (F) lattice, $mm2$:

$$\begin{matrix}\Phi_{m_a}(\mathbf{b}^{(i)}) \\ \Phi_{m_b}(\mathbf{b}^{(i)})\end{matrix} \equiv \begin{matrix}000 \\ 000\end{matrix} \text{ or } \begin{matrix}\tfrac{1}{2}00 \\ 0\tfrac{1}{2}0\end{matrix} \ . \tag{4.15}$$

Point group mmm (I^* (F) lattice). All of the conditions and gauge freedom used to arrive at (4.15) continue

TABLE XIX. The space groups on the orthorhombic P lattice. The mirror phase functions are given in a gauge in which $\Phi_{m_a}(\mathbf{b}^{(1)})$, $\Phi_{m_b}(\mathbf{b}^{(2)})$, and $\Phi_{m_c}(\mathbf{b}^{(3)})$ are zero. The first eight sets of phase functions listed for $mm2$ are grouped into four complementary pairs (the first and second entries constitute such a pair, the third and fourth another, etc.), and the first 12 sets of phase functions for mmm are grouped into six complementary pairs, as described in Sec. IV.C.4. (The remaining two sets of phase functions for $mm2$ and remaining four sets for mmm give the same space groups as their complements.) The meaning of the international space-group nomenclature is transparent for the P lattice, since it is always based on primitive indexing: m appears in the first (second, third) position if the phase function Φ_{m_a} (Φ_{m_b},Φ_{m_c}) is 000; n appears if the corresponding phase function has both entries $\frac{1}{2}$, and a, b, c indicate a single entry of $\frac{1}{2}$ (with the choice of letter clearly indicating which entry it is); 2 or 2_1 appears in the third position if $\Phi_{r_c}(\mathbf{b}^{(3)}) \equiv \frac{1}{2}$, and similarly for the other two positions, when $\mathbf{b}^{(1)}$ and $\mathbf{b}^{(2)}$ are also twofold axes. [One can verify from the group compatibility condition (2.11) that the phase functions for the unlisted twofold rotations are given by $\Phi_{r_c}(\mathbf{b}^{(i)}) \equiv \Phi_{m_a}(\mathbf{b}^{(i)}) + \Phi_{m_b}(\mathbf{b}^{(i)})$ and (when relevant) the two additional relations given by cyclically permuting a, b, and c.]

222 (D_2)		Φ_{r_a}	Φ_{r_b}
$P222$	16	000	000
$P2_122$	17	$\frac{1}{2}00$	000
$P2_12_12$	18	$\frac{1}{2}\frac{1}{2}0$	$0\frac{1}{2}0$
$P2_12_12_1$	19	$\frac{1}{2}\frac{1}{2}0$	$0\frac{1}{2}\frac{1}{2}$

$mm2$ (D_{2d})		Φ_{m_a}	Φ_{m_b}
$Pmm2$	25	000	000
$Pnn2$	34	$0\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}0\frac{1}{2}$
$Pma2$	28	000	$\frac{1}{2}00$
$Pnc2$	30	$0\frac{1}{2}\frac{1}{2}$	$00\frac{1}{2}$
$Pmc2_1$	26	000	$00\frac{1}{2}$
$Pna2_1$	33	$0\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}00$
$Pcc2$	27	$00\frac{1}{2}$	$00\frac{1}{2}$
$Pba2$	32	$0\frac{1}{2}0$	$\frac{1}{2}00$
$Pmn2_1$	31	000	$\frac{1}{2}0\frac{1}{2}$
$Pca2_1$	29	$00\frac{1}{2}$	$\frac{1}{2}00$

mmm (D_{2h})		Φ_{m_a}	Φ_{m_b}	Φ_{m_c}
$P\frac{2}{m}\frac{2}{m}\frac{2}{m}$	47	000	000	000
$P\frac{2}{n}\frac{2}{n}\frac{2}{n}$	48	$0\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}0\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}0$
$P\frac{2_1}{m}\frac{2}{m}\frac{2}{a}$	51	000	000	$\frac{1}{2}00$
$P\frac{2_1}{n}\frac{2}{n}\frac{2}{b}$	52	$0\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}0\frac{1}{2}$	$0\frac{1}{2}0$
$P\frac{2_1}{m}\frac{2_1}{m}\frac{2}{n}$	59	000	000	$\frac{1}{2}\frac{1}{2}0$
$P\frac{2_1}{n}\frac{2_1}{n}\frac{2}{m}$	58	$0\frac{1}{2}\frac{1}{2}$	$\frac{1}{2}0\frac{1}{2}$	000
$P\frac{2_1}{b}\frac{2_1}{a}\frac{2}{m}$	55	$0\frac{1}{2}0$	$\frac{1}{2}00$	000
$P\frac{2_1}{c}\frac{2_1}{c}\frac{2}{n}$	56	$00\frac{1}{2}$	$00\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}0$
$P\frac{2}{b}\frac{2_1}{c}\frac{2_1}{m}$	57	$0\frac{1}{2}0$	$00\frac{1}{2}$	000
$P\frac{2}{c}\frac{2_1}{a}\frac{2_1}{n}$	60	$00\frac{1}{2}$	$\frac{1}{2}00$	$\frac{1}{2}\frac{1}{2}0$
$P\frac{2}{c}\frac{2}{c}\frac{2}{m}$	49	$00\frac{1}{2}$	$00\frac{1}{2}$	000
$P\frac{2}{b}\frac{2}{a}\frac{2}{n}$	50	$0\frac{1}{2}0$	$\frac{1}{2}00$	$\frac{1}{2}\frac{1}{2}0$
$P\frac{2_1}{c}\frac{2}{c}\frac{2}{a}$	54	$00\frac{1}{2}$	$00\frac{1}{2}$	$\frac{1}{2}00$
$P\frac{2_1}{b}\frac{2_1}{c}\frac{2_1}{a}$	61	$0\frac{1}{2}0$	$00\frac{1}{2}$	$\frac{1}{2}00$
$P\frac{2_1}{c}\frac{2}{n}\frac{2}{m}$	53	$00\frac{1}{2}$	$\frac{1}{2}0\frac{1}{2}$	000
$P\frac{2_1}{b}\frac{2_1}{n}\frac{2_1}{m}$	62	$0\frac{1}{2}0$	$\frac{1}{2}0\frac{1}{2}$	000

to hold when we add a third independent generator m_c. In addition, as noted above, we can use a gauge in which

$$\Phi_{m_c}(\mathbf{b}^{(2)})\equiv 0 \ . \tag{4.16}$$

The condition (4.5) coming from the generating relation $m_a m_c = m_c m_a$ then gives

$$\Phi_{m_c}(b^{(3)})\equiv\Phi_{m_a}(\mathbf{b}^{(1)}) \ . \tag{4.17}$$

The corresponding condition coming from $m_b m_c = m_c m_b$ then holds automatically, and the final condition (4.5) coming from $m_c^2 = e$ gives

$$\Phi_{m_c}(\mathbf{b}^{(1)})\equiv 0 \ . \tag{4.18}$$

Consequently there continue to be just two space groups with phase functions given by

I^* (F) lattice, mmm:

$$\begin{matrix}\Phi_{m_a}(\mathbf{b}^{(i)}) & & 000 & & \frac{1}{2}00\\ \Phi_{m_b}(\mathbf{b}^{(i)}) & \equiv & 000 & \text{or} & 0\frac{1}{2}0 \ .\\ \Phi_{m_c}(\mathbf{b}^{(i)}) & & 000 & & 00\frac{1}{2}\end{matrix} \tag{4.19}$$

2. F^* (I) lattice

Everything follows from an examination of Table XIII:

Point group 222 (F^* (I) lattice). We pick a gauge in which[31]

$$\Phi_{r_a}(\mathbf{b}^{(3)})\equiv\Phi_{r_b}(\mathbf{b}^{(1)})\equiv\Phi_{r_c}(\mathbf{b}^{(2)})\equiv 0 \ . \tag{4.20}$$

(Since $r_c = r_a r_b$, the third of these gives an additional constraint on Φ_{r_a} and Φ_{r_b}, which we return to below.)

In the gauge (4.20), the conditions (4.5) associated with the generating relations $r_a^2\equiv e$ and $r_b^2 = e$ reduce to

$$\Phi_{r_a}(\mathbf{b}^{(1)})\equiv\Phi_{r_a}(\mathbf{b}^{(2)}) \ , \Phi_{r_b}(\mathbf{b}^{(2)}\equiv\Phi_{r_b}(\mathbf{b}^{(3)}) \ . \tag{4.21}$$

In view of Eqs. (4.20) and (4.21), the conditions (4.5) associated with $r_a r_b = r_b r_a$ give additionally

$$\Phi_{r_a}(\mathbf{b}^{(1)})\equiv 0,\tfrac{1}{2} \ . \tag{4.22}$$

The third gauge condition expands to

$$\begin{aligned}0\equiv\Phi_{r_c}(\mathbf{b}^{(2)})&\equiv\Phi_{r_a}(r_b\mathbf{b}^{(2)})+\Phi_{r_b}(\mathbf{b}^{(2)})\\ &\equiv-\Phi_{r_a}(\mathbf{b}^{(2)})+\Phi_{r_b}(\mathbf{b}^{(2)}) \ ,\end{aligned} \tag{4.23}$$

where we have noted (from Table XIII) that $r_b\mathbf{b}^{(2)} = -\mathbf{b}^{(2)}$.

We are thus left with a single choice of nonzero phase functions:

F^* (I) lattice, 222:

$$\begin{matrix}\Phi_{r_a}(\mathbf{b}^{(i)}) & & 000 & & \frac{1}{2}\frac{1}{2}0\\ \Phi_{r_b}(\mathbf{b}^{(i)}) & \equiv & & \text{or} & \\ & & 000 & & 0\frac{1}{2}\frac{1}{2}\end{matrix} \ . \tag{4.24}$$

As a direct check that the second possibility is not gauge equivalent to the first, note from Table XIII that the nonzero combination $\Phi_{r_a}(\mathbf{b}^{(2)})-\Phi_{r_b}(\mathbf{b}^{(1)})$ is gauge invariant. (As we shall note in Sec. VI, this is the only other[32] example of a nonsymmorphic crystallographic space group without extinctions.)

Point group $mm2$ (F^* (I) lattice). The generating relations $m_a^2 = e$ and $m_b^2 = e$ give

$$\Phi_{m_a}(\mathbf{b}^{(1)})\equiv 0,\tfrac{1}{2}, \ \ \Phi_{m_b}(\mathbf{b}^{(2)})\equiv 0,\tfrac{1}{2} \ , \tag{4.25}$$

and

$$\begin{aligned}&\Phi_{m_a}(\mathbf{b}^{(2)}-\mathbf{b}^{(3)})\equiv\Phi_{m_a}(\mathbf{b}^{(1)}) \ ,\\ &\Phi_{m_b}(\mathbf{b}^{(3)}-\mathbf{b}^{(1)})\equiv\Phi_{m_b}(\mathbf{b}^{(2)}) \ .\end{aligned} \tag{4.26}$$

[Since $-\frac{1}{2}\equiv\frac{1}{2}$, a third pair of conditions—the pair (4.26) with the signs of $\Phi_{m_a}(\mathbf{b}^{(1)})$ and $\Phi_{m_b}(\mathbf{b}^{(2)})$ reversed—gives nothing more.] The remaining generating relation, $m_a m_b = m_b m_a$, adds nothing new to these conditions. If we now pick a gauge in which

$$\Phi_{m_a}(\mathbf{b}^{(3)})\equiv\Phi_{m_b}(\mathbf{b}^{(3)})\equiv 0 \ , \tag{4.27}$$

then we end up with just four gauge-inequivalent families of phase functions. Because, however, the distinction between the a and b axis is conventional, the two choices (4.25) with a single nonzero phase do not specify distinct space groups.[33] There are thus just three space groups, associated with the gauge equivalence classes defined by the phase functions:

F^* (I) lattice, $mm2$:

$$\begin{matrix}\Phi_{m_a}(\mathbf{b}^{(i)}) & & 000 & & \frac{1}{2}\frac{1}{2}0 & & \frac{1}{2}\frac{1}{2}0\\ \Phi_{m_b}(\mathbf{b}^{(i)}) & \equiv & & \text{or} & & \text{or} & \\ & & 000 & & 000 & & \frac{1}{2}\frac{1}{2}0\end{matrix} \ . \tag{4.28}$$

[31]Note that this choice preserves the $\mathbf{a}\to\mathbf{b}\to\mathbf{c}\to\mathbf{a}$ symmetry but introduces a gauge-dependent handedness; the alternative choice $\Phi_{r_a}(\mathbf{b}^{(2)})\equiv\Phi_{r_b}(\mathbf{b}^{(3)})\equiv\Phi_{r_c}(\mathbf{b}^{(1)})\equiv 0$ would introduce the opposite handedness.

[32]We noted in Sec. III.G.6 a single example in the cubic system.

[33]This is a familiar phenomenon in the orthorhombic system. More formally, it is another consequence of the existence of an operation not in the point group that leaves the lattice invariant, as discussed in Sec. II.G. In this case the operation is a 90-degree rotation about $\mathbf{c}$ combined with an independent rescaling of the vectors $\mathbf{a}$ and $\mathbf{b}$ in such a way as to interchange their lengths.

Point group mmm (F (I) lattice).* Everything done above for the pair of generators m_a, m_b leading to Eqs. (4.25) and (4.26) applies equally well to the pairs m_b, m_c and m_c, m_a. If we cyclically permute a,b,c and with them 1,2,3 then we generate from (4.25) and (4.26) just two additional conditions:

$$\Phi_{m_c}(\mathbf{b}^{(3)})=0,\tfrac{1}{2} \tag{4.29}$$

and

$$\Phi_{m_c}(\mathbf{b}^{(1)}-\mathbf{b}^{(2)})\equiv\Phi_{m_c}(\mathbf{b}^{(3)})\ . \tag{4.30}$$

To maintain the symmetry it is now convenient to express the result in a gauge in which $\Phi_{m_a}(\mathbf{b}^{(3)}) \equiv\Phi_{m_b}(\mathbf{b}^{(1)})\equiv\Phi_{m_c}(\mathbf{b}^{(2)})\equiv 0$ (the existence of which is ensured by the upper part of Table XIII). The distinct classes of gauge-equivalent phase functions then result in just four space groups:

F^* (I) lattice, mmm:

$$\begin{array}{lccccccccc} \Phi_{m_a}(\mathbf{b}^{(i)}) & & 000 & & 000 & & \tfrac{1}{2}\tfrac{1}{2}0 & & \tfrac{1}{2}\tfrac{1}{2}0 \\ \Phi_{m_b}(\mathbf{b}^{(i)}) & \equiv & 000 & \text{or} & 000 & \text{or} & 0\tfrac{1}{2}\tfrac{1}{2} & \text{or} & 0\tfrac{1}{2}\tfrac{1}{2}\ . \\ \Phi_{m_c}(\mathbf{b}^{(i)}) & & 000 & & \tfrac{1}{2}0\tfrac{1}{2} & & 000 & & \tfrac{1}{2}0\tfrac{1}{2} \end{array} \tag{4.31}$$

3. *C* lattice

Everything follows from an examination of Table XIV:

Point group 222 (C lattice). We pick a gauge in which

$$\Phi_{r_a}(\mathbf{b}^{(3)})\equiv\Phi_{r_a}(\mathbf{b}^{(2)})\equiv\Phi_{r_b}(\mathbf{b}^{(1)})\equiv 0\ . \tag{4.32}$$

The conditions (4.5) associated with $r_a^2=e$ and $r_b^2=e$ then give

$$\Phi_{r_a}(\mathbf{b}^{(1)})\equiv\Phi_{r_b}(\mathbf{b}^{(2)})\equiv 0\ , \tag{4.33}$$

and $r_a r_b = r_b r_a$ gives

$$\Phi_{r_b}(\mathbf{b}^{(3)})\equiv 0,\tfrac{1}{2}\ , \tag{4.34}$$

so there are just two space groups with phase functions given by

C lattice, 222:

$$\begin{array}{lccccc} \Phi_{r_a}(\mathbf{b}^{(i)}) & & 000 & & 000 \\ \Phi_{r_b}(\mathbf{b}^{(i)}) & \equiv & 000 & \text{or} & 00\tfrac{1}{2}\ . \end{array} \tag{4.35}$$

Point groups mm2 or m2m (C lattice). In this single case there are two ways of orienting the point group with respect to the lattice: the unique twofold axis can lie either along or perpendicular to the distinguished lattice-generating vector $\mathbf{b}^{(3)}\equiv\mathbf{c}$. In the latter case, we take the twofold axis to lie along $\mathbf{b}$. We distinguish the two cases nomenclaturally by referring to the point group as $mm2$ or $m2m$.

In either case (or in the case of mmm) the mirror m_a is a generator, we can pick a gauge in which

$$\Phi_{m_a}(\mathbf{b}^{(2)})\equiv 0\ , \tag{4.36}$$

and the generating relation $m_a^2=e$ then gives

$$\Phi_{m_a}(\mathbf{b}^{(1)})\equiv 0\ ,\quad \Phi_{m_a}(\mathbf{b}^{(3)})\equiv 0,\tfrac{1}{2}\ . \tag{4.37}$$

In the case of $mm2$ (or in the case of mmm) we can do the same for the mirror m_b:

$$\Phi_{m_b}(\mathbf{b}^{(2)})\equiv 0\ ,\quad \Phi_{m_b}(\mathbf{b}^{(1)})\equiv 0\ ,\quad \Phi_{m_b}(\mathbf{b}^{(3)})\equiv 0,\tfrac{1}{2}\ . \tag{4.38}$$

The relation $m_a m_b = m_b m_a$ imposes no further constraints, so we have four gauge-inequivalent families of phase functions. In view of the interchangeability of the a and b axes these give three distinct space groups:

C lattice, $mm2$:

$$\begin{array}{lccccc} \Phi_{m_a}(\mathbf{b}^{(i)}) & & 000 & & 000 & & 00\tfrac{1}{2} \\ \Phi_{m_b}(\mathbf{b}^{(i)}) & \equiv & 000 & \text{or} & 00\tfrac{1}{2} & \text{or} & 00\tfrac{1}{2}\ . \end{array} \tag{4.39}$$

In the case of $m2m$ (or in the case of mmm) we can choose a gauge in which

$$\Phi_{m_c}(\mathbf{b}^{(3)})\equiv 0\ , \tag{4.40}$$

and the generating relation $m_c^2=e$ gives

$$\Phi_{m_c}(\mathbf{b}^{(1)})\equiv 0,\tfrac{1}{2},\quad \Phi_{m_c}(\mathbf{b}^{(2)})\equiv 0,\tfrac{1}{2}\ . \tag{4.41}$$

The relation $m_a m_c = m_c m_a$ imposes the additional constraint

$$\Phi_{m_c}(\mathbf{b}^{(1)})\equiv\Phi_{m_c}(\mathbf{b}^{(2)})\ , \tag{4.42}$$

so we have four space groups:

C lattice, $m2m$:

$$\begin{array}{lccccccccc} \Phi_{m_a}(\mathbf{b}^{(i)}) & & 000 & & 000 & & 00\tfrac{1}{2} & & 00\tfrac{1}{2} \\ \Phi_{m_c}(\mathbf{b}^{(i)}) & \equiv & 000 & \text{or} & \tfrac{1}{2}\tfrac{1}{2}0 & \text{or} & 000 & \text{or} & \tfrac{1}{2}\tfrac{1}{2}0 \end{array} \tag{4.43}$$

Point group mmm (C lattice). Since all three mirrors are generators, all of Eqs. (4.36)–(4.42) must hold, and the only remaining source of constraints is the generating relation $m_b m_c = m_c m_b$, which gives nothing new. The distinct space groups therefore arise from the three independent choices $0,\frac{1}{2}$ for $\Phi_{m_a}(\mathbf{b}^{(3)})$, $\Phi_{m_b}(\mathbf{b}^{(3)})$, and $\Phi_{m_c}(\mathbf{b}^{(1)})=\Phi_{m_c}(\mathbf{b}^{(2)})$. In view of the interchangeability of the a and b axes, the eight choices yield six distinct space groups:

C lattice, *mmm*:

$$\begin{array}{lcccccccccccc} \Phi_{m_a}(\mathbf{b}^{(i)}) & & 000 & & 000 & & 00\tfrac{1}{2} & & 000 & & 000 & & 00\tfrac{1}{2} \\ \Phi_{m_b}(\mathbf{b}^{(i)}) & \equiv & 000 & \text{or} & 00\tfrac{1}{2} & \text{or} & 00\tfrac{1}{2} & \text{or} & 000 & \text{or} & 00\tfrac{1}{2} & \text{or} & 00\tfrac{1}{2} \\ \Phi_{m_c}(\mathbf{b}^{(i)}) & & 000 & & 000 & & 000 & & \tfrac{1}{2}\tfrac{1}{2}0 & & \tfrac{1}{2}\tfrac{1}{2}0 & & \tfrac{1}{2}\tfrac{1}{2}0 \end{array} . \tag{4.44}$$

4. *P* lattice

Everything follows from an examination of Table XV:

Point group 222 (P lattice). As in the case of 222 on the *I* lattice, we preserve the $\mathbf{a}\to\mathbf{b}\to\mathbf{c}\to\mathbf{a}$ symmetry (at the price of introducing a gauge-dependent handedness) by picking the gauge

$$\Phi_{r_a}(\mathbf{b}^{(3)})\equiv\Phi_{r_b}(\mathbf{b}^{(1)})\equiv\Phi_{r_c}(\mathbf{b}^{(2)})\equiv 0 . \tag{4.45}$$

Since

$$\begin{aligned}\Phi_{r_c}(\mathbf{b}^{(2)})&\equiv\Phi_{r_b}(r_a\mathbf{b}^{(2)})+\Phi_{r_a}(\mathbf{b}^{(2)})\\ &\equiv-\Phi_{r_b}(\mathbf{b}^{(2)})+\Phi_{r_a}(\mathbf{b}^{(2)}) ,\end{aligned} \tag{4.46}$$

the third of these constrains the phase functions associated with the two independent generators by

$$\Phi_{r_b}(\mathbf{b}^{(2)})\equiv\Phi_{r_a}(\mathbf{b}^{(2)}) . \tag{4.47}$$

The generating relations $r_a^2=e$ and $r_b^2=e$ give

$$\Phi_{r_a}(\mathbf{b}^{(1)})\equiv 0,\tfrac{1}{2},\quad \Phi_{r_b}(\mathbf{b}^{(2)})\equiv 0,\tfrac{1}{2} , \tag{4.48}$$

and in view of the choice of gauge (4.45) the relation $r_a r_b = r_b r_a$ gives

$$\Phi_{r_b}(\mathbf{b}^{(3)}\equiv 0,\tfrac{1}{2} . \tag{4.49}$$

There are therefore eight distinct gauge equivalence classes associated with the three choices $0,\frac{1}{2}$ in Eqs. (4.48) and (4.49). The $\mathbf{a}\to\mathbf{b}\to\mathbf{c}\to\mathbf{a}$ symmetry reduces the number of distinct space groups to four, which is only evident if one displays the redundant phase function Φ_{r_c} along with those for the group generators r_a and r_b:[34,35]

[34]The phase Φ_{r_c} is easily evaluated from the group compatibility condition (2.11), which gives $\Phi_{r_c}(\mathbf{b}^{(i)})\equiv\Phi_{r_a}(r_b\mathbf{b}^{(i)})+\Phi_{r_b}(\mathbf{b}^{(i)})$. But for the *P* lattice $r_b\mathbf{b}^{(i)}=\pm\mathbf{b}^{(i)}$. Since we use a gauge in which the only values of Φ_{r_a} and Φ_{r_b} are 0 or $\frac{1}{2}$, it follows that $\Phi_{r_c}(\mathbf{b}^{(i)})\equiv\Phi_{r_a}(\mathbf{b}^{(i)})+\Phi_{r_b}(\mathbf{b}^{(i)})$.

[35]The other four gauge equivalence classes are given by the $\mathbf{a}\to\mathbf{b}\to\mathbf{c}\to\mathbf{a}$ permutations of the two that lack $\mathbf{a}\to\mathbf{b}\to\mathbf{c}\to\mathbf{a}$ symmetry.

P lattice, 222:

$$\begin{array}{lcccccccc} \Phi_{r_a}(\mathbf{b}^{(i)}) & & 000 & & \tfrac{1}{2}00 & & \tfrac{1}{2}\tfrac{1}{2}0 & & \tfrac{1}{2}\tfrac{1}{2}0 \\ \Phi_{r_b}(\mathbf{b}^{(i)}) & \equiv & 000 & \text{or} & 000 & \text{or} & 0\tfrac{1}{2}0 & \text{or} & 0\tfrac{1}{2}\tfrac{1}{2} \\ \Phi_{r_c}(\mathbf{b}^{(i)}) & & 000 & & \tfrac{1}{2}00 & & \tfrac{1}{2}00 & & \tfrac{1}{2}0\tfrac{1}{2} \end{array} . \tag{4.50}$$

Point group mm2 (P lattice). We choose a gauge in which

$$\Phi_{m_a}(\mathbf{b}^{(1)})\equiv\Phi_{m_b}(b^{(2)})\equiv 0 . \tag{4.51}$$

The generating relations $m_a^2=e$ and $m_b^2=e$ lead to four independent choices of $0,\frac{1}{2}$:

$$\begin{aligned}&\Phi_{m_a}(\mathbf{b}^{(2)})\equiv 0,\tfrac{1}{2} ,\quad \Phi_{m_a}(\mathbf{b}^{(3)})\equiv 0,\tfrac{1}{2} ,\\ &\Phi_{m_b}(\mathbf{b}^{(1)})\equiv 0,\tfrac{1}{2} ,\quad \Phi_{m_b}(\mathbf{b}^{(3)})\equiv 0,\tfrac{1}{2} ,\end{aligned} \tag{4.52}$$

in view of which the additional generating relation $m_a m_b = m_b m_a$ gives no additional constraints. There are thus 16 distinct gauge equivalence classes, four of which are symmetric under interchange of **a** and **b**, leading to 10 distinct space groups when one takes $\mathbf{a}\leftrightarrow\mathbf{b}$ symmetry into account.

In enumerating the cases it is convenient to define for every pair of phase functions Φ_{m_a} and Φ_{m_b} a "complementary" pair in which each of the four choices (4.52) for $0,\frac{1}{2}$ is replaced by its opposite. We can then enumerate the space groups by considering first the case where all the choices are 0 (and the complementary pair with all choices $\frac{1}{2}$), then the two cases in which only one choice is $\frac{1}{2}$ (and the complementary pairs with three choices of $\frac{1}{2}$), and finally the case in which two of the choices are $\frac{1}{2}$ (two of which form a complementary pair and two of which—listed last—give the same space groups as their complements). In the enumeration that follows complementary pairs are separated by commas:

P lattice, *mm*2:

$$\begin{matrix}\Phi_{m_a}(\mathbf{b}^{(i)})\\ \Phi_{m_b}(\mathbf{b}^{(i)})\end{matrix} \equiv \begin{matrix}000\\000\end{matrix}, \begin{matrix}0\tfrac{1}{2}\tfrac{1}{2}\\ \tfrac{1}{2}0\tfrac{1}{2}\end{matrix} \text{ or } \begin{matrix}000\\ \tfrac{1}{2}00\end{matrix}, \begin{matrix}0\tfrac{1}{2}\tfrac{1}{2}\\ 00\tfrac{1}{2}\end{matrix} \text{ or } \begin{matrix}000\\ 00\tfrac{1}{2}\end{matrix}, \begin{matrix}0\tfrac{1}{2}\tfrac{1}{2}\\ \tfrac{1}{2}00\end{matrix} \text{ or } \begin{matrix}00\tfrac{1}{2}\\ 00\tfrac{1}{2}\end{matrix}, \begin{matrix}0\tfrac{1}{2}0\\ \tfrac{1}{2}00\end{matrix} \text{ or } \begin{matrix}000\\ \tfrac{1}{2}0\tfrac{1}{2}\end{matrix} \text{ or } \begin{matrix}00\tfrac{1}{2}\\ \tfrac{1}{2}00\end{matrix}. \tag{4.53}$$

Note that the first, second, seventh, and eighth sets of phases are symmetric under interchange of **a** and **b**; the results of interchanging **a** and **b** on the remaining six entries give back the full set of 16 gauge equivalence classes.

Point group mmm (P lattice). We choose a gauge in which

$$\Phi_{m_a}(\mathbf{b}^{(1)})\equiv\Phi_{m_b}(\mathbf{b}^{(2)})\equiv\Phi_{m_c}(\mathbf{b}^{(3)})\equiv 0\ . \tag{4.54}$$

The generating relations $m_a^2=e$, $m_b^2=e$, and $mc^2=e$ lead to six independent choices of $0,\frac{1}{2}$:

$$\begin{aligned}&\Phi_{m_a}(\mathbf{b}^{(2)})\equiv 0,\tfrac{1}{2}\ ,\quad \Phi_{m_a}(\mathbf{b}^{(3)})\equiv 0,\tfrac{1}{2}\ ,\\ &\Phi_{m_b}(\mathbf{b}^{(3)})\equiv 0,\tfrac{1}{2},\quad \Phi_{m_b}(\mathbf{b}^{(1)})\equiv 0,\tfrac{1}{2}\ ,\\ &\Phi_{m_c}(\mathbf{b}^{(1)})\equiv 0,\tfrac{1}{2}\ ,\quad \Phi_{m_c}(\mathbf{b}^{(2)})\equiv 0,\tfrac{1}{2}\ ,\end{aligned} \tag{4.55}$$

in view of which the additional generating relations $m_bm_c=m_cm_b$, $m_cm_a=m_am_c$, $m_am_b=m_bm_a$ give no additional constraints. There are thus 64 distinct gauge equivalence classes, which reduce to 16 distinct space groups when the $\mathbf{a}\to\mathbf{b}\to c\to\mathbf{a}$ symmetry is taken into account.

We enumerate the 16 sets of phase functions below, grouping each of the first 12 with a complementary set in which each of the six choices (4.55) for $0,\frac{1}{2}$ is replaced by its opposite. (The last four on the list give the same space groups as their complements.) The enumeration is made systematic by considering first the case where all the choices are 0 (and the complementary set with all choices $\frac{1}{2}$), then the case in which only one choice is $\frac{1}{2}$ (and the complementary sets with five choices of $\frac{1}{2}$), then the four cases with two choices of $\frac{1}{2}$ (and the complementary sets with four choices of $\frac{1}{2}$), and finally the four cases in which three of the choices are $\frac{1}{2}$ (each of which gives the same space group as its complement). In the enumeration that follows complementary pairs separated by commas:

P lattice, *mmm*:

$$\begin{matrix}\Phi_{m_a}(\mathbf{b}^{(i)})\\ \Phi_{m_b}(\mathbf{b}^{(i)})\\ \Phi_{m_c}(\mathbf{b}^{(i)})\end{matrix} \equiv \begin{matrix}000\\000\\000\end{matrix}, \begin{matrix}0\tfrac{1}{2}\tfrac{1}{2}\\ \tfrac{1}{2}0\tfrac{1}{2}\\ \tfrac{1}{2}\tfrac{1}{2}0\end{matrix} \text{ or } \begin{matrix}000\\ \tfrac{1}{2}00\\ 0\tfrac{1}{2}0\end{matrix}, \begin{matrix}0\tfrac{1}{2}\tfrac{1}{2}\\ \tfrac{1}{2}0\tfrac{1}{2}\\ \tfrac{1}{2}\tfrac{1}{2}0\end{matrix} \text{ or } \begin{matrix}000\\ 000\\ \tfrac{1}{2}\tfrac{1}{2}0\end{matrix}, \begin{matrix}0\tfrac{1}{2}\tfrac{1}{2}\\ \tfrac{1}{2}0\tfrac{1}{2}\\ 000\end{matrix} \text{ or } \begin{matrix}\tfrac{1}{2}00\\ 000\\ \tfrac{1}{2}\tfrac{1}{2}0\end{matrix}, \begin{matrix}0\tfrac{1}{2}0\\ 00\tfrac{1}{2}\\ \tfrac{1}{2}\tfrac{1}{2}0\end{matrix}$$
$$\text{or } \begin{matrix}0\tfrac{1}{2}0\\ 00\tfrac{1}{2}\\ 000\end{matrix}, \begin{matrix}00\tfrac{1}{2}\\ \tfrac{1}{2}00\\ \tfrac{1}{2}\tfrac{1}{2}0\end{matrix} \text{ or } \begin{matrix}00\tfrac{1}{2}\\ 0\tfrac{1}{2}0\\ 000\end{matrix}, \begin{matrix}0\tfrac{1}{2}0\\ \tfrac{1}{2}00\\ \tfrac{1}{2}\tfrac{1}{2}0\end{matrix} \text{ or } \begin{matrix}00\tfrac{1}{2}\\ 00\tfrac{1}{2}\\ \tfrac{1}{2}00\end{matrix} \text{ or } \begin{matrix}0\tfrac{1}{2}0\\ 00\tfrac{1}{2}\\ \tfrac{1}{2}00\end{matrix} \text{ or } \begin{matrix}00\tfrac{1}{2}\\ \tfrac{1}{2}0\tfrac{1}{2}\\ 000\end{matrix} \text{ or } \begin{matrix}\tfrac{1}{2}0\tfrac{1}{2}\\ 0\tfrac{1}{2}0\\ 000\end{matrix}. \tag{4.56}$$

The results are collected together in Tables XVI–XIX, which list the orthorhombic space groups in terms of gauge equivalence classes of phase functions.

V. THE MONOCLINIC AND TRICLINIC SPACE GROUPS

A. Generators for the monoclinic point groups

The three monoclinic point groups are characterized either by a unique twofold axis (which we take to be along *c*), a unique mirror plane (which we take to be orthogonal to *c*), or both. The generators are therefore r_c, m_c, or both. The point-group nomenclature and generating relations are summarized in Table XX.

B. The monoclinic lattices

There are two monoclinic lattices, which we specify in terms of their primitive generating vectors. These can be expressed in terms of two vectors **a** and **b** bearing no special relation to one another and a third vector **c** normal to the plane of **a** and **b**. For the simple monoclinic lattice we have

TABLE XX. Generators for the Monoclinic Point Groups. The subscript c refers to the unique direction $\mathbf{c}$ of the axis of the twofold rotation r_c, or the normal to the mirror $m_c = ir_c$.

Schön-flies	Interna-tional	Gener-ators	Point-Group Generating Relations
C_2	2	r_c	$r_c^2 = e$
C_{1h}	m $(\bar{2})$	m_c	$m_c^2 = e$
C_{2h}	$\frac{2}{m}$	r_c, m_c	$m_c^2 = e$, $r_c^2 = e$, $m_c r_c = r_c m_c$

P lattice:

$$\mathbf{b}^{(1)}=\mathbf{a}\ ,\quad \mathbf{b}^{(2)}=\mathbf{b}\ ,\quad \mathbf{b}^{(3)}=\mathbf{c}\ . \tag{5.1}$$

There is also a single centered lattice given by

C lattice:

$$\mathbf{b}^{(1)}=\mathbf{a}\ ,\quad \mathbf{b}^{(2)}=\mathbf{b}\ ,\quad \mathbf{b}^{(3)}=\mathbf{c}+\tfrac{1}{2}(\mathbf{a}+\mathbf{b})\ . \tag{5.2}$$

C. The monoclinic space groups

As earlier, we determine the space groups by applying the group compatibility condition (2.11) to the generating relations, always selecting a gauge to make the analysis simple.

1. P lattice

Point group 2 (P lattice). Since r_c takes $\mathbf{a}$ and $\mathbf{b}$ into their negatives, we have

$$\Delta\Phi_{r_c}(\mathbf{b}^{(i)})\equiv\chi([r_c-1]\mathbf{b}^{(i)})\equiv-2\chi(\mathbf{b}^{(i)})\ ,\quad i=1,2\ . \tag{5.3}$$

We can therefore pick a gauge in which

$$\Phi_{r_c}(\mathbf{b}^{(1)})\equiv\Phi_{r_c}(\mathbf{b}^{(2)})\equiv 0\ . \tag{5.4}$$

On the other hand the generating relation $r_c^2=e$ gives, with the group compatibility condition (2.11),

$$\Phi_{r_c}(\mathbf{b}^{(3)})\equiv 0,\tfrac{1}{2}\ ,$$

so there are two space groups, as noted in Table XXI.

Point group m (P lattice). Since m_c takes $\mathbf{c}$ into $-\mathbf{c}$,

$$\Delta\Phi_{m_c}(\mathbf{b}^{(3)})\equiv\chi([m_c-1]\mathbf{b}^{(3)})\equiv-2\chi(\mathbf{b}^{(3)}\ . \tag{5.5}$$

We can therefore pick a gauge in which

$$\Phi_{m_c}(\mathbf{b}^{(3)})\equiv 0\ . \tag{5.6}$$

Since m_c leaves $\mathbf{a}$ and $\mathbf{b}$ invariant, the group compatibility condition, applied to the generating relation $m_c^2=e$, gives

$$\Phi_{m_c}(\mathbf{b}^{(1)})\equiv 0,\tfrac{1}{2}\ ,\quad \Phi_{m_c}(\mathbf{b}^{(2)})=0,\tfrac{1}{2}\ . \tag{5.7}$$

Because there is no relation between $\mathbf{a}$ and $\mathbf{b}$, the choices with one or both of the phases equal to $\frac{1}{2}$ all give a single space group. If only one of the two is $\frac{1}{2}$, this is an immediate consequence of the interchangeability of $\mathbf{a}$ and $\mathbf{b}$. If both are $\frac{1}{2}$, it follows because $\mathbf{a},\mathbf{a}+\mathbf{b}$ is as valid a choice of primitive generating vectors as $\mathbf{a}$, $\mathbf{b}$, but with this new choice, $\Phi_{m_c}(\mathbf{a}+\mathbf{b})\equiv 0$. We represent the single nonsymmorphic space group by the symmetric choice in which both phases are taken to be $\frac{1}{2}$ and record the two space groups in Table XXI.

Point group $\frac{2}{m}$ (P lattice). Both r_c and m_c are generators, but since the choice of gauge leading to Eq. (5.4) fixed only $\chi(\mathbf{b}^{(1)})$ and $\chi(\mathbf{b}^{(2)})$, while the choice of gauge leading to Eq. (5.6) fixed only $\chi(\mathbf{b}^{(3)})$, we can work in a gauge in which both sets of conditions hold. We there-

TABLE XXI. The space groups on the monoclinic P lattice.

2 (C_2)		Φ_{r_c}	
$P2$	3	000	
$P2_1$	4	$00\frac{1}{2}$	
m (C_{1h})			Φ_{m_c}
Pm	6		000
Pc	7		$\frac{1}{2}\frac{1}{2}0$
$\frac{2}{m}$ (C_{2h})		Φ_{r_c}	Φ_{m_c}
$P\frac{2}{m}$	10	000	000
$P\frac{2_1}{m}$	11	$00\frac{1}{2}$	000
$P\frac{2}{c}$	13	000	$\frac{1}{2}\frac{1}{2}0$
$P\frac{2_1}{c}$	14	$00\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}0$

fore begin with the possible nonzero phases being $\Phi_{r_c}(\mathbf{b}^{(3)})\equiv 0,\frac{1}{2}$ and, independently, $\Phi_{m_c}(\mathbf{b}^{(1)})\equiv\Phi_{m_c}(\mathbf{b}^{(2)})\equiv 0,\frac{1}{2}$. We have one additional constraint, coming from the application of the group compatibility condition (2.11) to $r_c m_c = m_c r_c$. This requires

$$\Phi_{m_c}([r_c-1]\mathbf{b}^{(i)})\equiv\Phi_{r_c}([m_c-1]\mathbf{b}^{(i)}) . \tag{5.8}$$

But since each $\mathbf{b}^{(i)}$ is either invariant or changes sign under r_c or m_c, and since all the possible phases are 0 or $\frac{1}{2}$, Eq. (5.8) always holds, and there is no further constraint. The four space groups are recorded in Table XXI.

2. *C* lattice

Point group 2 (C lattice). Since r_c preserves **c** and takes **a** and **b** into their negatives, we have

$$\Delta\Phi_{r_c}(\mathbf{b}^{(i)})\equiv\chi([r_c-1]\mathbf{b}^{(i)})\equiv -2\chi(\mathbf{b}^{(i)}),\quad i=1,2 , \tag{5.9}$$

and

$$\begin{aligned}\Delta\Phi_{r_c}(\mathbf{b}^{(3)})&=\chi([r_c-1][c+\tfrac{1}{2}(\mathbf{a}+\mathbf{b})])\\ &\equiv -\chi(\mathbf{b}^{(1)})-\chi(\mathbf{b}^{(2)}) .\end{aligned} \tag{5.10}$$

We can therefore pick a gauge in which $\Phi_{r_c}(\mathbf{b}^{(1)})$ and $\Phi_{r_c}(\mathbf{b}^{(2)})$ vanish and be left with enough gauge freedom to shift $\Phi_{r_c}(\mathbf{b}^{(3)})$ by $\frac{1}{2}$. But the generating relation $r_c^2=e$ gives, with the group compatibility condition (2.11).

$$0\equiv\Phi_{r_c}([r_c+1]\mathbf{b}^{(3)})\equiv\Phi_{r_c}(2c) , \tag{5.11}$$

and therefore

$$2\Phi_{r_c}(\mathbf{b}^{(3)})\equiv\Phi_{r_c}(\mathbf{b}^{(1)})+\Phi_{r_c}(\mathbf{b}^{(2)})\equiv 0 , \tag{5.12}$$

which restricts $\Phi_{r_c}(\mathbf{b}^{(3)})$ to be 0 or $\frac{1}{2}$. Consequently we can pick a gauge in which all the phases are zero. This is recorded in Table XXII.

Point group m (C lattice). Since m_c leaves **a** and **b** invariant, we have

$$\Delta\Phi_{m_c}(\mathbf{b}^{(3)})\equiv\chi([m_c-1]\mathbf{b}^{(3)})\equiv -\chi(2\mathbf{c}) , \tag{5.13}$$

so we can take $\Phi_{m_c}(\mathbf{b}^{(3)})\equiv 0$. The generating relation $m_c^2=e$ gives

$$0\equiv\Phi_{m_c}([m_c+1]\mathbf{b}^{(i)}) , \tag{5.14}$$

which applied to $\mathbf{b}^{(1)}$, $\mathbf{b}^{(2)}$, and $\mathbf{b}^{(3)}$ requires that

$$\begin{aligned}&\Phi_{m_c}(\mathbf{b}^{(1)})\equiv 0,\tfrac{1}{2} ,\quad \Phi_{m_c}(\mathbf{b}^{(2)})\equiv 0,\tfrac{1}{2} ,\\ &\Phi_{m_c}(\mathbf{b}^{(1)}+\mathbf{b}^{(2)})\equiv 0 ,\end{aligned} \tag{5.15}$$

so we can have

$$\Phi_{m_c}(\mathbf{b}^{(1)})\equiv\Phi_{m_c}(\mathbf{b}^{(2)})\equiv 0,\tfrac{1}{2} . \tag{5.16}$$

TABLE XXII. The space groups on the monoclinic *C* lattice.

2 (C_2)	Φ_{r_c}	
$C2$ 5	000	
m (C_1h)		Φ_{m_c}
Cm 8		000
Cc 9		$\frac{1}{2}\frac{1}{2}0$
$\frac{2}{m}$ (C_{2h})	Φ_{r_c}	Φ_{m_c}
$C\frac{2}{m}$ 12	000	000
$C\frac{2}{c}$ 15	000	$\frac{1}{2}\frac{1}{2}0$

There are thus two space groups, noted in Table XXII.

Point group $\frac{2}{m}$ *(C lattice).* If we add to m_c the generator r_c, we can pick a gauge in which all of the preceding gauge conditions hold. Since all phases are zero or $\frac{1}{2}$, the one additional condition coming from $r_c m_c = m_c r_c$ gives nothing new. Consequently we get just the two space groups listed in Table XXII.

D. The triclinic space groups

The triclinic lattice has no symmetries beyond the inversion *i*, which any lattice must possess. If $\mathbf{b}^{(i)}$ are primitive generating vectors then we have

$$\Delta\Phi_i(\mathbf{b}^{(i)})\equiv\chi([i-1]\mathbf{b}^{(i)})\equiv -2\chi(\mathbf{b}^{(i)}) , \tag{5.17}$$

so we can always choose a gauge in which $\Phi_i(\mathbf{b}^{(i)})\equiv 0$. There are thus only two triclinic space groups, depending on whether the point group does or does not contain *i*, both symmorphic, as duly noted in Table XXIII.

VI. EXTINCTIONS

As noted in Sec. II.D, the phase functions for a given space group immediately determine the extinctions. These have a somewhat different character when viewed from the perspective of Fourier space. Conventional crystallography starts with a direct lattice, the template for the periodicity of a real-space structure. Dual to this

TABLE XXIII. The space groups on the triclinic lattice.

	Φ_i
$P1$ 1	
$P\bar{1}$ 2	000

is a lattice of wave vectors, and associated with each wave vector is a Bragg peak. Certain peaks may be missing from the diffraction pattern—extinct—as a consequence of the space-group symmetry.

In Fourier-space crystallography, on the other hand, one begins with the diffraction pattern itself. Peaks are "missing" only when their intensity is beneath the threshold for detection. The lattice is not a template for the diffraction pattern, but an extension of it—the set of all integral linear combinations of the observed vectors. Every lattice vector is a candidate for an additional Bragg peak, but for a given space group certain such integral linear combinations of observed peaks cannot consistently be associated with a density Fourier coefficient and therefore cannot be associated with a Bragg peak. The emphasis thus shifts from extinctions as "missing" Bragg peaks to extinctions as peaks that can never be added to the pattern, no matter how much the resolution is improved.

Extinctions occur at wave vectors $\mathbf{k}$ in the invariant subspace of a point-group operation g for which the phase $\Phi_g(\mathbf{k})$ is nonintegral. The vanishing of $\rho(\mathbf{k})$ follows directly from the definition (2.9) of the phase function. Since it follows from the definition (2.10) of a gauge transformation that the phase functions are gauge invariant on their invariant subspaces, we can find the extinctions in any convenient gauge and thus directly from the phase functions given in the tables.

As in determining the phase functions themselves, the primary analytic effort consists of an elementary geometrical exercise, in this case specifying the form of a general lattice vector in each invariant subspace of the point group in terms of the primitive generating vectors $\mathbf{b}^{(i)}$ of the lattice. In a few cases it is also necessary to use the point-group generating relations and the group compatibility condition to express the phase function for a general element g of G in terms of the phase functions for the point-group generators.

A. Cubic and icosahedral extinctions

Because the magnitudes of the density Fourier coefficients have the symmetry of the point group, it is enough to determine the extinctions for one specimen of each of the invariant subspaces.[36] These invariant subspaces are either rotation axes or mirror planes.

In both the cubic and icosahedral cases, there are never extinctions on the threefold axes because Φ_{r_3} can always be taken to vanish. This has already been noted and exploited when the point group has r_3 as a generator. When the generator is $\bar{r}_3$, then $\Phi_{\bar{r}_3}$ can be taken to vanish (Sec. III.B.1), and the vanishing of Φ_{r_3} then follows from applying the group compatibility condition (2.11) to the identity $r_3=\bar{r}_3^4$.

The group compatibility condition can also be used to express the phase functions associated with the remaining invariant subspaces in terms of the phase function Φ_{g_2} associated with the twofold generator of the point group. In all but two cases (noted below) those other phase functions can be taken to be identical to Φ_{g_2}.

1. Cubic extinctions

The specimens of the remaining invariant subspaces can be taken to be the twofold axis of r_2, the plane of the perpendicular mirror m, the fourfold axis of r_4 (which is also the twofold axis of r_2' in the tetrahedral groups), and the plane of the perpendicular mirror m'. (See Fig. 1.) The general forms of vectors in those four subspaces are given for each of the three cubic lattices at the top of Table XXIV (and again at the top of Table XXV, except that m' is omitted because none of the point groups in Table XXV contain it.)

The entries in Tables XXIV–XXVI are the values in the invariant subspaces of the associated phase functions. With two exceptions, they are constructed by taking the inner product of the phase-function vector Φ_{g_2} (listed explicitly for each space group) with the form of a general vector in the invariant space specified for the appropriate lattice at the top of each column. The first exception is the invariant subspace of m' of the point group O_h, whose twofold generator we have taken to be m. Since $r_4=\bar{r}_3 m$ and $r_2=im=\bar{r}_3^3 m$, it follows from the vanishing of $\Phi_{\bar{r}_3}$ and the group compatibility condition (2.11) that $\Phi_{r_4}\equiv\Phi_m$ and $\Phi_{r_2}\equiv\Phi_m$. Because, however, $m'=ir_4^2$, Eq. (2.11) gives

$$\Phi_{m'}(\mathbf{k})\equiv\Phi_{r_4}([1+r_4]\mathbf{k})\equiv\Phi_m([1+r_4]\mathbf{k})\ . \tag{6.1}$$

The second exception is the invariant subspace of r_2' for the point group T_d, whose twofold generator we have taken to be m. The phase function $\Phi_{r_2'}$ is not given by Φ_m, but because $r_2'=\bar{r}_4^2$ the group compatibility condition (2.11) gives

$$\Phi_{r_2'}(\mathbf{k})\equiv\Phi_{\bar{r}_4}([1+\bar{r}_4]\mathbf{k})\ , \tag{6.2}$$

which vanishes (modulo 1) on the invariant subspace of r_2', since the rotoinversion $\bar{r}_4$ reverses the sign of any vector on its axis.

In all other cubic cases (and all the icosahedral cases considered below) the phase functions associated with the invariant subspaces are identical to those for the twofold generator.

Extinctions for the cubic space groups occur for values of the arbitrary integers u and v that give nonintegral entries in Tables XXIV or XXV. Note the interesting case of space group $I2_13$ (No. 199) in Table XXV, a rare example[37] of a nonsymmorphic space group with no extinctions.

[36] More abstractly, the phases $\Phi_g(\mathbf{k})$ and $\Phi_{hgh}^{-1}(h\mathbf{k})$ necessarily agree when $g\mathbf{k}=\mathbf{k}$ as a consequence of Eqs. (2.13) and (2.16).

[37] The only other is $I2_12_12_1$ (No. 24) in the orthorhombic system, as noted below.

2. Icosahedral extinctions

The extinctions for the icosahedral space groups are given in Table XXVI. The only effort in constructing the table is in specifying the primitive generating vectors for the invariant subspaces of r_5, r_2, and m. The icosahedral case is simpler than the cubic because there are at most three invariant subspaces and because the phase func-

TABLE XXIV. Extinctions for the cubic space groups with point groups O_h and T_h. The four invariant subspaces are listed in the top row. [Since $\Phi_{\bar{r}_3}\equiv 0$ and since $r_3\equiv\bar{r}_3^4$, it follows from the group compatibility condition (2.11) that $\Phi_{r_3}\equiv 0$, so there are no extinctions on threefold axes.] Immediately below are the general forms for vectors in each of the invariant subspaces, for each of the three lattice types. An entry (u,v,w) means a lattice vector of the form $u\mathbf{b}^{(1)}+v\mathbf{b}^{(2)}+w\mathbf{b}^{(3)}$ where the $\mathbf{b}^{(i)}$ are the threefold-symmetric sets of primitive generating vectors given in Eq. (3.17) [P lattice], Eq. (3.18) [F^* (I) lattice], or Eq. (3.19) [I^* (F) lattice] and u, v, and w are arbitrary integers.

The nonsymmorphic space groups with point groups O_h and T_h are listed by number, international symbol, and the phases $\Theta_i=\Phi_m(\mathbf{b}^{(i)})$ (O_h) or $\Phi_{m'}(\mathbf{b}^{(i)})$ (T_h) in the form $\Theta_1\Theta_2\Theta_3$ (taken directly from Table VIII).

The Table entries are the values (modulo unity) of the phase functions Φ_{r_2}, Φ_m, Φ_{r_4}, $\Phi_{r_2'}$, or $\Phi_{m'}$ in the invariant subspace of the operation with which they are associated. [A dash(–) indicates that the operation is not in that point group.] In every case but one the appropriate phase function is identical to the one given by the Θ_i, so if a point in an invariant subspace of a lattice is specified by (u,v,w), then the entry in the table is just $u\Theta_1+v\Theta_2+w\Theta_3$. The only exceptions to this rule are the entries in the invariant subspace of m' for O_h. In this one case the phase function $\Phi_{m'}$ associated with the invariant subspace is not identical to the phase function Φ_m specified by the phases $\Theta_1\Theta_2\Theta_3$, but is given by Eq. (6.1). As a result, to get the extinctions in the plane of m' one must evaluate the phase function Φ_m not at the vectors listed under m', but at the result of applying $(1+r_4)$ to those vectors. These are easily verified to be given by $(1+r_4)(u,0,v)=(u-v,0,u+v)$ [P lattice], $(1+r_4)(u,v,\bar{u})=(u+v,\bar{u}+v,\bar{u}+\bar{v})$ [F^* (I) lattice], $(1+r_4)(u,u+v,v)=(u+v,2v,\bar{u}+v)$ [I^* (F) lattice].

		r_2	m	r_4 or r_2'	m'
P lattice		$(u,u,0)$	$(u,\bar{u},v)$	$(0,u,0)$	$(u,0,v)$
F^* (I) lattice		$(0,0,u)$	$(u+v,\bar{u}+v,\bar{v})$	$(u,\bar{u},u)$	$(u,v,\bar{u})$
I^* (F) lattice		$(u,u,2u)$	$(u,v,0)$	$(u,0,u)$	$(u,u+v,v)$
$\frac{4}{m}\bar{3}\frac{2}{m}$ (O_h)	Φ_m				
222 $P\frac{4}{n}\bar{3}\frac{2}{n}$	$\frac{1}{2}(001)$	0	$\frac{1}{2}v$	0	$\frac{1}{2}(u+v)$
224 $P\frac{4_2}{n}\bar{3}\frac{2}{m}$	$\frac{1}{2}(110)$	0	0	$\frac{1}{2}u$	$\frac{1}{2}(u+v)$
223 $P\frac{4_2}{m}\bar{3}\frac{2}{n}$	$\frac{1}{2}(111)$	0	$\frac{1}{2}v$	$\frac{1}{2}u$	0
230 $I\frac{4_1}{a}\bar{3}\frac{2}{d}$	$\frac{1}{2}(100)$	0	$\frac{1}{2}(u+v)$	$\frac{1}{2}u$	$\frac{1}{2}(u+v)$
227 $F\frac{4_1}{d}\bar{3}\frac{2}{m}$	$\frac{1}{2}(001)$	0	0	$\frac{1}{2}u$	$\frac{1}{2}(u+v)$
228 $F\frac{4_1}{d}\bar{3}\frac{2}{n}$	$\frac{1}{2}(110)$	0	$\frac{1}{2}(u+v)$	$\frac{1}{2}u$	$\frac{1}{2}(u+v)$
226 $F\frac{4}{m}\bar{3}\frac{2}{c}$	$\frac{1}{2}(111)$	0	$\frac{1}{2}(u+v)$	0	0
$\frac{2}{m}\bar{3}$ (T_h)	$\Phi_{m'}$				
201 $P\frac{2}{n}\bar{3}$	$\frac{1}{2}(101)$	—	—	0	$\frac{1}{2}(u+v)$
205 $P\frac{2_1}{a}\bar{3}$	$\frac{1}{2}(110)$	—	—	$\frac{1}{2}u$	$\frac{1}{2}u$
206 $I\frac{2_1}{a}\bar{3}$	$\frac{1}{2}(110)$	—	—	0	$\frac{1}{2}(u+v)$
203 $F\frac{2}{d}\bar{3}$	$\frac{1}{2}(010)$	—	—	0	$\frac{1}{2}(u+v)$

tions associated with all of them can be taken to be identical. It is more complicated because the lattice vectors on the invariant rotation axes are the integral linear combinations of two integrally independent vectors on those axes, while those in the invariant plane of m are the integral linear combinations of four vectors in the plane.

Sets of vectors whose integral linear combinations give the three invariant subspaces are listed in the upper part of the table. The phase functions Φ_{g_2} for the five nonsymmorphic icosahedral space groups are given in the

TABLE XXV. Extinctions for the cubic space groups with point groups O, T_d, and T. The three possible invariant subspaces are listed in the top row. (Since $\Phi_{r_3} \equiv 0$ there are no extinctions on threefold axes.) Immediately below are the general forms for vectors in each of the invariant subspaces, for each of the three lattice types. An entry (u,v,w) means a lattice vector of the form $u\mathbf{b}^{(1)}+v\mathbf{b}^{(2)}+w\mathbf{b}^{(3)}$ where the $\mathbf{b}^{(i)}$ are the threefold-symmetric sets of primitive generating vectors given in Eq. (3.17). [P lattice], Eq. (3.18) [F^* (I) lattice], or Eq. (3.19) [I^* (F) lattice].

For each point group the nonsymmorphic space groups are identified by number and by their international space-group symbol (to facilitate comparison with the calculated extinctions). Immediately after the number and symbol of each space group are listed the phases $\Theta_i = \Phi_{g_2}(\mathbf{b}^{(i)})$ in the form $\Theta_1\Theta_2\Theta_3$, where $g_2 = r_2$ for O and T_d, and $g_2 = r_2'$ for T. (These phases are taken directly from Tables IX and X.)

The entries in the table are the values (modulo unity) of the phase functions Φ_{r_2}, Φ_m, Φ_{r_4}, or $\Phi_{r_2'}$, in the invariant subspace of the operation with which they are associated. [A dash (–) indicates that the operation is not in that point group.] In every case but one, if the phases are $\Theta_1\Theta_2\Theta_3$ and the vector in the invariant subspace is specified by (u,v,w) for the appropriate lattice, then the entry in the table is just $u\Theta_1+v\Theta_2+w\Theta_3$. The exceptions to this rule are the zero entries in the invariant subspace of r_2' for T_d. In this one case the phase function $\Phi_{r_2'}$ associated with the invariant subspace is not identical to the phase function Φ_m specified by the phases $\Theta_1\Theta_2\Theta_3$. It must, however, vanish as an immediate consequence of Eq. (6.2).

Note the rare example of a nonsymmorphic space group (No. 199) with no extinctions. The only other example is $I2_12_12_1$ (No. 24) in the orthorhombic system.

		r_2	m	r_4 or r_2'
P lattice		$(u,u,0)$	$(u,\bar{u},v)$	$(0,u,0)$
F^* (I) lattice		$(0,0,u)$	$(u+v,\bar{u}+v,\bar{v})$	$(u,\bar{u},u)$
I^* (F) lattice		$(u,u,2u)$	$(u,v,0)$	$(u,0,u)$
432 (O)	Φ_{r_2}			
213 $P4_132$	$\frac{1}{4}(1\bar{1}0)$	0	—	$\frac{1}{4}\bar{u}$
208 $P4_232$	$\frac{1}{2}(1\bar{1}0)$	0	—	$\frac{1}{2}\bar{u}$
212 $P4_332$	$\frac{3}{4}(1\bar{1}0)$	0	—	$\frac{1}{4}u$
214 $I4_132$	$\frac{1}{2}(100)$	0	—	$\frac{1}{2}u$
210 $F4_132$	$\frac{1}{2}(1\bar{1}0)$	0	—	$\frac{1}{2}\bar{u}$
$\bar{4}3m$ (T_d)	Φ_m			
218 $P\bar{4}3n$	$\frac{1}{2}(001)$	—	$\frac{1}{2}v$	0
220 $I\bar{4}3d$	$\frac{1}{2}(010)$	—	$\frac{1}{2}(u+v)$	0
219 $F\bar{4}3c$	$\frac{1}{2}(110)$	—	$\frac{1}{2}(u+v)$	0
23 (T)	$\Phi_{r_2'}$			
198 $P2_13$	$\frac{1}{2}(01\bar{1})$	—	—	$\frac{1}{2}u$
199 $I2_13$	$\frac{1}{2}(011)$	—	—	0

lower half. In the case of Y_h we have $\Phi_{g_2} \equiv \Phi_m \equiv \Phi_{r_2} \equiv \Phi_{r_5}$, while for Y we have $\Phi_{g_2} = \Phi_{r_2} \equiv \Phi_{r_5}$. Extinctions occur at points in an invariant subspace of a lattice that have nonintegral inner products with the 6-vector specifying the phase function for that lattice. One verifies directly from the table that Y_h has nonvanishing inner products only in the mirror planes, and Y only along the fivefold axes. The coordinates of extinct vectors in those subspaces (i.e., the values of those nonvanishing inner products) are given in the lower half of the table.

B. Orthorhombic extinctions

To determine the extinctions we require the values of the phase function $\Phi_g(\mathbf{k})$ at vectors $\mathbf{k}$ in the invariant

TABLE XXVI. Extinctions for the icosahedral space groups. For each of the three icosahedral lattices, the upper half of the table gives the invariant subspaces of Y_h and Y. Each invariant subspace is specified by giving a set of primitive generating vectors for that subspace. Two vectors are required for each of the invariant subspaces of r_5 and r_2, and four for the invariant subspace of m (relevant only to Y_h). the subset of a given lattice lying in a given invariant subspace is just the set of all integral linear combinations of the specified vectors. That the subspaces are as stated can be confirmed directly from Fig. 2 for the P lattice, and from the expressions (3.21) and (3.22) that give the generating vectors for the F^* and I^* lattices in terms of the generating vectors $\mathbf{v}^{(i)}$ of the P lattice.

The lower half of the table lists the nonzero phase functions for the five nonsymmorphic icosahedral space groups, taken directly from Tables VIII and IX. Since $\Phi_{r_5} \equiv \Phi_{r_2}$ for Y and $\Phi_{r_5} \equiv \Phi_{r_2} \equiv \Phi_m$ for Y_h, extinctions can be computed directly from the upper part of the table by examining the inner products of these 6-vectors with the 6-vectors specifying the invariant subspaces. One immediately verifies that the only extinctions are in the mirror plane for Y_h and along the fivefold axis for Y, and that the extinguished points are as specified by the entries in the lower part of the table.

	r_5	m	r_2
P	$(000,010) = \mathbf{v}^{(5)}$ $(1\bar{1}1,121) = \tau^3\mathbf{v}^{(5)}$	$(100,000) = \mathbf{v}^{(1)}$ $(010,000) = \mathbf{v}^{(2)}$ $(001,00\bar{1}) = \mathbf{v}^{(3)} - \mathbf{v}^{(6)}$ $(000,1\bar{1}0) = \mathbf{v}^{(4)} - \mathbf{v}^{(5)}$	$(001,001) = \mathbf{v}^{(3)} + \mathbf{v}^{(6)}$ $(000,110) = \tau(\mathbf{v}^{(3)} + \mathbf{v}^{(6)})$
F^*	$(1\bar{1}1,020) = 2\mathbf{v}^{(5)}$ $(020,111) = \tau(2\mathbf{v}^{(5)})$	$(001,000) = \mathbf{v}^{(1)} + \mathbf{v}^{(2)}$ $(000,001) = \tau(\mathbf{v}^{(1)} + \mathbf{v}^{(2)})$ $(1\bar{1}0,000) = \mathbf{v}^{(2)} - \mathbf{v}^{(1)}$ $(000,1\bar{1}0) = \tau(\mathbf{v}^{(2)} - \mathbf{v}^{(1)})$	$(11\bar{1},001) = \mathbf{v}^{(3)} + \mathbf{v}^{(6)}$ $(001,110) = \tau(\mathbf{v}^{(3)} + \mathbf{v}^{(6)})$
I^*	$(010,101) = 2\mathbf{v}^{(5)}$ $(101,111) = \tau(2\mathbf{v}^{(5)})$	$(100,000) = 2\mathbf{v}^{(1)}$ $(000,100) = \tau(2\mathbf{v}^{(1)})$ $(010,000) = 2\mathbf{v}^{(2)}$ $(000,010) = \tau(2\mathbf{v}^{(2)})$	$(002,110) = 2(\mathbf{v}^{(3)} + \mathbf{v}^{(6)})$ $(110,112) = 2\tau(\mathbf{v}^{(3)} + \mathbf{v}^{(6)})$
$\bar{5}\bar{3}\frac{2}{m}$ (Y_h)	Φ_m	Vectors in plane of m	Extinctions
$P\bar{5}\bar{3}\frac{2}{q}$	$\frac{1}{2}(110,000)$	$u\mathbf{v}^{(1)} + s(\mathbf{v}^{(3)} - \mathbf{v}^{(6)})$ $+v\mathbf{v}^{(2)} + t(\mathbf{v}^{(4)} - \mathbf{v}^{(5)})$	$u + v$ odd
$I^*\bar{5}\bar{3}\frac{2}{q}$	$\frac{1}{2}(110,001)$	$2u\mathbf{v}^{(1)} + 2s\tau\mathbf{v}^{(1)}$ $+2v\mathbf{v}^{(2)} + 2t\tau\mathbf{v}^{(2)}$	$u + v$ odd
532 (Y)	$\Phi_{r_5} \equiv \Phi_{r_2}$	Vectors on 5–fold axis	Extinctions
$P5_132$	$\frac{1}{5}(100,\bar{1}10)$	$u\mathbf{v}^{(5)} + v\tau^3\mathbf{v}^{(5)}$	$u \not\equiv 3v \pmod 5$
F^*5_132	$\frac{1}{5}(012,0\bar{2}1)$	$2(u\mathbf{v}^{(5)} + v\tau\mathbf{v}^{(5)})$	$u \not\equiv 2v \pmod 5$
I^*5_132	$\frac{1}{5}(101,\bar{2}0\bar{2})$	$2(u\mathbf{v}^{(5)} + v\tau\mathbf{v}^{(5)})$	$u \not\equiv 2v \pmod 5$

subspace of g, for every point-group operation g. Tables XVI–XIX list the phase functions only for the point-group generators. The unspecified phase functions must then be determined from the group compatibility condition (2.11):

$$\Phi_{g_1g_2}(\mathbf{k})\equiv\Phi_{g_1}(g_2\mathbf{k})+\Phi_{g_2}(\mathbf{k})\ . \tag{6.3}$$

The invariant subspaces of the orthorhombic point groups are the twofold axes **a**, **b**, and **c** and the planes orthogonal to those axes. The result of any orthorhombic point-group operation in any of these invariant subspaces is to leave **k** invariant or take it into $-\mathbf{k}$, so when **k** is in any of the invariant subspaces of an orthorhombic point group, Eq. (6.3) simplifies to one of the two forms

$$\Phi_{g_1g_2}(\mathbf{k})\equiv\pm\Phi_{g_1}(\mathbf{k})+\Phi_{g_2}(\mathbf{k})\ . \tag{6.4}$$

When, however, g_1 is a generator of an orthorhombic space group and the phases are as in Tables XVI–XIX, then an examination of those tables reveals that the only values $\Phi_{g_1}(\mathbf{k})$ can have are 0 or $\frac{1}{2}$. Since $\frac{1}{2}\equiv-\frac{1}{2}$, we can drop the $\pm$ from Eq. (6.4):

$$\Phi_{g_1g_2}(\mathbf{k})\equiv\Phi_{g_1}(\mathbf{k})+\Phi_{g_2}(\mathbf{k})\ . \tag{6.5}$$

Since we always take all the mirrors in each orthorhombic point group to be generators, we need apply Eq. (6.5) only to find the unlisted phase functions associated with twofold rotations. These rotations are given in terms of the point-group generators by

$$\begin{aligned}
&G=222:\ r_c=r_ar_b\ ,\\
&G=mmm\ \text{or}\ mm2:\ r_c=m_am_b\ ,\\
&G=mmm\ \text{or}\ 2mm:\ r_a=m_bm_c\ ,\\
&G=mmm\ \text{or}\ m2m:\ r_b=m_cm_a\ .
\end{aligned} \tag{6.6}$$

Since a general vector in the invariant subspace of a twofold rotation is just an integral multiple of the vector **a**, **b**, or **c** along its axis, it follows from Eqs. (6.5) and (6.6) that the extinctions for the unlisted rotations are determined by adding two of the phases listed in Tables XVI–XIX according to the following rules:

$$\begin{aligned}
&G=222:\ \Phi_{r_c}(n\mathbf{c})\equiv\Phi_{r_a}(n\mathbf{c})+\Phi_{r_b}(n\mathbf{c})\ ,\\
&G=mmm\ \text{or}\ mm2:\ \Phi_{r_c}(n\mathbf{c})\equiv\Phi_{m_a}(n\mathbf{c})+\Phi_{m_b}(n\mathbf{c})\ ,\\
&G=mmm\ \text{or}\ 2mm:\ \Phi_{r_a}(n\mathbf{a})\equiv\Phi_{m_b}(n\mathbf{a})+\Phi_{m_c}(n\mathbf{a})\ ,\\
&G=mmm\ \text{or}\ m2m:\ \Phi_{r_b}(n\mathbf{b})\equiv\Phi_{m_c}(n\mathbf{b})+\Phi_{m_a}(n\mathbf{c})\ .
\end{aligned} \tag{6.7}$$

Note that in the last three cases the phase functions associated with a twofold axis can be nonintegral on that axis only if one of the two phase functions associated with the mirrors leaving that axis invariant is also nonin-

TABLE XXVII. Invariant sublattices of the orthorhombic lattices. For each of the four orthorhombic lattices, we list primitive generating vectors for the one-dimensional sublattices invariant under each of the twofold rotations, and for the two-dimensional sublattices invariant under each of the mirrorings. The primitive generating vectors for the sublattices are specified both in terms of the three orthogonal vectors **a**, **b**, and **c** and in terms of the primitive lattice-generating vectors $\mathbf{b}^{(1)}$,$\mathbf{b}^{(2)}$, and $\mathbf{b}^{(3)}$, related to **a**, **b**, and **c** through Eqs. (4.1)–(4.4).

Lattice	Two-fold Axes	Mirror Planes
P	r_a : $\mathbf{a}=\mathbf{b}^{(1)}$	m_a : $\mathbf{b}=\mathbf{b}^{(2)},\ \mathbf{c}=\mathbf{b}^{(3)}$
	r_b : $\mathbf{b}=\mathbf{b}^{(2)}$	m_b : $\mathbf{c}=\mathbf{b}^{(3)},\ \mathbf{a}=\mathbf{b}^{(1)}$
	r_c : $\mathbf{c}=\mathbf{b}^{(3)}$	m_c : $\mathbf{a}=\mathbf{b}^{(1)},\ \mathbf{b}=\mathbf{b}^{(2)}$
F^* (I)	r_a : $2\mathbf{a}=\mathbf{b}^{(2)}+\mathbf{b}^{(3)}-\mathbf{b}^{(1)}$	m_a : $\mathbf{b}+\mathbf{c}=\mathbf{b}^{(1)},\ \mathbf{b}-\mathbf{c}=\mathbf{b}^{(3)}-\mathbf{b}^{(2)}$
	r_b : $2\mathbf{b}=\mathbf{b}^{(3)}+\mathbf{b}^{(1)}-\mathbf{b}^{(2)}$	m_b : $\mathbf{c}+\mathbf{a}=\mathbf{b}^{(2)},\ \mathbf{c}-\mathbf{a}=\mathbf{b}^{(1)}-\mathbf{b}^{(3)}$
	r_c : $2\mathbf{c}=\mathbf{b}^{(1)}+\mathbf{b}^{(2)}-\mathbf{b}^{(3)}$	m_c : $\mathbf{a}+\mathbf{b}=\mathbf{b}^{(3)},\ \mathbf{a}-\mathbf{b}=\mathbf{b}^{(2)}-\mathbf{b}^{(1)}$
I^* (F)	r_a : $2\mathbf{a}=\mathbf{b}^{(2)}+\mathbf{b}^{(3)}$	m_a : $2\mathbf{b}=\mathbf{b}^{(3)}+\mathbf{b}^{(1)},\ 2\mathbf{c}=\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$
	r_b : $2\mathbf{b}=\mathbf{b}^{(3)}+\mathbf{b}^{(1)}$	m_b : $2\mathbf{c}=\mathbf{b}^{(1)}+\mathbf{b}^{(2)},\ 2\mathbf{a}=\mathbf{b}^{(2)}+\mathbf{b}^{(3)}$
	r_c : $2\mathbf{c}=\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$	m_c : $2\mathbf{a}=\mathbf{b}^{(2)}+\mathbf{b}^{(3)},\ 2\mathbf{b}=\mathbf{b}^{(3)}+\mathbf{b}^{(1)}$
C	r_a : $2\mathbf{a}=\mathbf{b}^{(1)}-\mathbf{b}^{(2)}$	m_a : $2\mathbf{b}=\mathbf{b}^{(1)}+\mathbf{b}^{(2)},\ \mathbf{c}=\mathbf{b}^{(3)}$
	r_b : $2\mathbf{b}=\mathbf{b}^{(1)}+\mathbf{b}^{(2)}$	m_b : $2\mathbf{a}=\mathbf{b}^{(1)}-\mathbf{b}^{(2)},\ \mathbf{c}=\mathbf{b}^{(3)}$
	r_c : $\mathbf{c}=\mathbf{b}^{(3)}$	m_c : $\mathbf{a}+\mathbf{b}=\mathbf{b}^{(1)},\ \mathbf{b}-\mathbf{a}=\mathbf{b}^{(2)}$

tegral. Therefore, except for the point group 222, which contains no mirrors, extinctions on twofold axes can only arise for points that are already extinct by virtue of being in mirror planes. Therefore extinctions arising from the phase functions Φ_{r_a}, Φ_{r_b}, or Φ_{r_c} need only be considered when the point group is 222.

In Table XXVII we list primitive generating vectors for the sublattices of the four orthorhombic lattices invariant under the orthorhombic point-group operations, giving them as linear combinations of the primitive lattice-generating vectors $\mathbf{b}^{(i)}$ in terms of which the phase functions are specified in Tables XVI–XIX. One finds the extinctions for any orthorhombic space group from Table XXVII, Tables XVI–XIX, and (in the case of 222) the first of rules (6.7) giving $\Phi_{r_c}(n\mathbf{c})$ in terms of the tabulated phase functions.

1. *P* lattice

Here the content of Table XXVII is trivial and one can read the extinctions directly from Table XIX:

Screw axes (222). Along twofold axes the lattice contains all integral multiples of **a**, **b**, and **c**. Odd multiples of **a** are extinct if and only if $\Phi_{r_a}(\mathbf{a})\equiv\frac{1}{2}$, and similarly for **b** and **c**. The relevant phases are either listed in Table XIX or inferred from it directly through the rule $\Phi_{r_c}(\mathbf{c})\equiv\Phi_{r_a}(\mathbf{c})+\Phi_{r_b}(\mathbf{c})$.

Glide planes. In the mirror plane orthogonal to **a** the lattice contains all integral linear combinations $m\mathbf{b}+n\mathbf{c}$. If only $\Phi_{m_a}(\mathbf{b})\equiv\frac{1}{2}$ then points with odd m are extinct; if only $\Phi_{m_a}(\mathbf{c})\equiv\frac{1}{2}$ then points with odd n are extinct; if both phases are $\frac{1}{2}$ then points with odd $(m+n)$ are extinct. All relevant phases can be read directly from Table XIX. The same rule applies, *mutatis mutandis,* to the planes orthogonal to **b** and **c**.

2. *C* lattice

Screw axes along **c** *(222).* The lattice contains all integral multiples of **c**. Since $\Phi_{r_c}(\mathbf{c})\equiv\Phi_{r_a}(\mathbf{c})+\Phi_{r_b}(\mathbf{c})$, Table XVIII shows that odd multiples are extinct for the one nonsymmorphic space group No. 20.

Screw axes along **a** *or* **b** *(222).* These axes contain integral multiples of 2**a** or 2**b**. since Φ_{r_a} and Φ_{r_b} vanish at $\mathbf{b}^{(1)}$ and $\mathbf{b}^{(2)}$ for space group No. 20, Table XVIII shows that there are no extinctions along these axes for the point group 222.

Glide planes normal to **c**. The sublattice consists of all integral linear combinations $m(\mathbf{a}+\mathbf{b})+n(\mathbf{b}-\mathbf{a})$, and according to Table XXVII the relevant phase is $m\Phi_{m_c}(\mathbf{b}^{(1)})+n\Phi_{m_c}(\mathbf{b}^{(2)})$. According to Table XVIII this can be nonzero only in space groups Nos. 39, 41, 64, 67, and 68. In all five cases both $\Phi_{m_c}(\mathbf{b}^{(1)})$ and $\Phi_{m_c}(\mathbf{b}^{(2)})$ are $\frac{1}{2}$, and the extinct points are therefore those with $m+n$ odd. (Alternatively, the sublattice can be viewed as the set of integral linear combinations of **a** and **b** with both integers of the same parity, and the extinct points are those with both integers odd.)

Glide planes normal to **b** *or* **a**. The sublattice normal to **b** consists of all integral linear combinations $m\mathbf{c}+2n\mathbf{a}$. According to Table XXVII the relevant phase is $m\Phi_{m_b}(\mathbf{b}^{(3)})+n[\Phi_{m_b}(\mathbf{b}^{(1)})+\Phi_{m_b}(\mathbf{b}^{(2)})]$, but according to table XVIII $\Phi_{m_b}(\mathbf{b}^{(1)})$ and $\Phi_{m_b}(\mathbf{b}^{(2)})$ are always both 0, so points with odd m are extinct if and only if $\Phi_{m_b}(\mathbf{b}^{(3)})\equiv\frac{1}{2}$, which happens in Nos. 36, 37, 63, 64, 66, and 68. In the same way, the lattice normal to **a** consists of all integral linear combinations $m\mathbf{c}+2n\mathbf{a}$, and points with odd m are extinct if and only if $\Phi_{m_a}(\mathbf{b}^{(3)})\equiv\frac{1}{2}$, as in Nos. 37, 40, 41, 66, and 68.

3. $F^*(I)$ and $I^*(F)$ lattices

For the other two orthorhombic lattices we can further simplify Table XXVII. Because every phase $\Phi_g(\mathbf{b}^{(i)})$ is

TABLE XXVIII. Mirror phase functions on their invariant sublattices for the orthorhombic I^* and F^* lattices. Using (6.11) we list the phase functions Φ_m evaluated at the vectors that primitively generate the invariant subspace of m, in terms of the values of phase functions tabulated in Tables XVII and XVIII at the lattice primitive vectors $\mathbf{b}^{(i)}$.

	Mirror Planes
F^*	$\Phi_{m_a}(\mathbf{b}+\mathbf{c})\equiv\Phi_{m_a}(\mathbf{b}-\mathbf{c})\equiv\Phi_{m_a}(\mathbf{b}^{(1)})$
(I)	$\Phi_{m_b}(\mathbf{c}+\mathbf{a})\equiv\Phi_{m_b}(\mathbf{c}-\mathbf{a})\equiv\Phi_{m_b}(\mathbf{b}^{(2)})$
	$\Phi_{m_c}(\mathbf{a}+\mathbf{b})\equiv\Phi_{m_c}(\mathbf{a}-\mathbf{b})\equiv\Phi_{m_c}(\mathbf{b}^{(3)})$
I^*	$\Phi_{m_a}(2\mathbf{b})\equiv\Phi_{m_a}(\mathbf{b}^{(2)})+\frac{1}{2}$, $\Phi_{m_a}(2\mathbf{c})\equiv\Phi_{m_a}(\mathbf{b}^{(3)})+\frac{1}{2}$
(F)	$\Phi_{m_b}(2\mathbf{c})\equiv\Phi_{m_b}(\mathbf{b}^{(3)})+\frac{1}{2}$, $\Phi_{m_b}(2\mathbf{a})\equiv\Phi_{m_b}(\mathbf{b}^{(1)})+\frac{1}{2}$
	$\Phi_{m_c}(2\mathbf{a})\equiv\Phi_{m_c}(\mathbf{b}^{(1)})+\frac{1}{2}$, $\Phi_{m_c}(2\mathbf{b})\equiv\Phi_{m_c}(\mathbf{b}^{(2)})+\frac{1}{2}$

either 0 or $\frac{1}{2}$,[38] in evaluating

$$\Phi_g(n_1\mathbf{b}^{(1)}+n_2\mathbf{b}^{(2)}+n_3\mathbf{b}^{(3)}) \tag{6.8}$$

we can shift any of the n_i by arbitrary multiples of 2. In particular, any expression of the form (6.8) with three odd coefficients reduces to

$$\Phi_g(\mathbf{b}^{(1)}+\mathbf{b}^{(2)}+\mathbf{b}^{(3)}) \tag{6.9}$$

and any with two odd coefficients can be reduced to

$$\Phi_g(\mathbf{b}^{(1)}+\mathbf{b}^{(2)}+\mathbf{b}^{(3)})+\Phi_g(\mathbf{b}^{(i)})\ , \tag{6.10}$$

where $\mathbf{b}^{(i)}$ is the one without the odd coefficient. But an inspection of Tables XVI and XVII reveals that

$$\begin{aligned}&\Phi_m(\mathbf{b}^{(1)}+\mathbf{b}^{(2)}+\mathbf{b}^{(3)})\equiv 0,\quad m=m_a,m_b,m_c,\quad F^*\ (I)\ \text{lattice};\\ &\Phi_m(\mathbf{b}^{(1)}+\mathbf{b}^{(2)}+\mathbf{b}^{(3)})\equiv \tfrac{1}{2},\quad m=m_a,m_b,m_c,\quad I^*\ (F)\ \text{lattice},\quad \text{nonsymmorphic space groups}\ .\end{aligned} \tag{6.11}$$

Table XXVIII lists the phase functions Φ_m on the invariant subspaces of m, where the expressions for the invariant subspaces are taken from Table XXVII and the resulting expressions are simplified through the use of Eq. (6.11).

a. F^* (I) lattice

Screw axes (222). Along twofold axes the lattice contains all integral multiples of 2**a**, 2**b**, and 2**c**. It follows from Tables XVII and XXVII that the corresponding phase functions $\Phi_{r_a}(2\mathbf{a})$, $\Phi_{r_b}(2\mathbf{b})$, $\Phi_{r_c}(2\mathbf{c})$ vanish. Therefore the twofold axes in the F^* (I) orthorhombic lattice imply no extinctions. Note, in particular, space group $I2_12_12_1$ (No. 24), a rare specimen of a nonsymmorphic space group with no extinctions.[39]

Glide planes. A general lattice point in the plane perpendicular to **a** is $m(\mathbf{b}+\mathbf{c})+n(\mathbf{b}-\mathbf{c})$. According to Table XXVIII it will be extinct if and only if $\Phi_{m_a}(\mathbf{b}^{(1)})\equiv\frac{1}{2}$ (as in Nos. 45, 46, 72, and 73) and $m+n$ is odd. (Alternatively one can characterize the sublattice as integral linear combinations of **a** and **b** with both integers of the same parity, and the extinct points are those with both integers odd.) The rule for extinctions in the planes perpendicular to **b** (Nos. 45, 72, and 73) and **c** (Nos. 73 and 74) are the same, except for cyclic permutations of **a**, **b**, **c** and $\mathbf{b}^{(1)},\mathbf{b}^{(2)},\mathbf{b}^{(3)}$.

b. I^* (F) lattice

There are no nonsymmorphic space groups with point group 222, so we need only consider glide planes.

Glide planes. The sublattice in the mirror plane perpendicular to **a** consists of integral linear combinations $2m\mathbf{b}+2n\mathbf{c}$. Table XXVIII specifies the value of Φ_{m_a} at such a point to be $\frac{1}{2}(m+n)+m\Phi_{m_a}(\mathbf{b}^{(2)})+n\Phi_{m_a}(\mathbf{b}^{(3)})$. But according to Table XVI, $\Phi_{m_a}(\mathbf{b}^{(2)})$ and $\Phi_{m_a}(\mathbf{b}^{(3)})$ vanish for both nonsymmorphic space groups, so points are extinct if and only if $m+n$ is odd. The analogous state of affairs holds for the other two mirror planes.

C. Monoclinic extinctions

The only point-group operations are the twofold rotation r_c and/or the orthogonal mirror m_c.

Screw axes. The primitive lattice contains all integral multiples of $\mathbf{c}=\mathbf{b}^{(3)}$. Odd multiples are extinct if $\Phi_{r_c}(\mathbf{b}^{(3)})\equiv\frac{1}{2}$, which it does, according to Table XXI, in Nos. 4, 11, and 14. The centered lattice contains all integral multiples of $2\mathbf{c}=2\mathbf{b}^{(3)}-\mathbf{b}^{(1)}-\mathbf{b}^{(2)}$. According to Table XXII the phase function Φ_{r_c} always vanishes on the centered lattice, so none of these points is extinct.

Glide planes. In both the primitive and the centered lattice, points in the mirror plane are of the form $m\mathbf{b}^{(1)}+n\mathbf{b}^{(2)}$ for arbitrary integers m and n. According to Tables XXI and XXII all space groups with nonzero Φ_{m_c} have $\Phi_{m_c}(\mathbf{b}^{(1)})=\Phi_{m_c}(\mathbf{b}^{(2)})=\frac{1}{2}$, so for those space groups (Nos. 7, 9, 13, 14, and 15) points with odd $m+n$ in the mirror plane are extinct.

D. Triclinic extinctions

Both space groups (Table XXIII) are symmorphic, so there are no extinctions.

VII. CONCLUSIONS

Friends shook their heads sadly when, in response to polite inquiries, I cheerily informed them I was spending a significant part of my sabbatical year 1990–91 rederiving all the 230 crystallographic space groups. There are two answers[40] to their implied question: Why did you choose that particular way to waste your time?

[38] As noted above this is true whenever g is a generator, and is therefore true for arbitrary g since an arbitrary phase function can be expressed as an integral linear combination of phase functions associated with generators.

[39] The only other example is $I2_13$ (No. 199 in the cubic system), as noted above.

[40] There is also, of course, Hillary's answer: Because they are there!

(1) On the practical level, there is the matter of space-group theory for incommensurately modulated crystals. These can be regarded as materials with ordinary crystallographic point groups, but with lattices whose indexing dimension D is higher than 3. The analysis described here leads directly and efficiently to the classes of gauge-equivalent phase functions on such lattices, and a major part of the computation simply repeats the computation of the phase function for the crystallographic sublattices they contain. The tables of phase functions derived here and in RMRW therefore greatly simplify that process.

Much work on the lattices and space groups of incommensurately modulated crystals has been done by Janner, Janssen, and de Wolff, (de Wolff, Janssen, and Janner, 1981; Janner, Janssen, and de Wolff, 1983a, 1983b, 1983c; Janner, 1991) but their catalogues of lattices and space groups fail to take full advantage of the fact that from the point of view of symmetry there are no grounds for drawing distinctions within the lattice of wave vectors between a basic lattice (corresponding to an underlying crystal) and a set of satellites, corresponding to modulations of that crystal. From the present perspective many of their distinct "Bravais classes" contain identical Fourier-space lattices, and many of their distinct space groups are equivalent.[41]

(2) More importantly, on the visionary level, there is the matter of rescuing crystallographers from the abyss. I launched into a recomputation of the *International Tables* because I believe the conventional approach to space groups based on real space periodicity is a pedagogical disaster for students and a source of torment for anyone wishing to make use of them.[42] Much of the information contained in the vast expanses of the *International Tables for Crystallography* (International Union of Crystallography, 1987), together with all of the analogous information for standard quasicrystals of arbitrary rotational order, can be concisely summarized in a few tables of phase functions—Tables VIII–X, XVI–XIX, XXI, XXII of the present paper together with two short tables (V and VI) from RMRW—and a few rules on how to extract the useful information in those tables. How better to convince those addicted to established methods to try something else, than by writing two brief (on the scale of the *International Tables)* essays that do everything?

I would not dare to suggest that even in the matter of nomenclature it would be better to specify the space groups by simply giving the values, in a suitable gauge, of the phase functions associated with the point-group generators. Though it would be.

[41]These matters are discussed in Mermin and Lifshitz, 1992.

[42]See, for example, the charming *obiter dicta* on the *International Tables* scattered through Wilson, 1990.

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APPENDIX A: SCALE INVARIANCE OF THE ICOSAHEDRAL *P* LATTICE

Since we have noted (Sec. III.E) that the icosahedral F^* lattice is invariant under a scaling by τ, an easy way to establish the scaling properties of the P lattice is to represent it as a sublattice of the F^* lattice. It follows from inverting the definition (3.21) of the generating vectors $\mathbf{b}^{(i)}$ of the F^* lattice in terms of the generating vectors $\mathbf{v}^{(i)}$ of the P lattice, that[43]

$$2\mathbf{v}^{(1)}=(\bar{1}11,000)\ ,\quad 2\mathbf{v}^{(2)}=(1\bar{1}1,000)\ ,\quad 2\mathbf{v}^{(3)}=(11\bar{1},000),$$
$$2\mathbf{v}^{(4)}=(\bar{1}11,200)\ ,\quad 2\mathbf{v}^{(2)}=(1\bar{1}1,020)\ ,\quad 2\mathbf{v}^{(3)}=(11\bar{1},002), \tag{A1}$$

where by $(a_1a_2a_3,a_4a_5a_6)$ we mean $\sum a_i\mathbf{b}^{(i)}$. Thus a P lattice (scaled up by a factor of 2 from the one we started with) can be viewed as a sublattice of the F^* lattice subject to the constraint that the last three coordinates are all even, while the first three are either all even or all odd.

Since F^* lattice vectors satisfy

$$\tau(a_1a_2a_3,a_4a_5a_6)$$
$$=(a_4a_5a_6,[a_1+a_4][a_2+a_5][a_3+a_6])\ , \tag{A2}$$

we can readily establish the behavior of the P sublattice under successive scalings by τ. We have

[43]It is convenient to write -1 as $\bar{1}$, etc.

$$
\begin{aligned}
&2\tau\mathbf{v}^{(1)}=\tau(\bar{1}11,000)=(000,\bar{1}11)\ \text{(not in lattice)}\,,\\
&2\tau^2\mathbf{v}^{(1)}=\tau(\bar{0}00,\bar{1}11)=(\bar{1}11,\bar{1}11)\ \text{(not in lattice)}\,,\\
&2\tau^3\mathbf{v}^{(1)}=\tau(\bar{1}11,\bar{1}11)=(\bar{1}11,\bar{2}22)\ \text{(in lattice)}\,;\\
&2\tau\mathbf{v}^{(4)}=\tau(\bar{1}11,200)=(200,111)\ \text{(not in lattice)}\,,\\
&2\tau^2\mathbf{v}^{(4)}=\tau(200,111)=(111,311)\ \text{(not in lattice)}\,,\\
&2\tau^3\mathbf{v}^{(4)}=\tau(111,311)=(311,422)\ \text{(in lattice)}\,.
\end{aligned}
\tag{A3, A4}
$$

Similar expressions (given by cyclical permutations within the first and second three sets of coordinates) hold for $\mathbf{v}^{(2)}$ and $\mathbf{v}^{(5)}$ and for $\mathbf{v}^{(3)}$ and $\mathbf{v}^{(6)}$.

It follows that scaling the P lattice by τ or τ^2 gives vectors not in the P lattice, but scaling it by τ^3 yields only P-lattice vectors:

$$
\begin{aligned}
&2\tau^3\mathbf{v}^{(1)}=(\bar{1}11,\bar{2}22)\,,\quad 2\tau^3\mathbf{v}^{(2)}=(1\bar{1}1,2\bar{2}2)\,,\\
&2\tau^3\mathbf{v}^{(3)}=(11\bar{1},22\bar{2})\,;\\
&2\tau^3\mathbf{v}^{(4)}=(311,422),\quad 2\tau^3\mathbf{v}^{(5)}=(131,242)\,,\\
&2\tau^3\mathbf{v}^{(6)}=(113,224)\,.
\end{aligned}
\tag{A5}
$$

Furthermore, scaling the original lattice by τ^3 yields all the original lattice vectors. This can be confirmed by noting that the original vectors $2\mathbf{v}^{(i)}$, expressed in the form (A1), can be extracted as integral linear combinations of the vectors $2\tau^3\mathbf{v}^{(i)}$ expressed in the form (A5).

The explicit relations are

$$
\begin{pmatrix}\mathbf{v}^{(1)}\\ \mathbf{v}^{(2)}\\ \mathbf{v}^{(3)}\\ \mathbf{v}^{(4)}\\ \mathbf{v}^{(5)}\\ \mathbf{v}^{(6)}\end{pmatrix}=\begin{pmatrix}\bar{2}&\bar{1}&\bar{1}&\bar{1}&1&1\\ \bar{1}&\bar{2}&\bar{1}&1&\bar{1}&1\\ \bar{1}&\bar{1}&\bar{2}&1&1&\bar{1}\\ \bar{1}&1&1&\bar{2}&1&1\\ 1&\bar{1}&1&1&\bar{2}&1\\ 1&1&\bar{1}&1&1&\bar{2}\end{pmatrix}\begin{pmatrix}\tau^3\mathbf{v}^{(1)}\\ \tau^3\mathbf{v}^{(2)}\\ \tau^3\mathbf{v}^{(3)}\\ \tau^3\mathbf{v}^{(4)}\\ \tau^3\mathbf{v}^{(5)}\\ \tau^3\mathbf{v}^{(6)}\end{pmatrix}
\tag{A6}
$$

and

$$
\begin{pmatrix}\tau^3\mathbf{v}^{(1)}\\ \tau^3\mathbf{v}^{(2)}\\ \tau^3\mathbf{v}^{(3)}\\ \tau^3\mathbf{v}^{(4)}\\ \tau^3\mathbf{v}^{(5)}\\ \tau^3\mathbf{v}^{(6)}\end{pmatrix}=\begin{pmatrix}2&\bar{1}&\bar{1}&\bar{1}&1&1\\ \bar{1}&2&\bar{1}&1&\bar{1}&1\\ \bar{1}&\bar{1}&2&1&1&\bar{1}\\ \bar{1}&1&1&2&1&1\\ 1&\bar{1}&1&1&2&1\\ 1&1&\bar{1}&1&1&2\end{pmatrix}\begin{pmatrix}\mathbf{v}^{(1)}\\ \mathbf{v}^{(2)}\\ \mathbf{v}^{(3)}\\ \mathbf{v}^{(4)}\\ \mathbf{v}^{(5)}\\ \mathbf{v}^{(6)}\end{pmatrix}\,.
\tag{A7}
$$

APPENDIX B: SIX-DIMENSIONAL DUALITY OF ICOSAHEDRAL PRIMITIVE VECTORS

We record here the sets of dual 6-vectors, Eq. (2.21), appropriate to the three icosahedral lattices, because, although no use is made of them in this essay, they have an appealing form when expressed in terms of the threefold-symmetric sets of primitive vectors. The only feature of icosahedral geometry required in their construction is that a unit vector along a fivefold axis (say $\mathbf{v}^{(1)}$) is orthogonal to the sum of unit vectors along nearest neighboring (say $\mathbf{v}^{(5)}$) and next-nearest neighboring (say $\mathbf{v}^{(3)}$) fivefold axes, as is evident from the imbedding of the icosahedron in a cube in Fig. 4. As a result, the inner products $\mathbf{v}^{(i)}\cdot\mathbf{v}^{(j)}$ have one value for $ij=45$, 56, 64, 15, 16, 26, 24, 34, and 35, and the negative of that value for $ij=12$, 23, 31, 14, 25, and 36.

It follows immediately that an orthornormal 6-space extension of the P-lattice primitive generating vectors is given, to within a normalization constant, by

$$
\begin{aligned}
&(\mathbf{v}^{(1)},\mathbf{v}^{(4)})\,,\quad(\mathbf{v}^{(2)},\mathbf{v}^{(5)})\,,\quad(\mathbf{v}^{(3)},\mathbf{v}^{(6)})\,,\\
&(\mathbf{v}^{(4)},-\mathbf{v}^{(1)})\,,\quad(\mathbf{v}^{(5)},-\mathbf{v}^{(2)})\,,\quad(\mathbf{v}^{(6)},-\mathbf{v}^{(3)})\,.
\end{aligned}
\tag{B1}
$$

The primitive vectors (3.22) for the I^* (F) lattice are just $\mathbf{b}^{(i)}=2\mathbf{v}^{(i)}$, $i=1,2,3$ and $\mathbf{b}^{(i)}=\tau\mathbf{b}^{(i-3)}$, $i=4,5,6$. If we define a set of 3-vectors by (see Fig. 2)

$$
\begin{aligned}
&\mathbf{a}^{(1)}=\mathbf{v}^{(1)}+\mathbf{v}^{(4)}\,,\quad\mathbf{a}^{(4)}=\mathbf{v}^{(5)}+\mathbf{v}^{(6)}=\tau\mathbf{a}^{(1)}\,,\\
&\mathbf{a}^{(2)}=\mathbf{v}^{(2)}+\mathbf{v}^{(5)}\,,\quad\mathbf{a}^{(5)}=\mathbf{v}^{(6)}+\mathbf{v}^{(4)}=\tau\mathbf{a}^{(2)}\,,\\
&\mathbf{a}^{(3)}=\mathbf{v}^{(3)}+\mathbf{v}^{(6)}\,,\quad\mathbf{a}^{(6)}=\mathbf{v}^{(4)}+\mathbf{v}^{(5)}=\tau\mathbf{a}^{(3)}\,,
\end{aligned}
\tag{B2}
$$

then for $1\le i,j\le 3$ we have $\mathbf{a}^{(i)}\cdot\mathbf{b}^{(j)}=0$, $i\neq j$. It follows that to within a normalization constant the 6-vectors $\mathbf{A}^{(i)}$ and $\mathbf{B}^{(i)}$ of Eq. (2.21) are given by

$$
\begin{aligned}
&(\mathbf{a}^{(1)},\tau\mathbf{a}^{(1)})\,,\quad(\mathbf{a}^{(2)},\tau\mathbf{a}^{(2)})\,,\quad(\mathbf{a}^{(3)},\tau\mathbf{a}^{(3)})\,,\\
&(\tau\mathbf{a}^{(1)},-\mathbf{a}^{(1)})\,,\quad(\tau\mathbf{a}^{(2)},-\mathbf{a}^{(2)})\,,\quad(\tau\mathbf{a}^{(3)},-\mathbf{a}^{(3)})\,,
\end{aligned}
\tag{B3}
$$

and

$$
\begin{aligned}
&(\mathbf{b}^{(1)},\tau\mathbf{b}^{(1)})\,,\quad(\mathbf{b}^{(2)},\tau\mathbf{b}^{(2)})\,,\quad(\mathbf{b}^{(3)},\tau\mathbf{b}^{(3)})\,,\\
&(\tau\mathbf{b}^{(1)},-\mathbf{b}^{(1)})\,,\quad(\tau\mathbf{b}^{(2)},-\mathbf{b}^{(2)})\,,\quad(\tau\mathbf{b}^{(3)},-\mathbf{b}^{(3)})\,.
\end{aligned}
\tag{B4}
$$

Note, finally, that with the $\mathbf{A}^{(i)}$ and $\mathbf{B}^{(i)}$ interchanged, the sets (B3) and (B4) serve equally well for the F^* (I) lattice, since the vectors (B2) can be taken as a primitive generating set alternative to the set given in Eq. (3.21).

APPENDIX C: INDEX OF TECHNICAL TERMS

I give below an index of the major technical terms used in quasicrystallography. Although most of them are routinely familiar to crystallographers and solid-state physicists, I emphasize that some—notably "point group," "lattice," and "space group"—are defined here more broadly than they are in conventional crystallography

(although, of course, they reduce to the conventional definitions in the narrower contexts in which conventional crystallography applies).

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