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On the arithmetic classification of crystal structures

Giuseppe Fadda and Giovanni Zanzotto*

Dipartimento di Metodi e Modelli Matematici per le Scienze Applicate – DMMMSA, Università di Padova, Via Belzoni 7, 35131 Padova, Italy. Correspondence e-mail: zanzotto@dmsa.unipd.it

An arithmetic criterion for the classification of crystal structures with n points in their unit cell ('n-lattices') was described by Pitteri & Zanzotto [*Acta Cryst.* (1998), A**54** 359–373]. In this paper, a systematic analysis of monoatomic 2-lattices is given, showing that there exist 29 distinct arithmetic types of these structures, some of which share the same space groups. As all monoatomic 2-lattices are constituted by a single crystallographic orbit, these structures are also classified by the established criterion of Fischer & Koch [Koch & Fischer (1975). *Acta Cryst.* A**31**, 88–95; Fischer & Koch (1996). *International Tables for Crystallography*, Vol. A. Dordrecht: Kluwer] involving the lattice complexes. The two classifications are found to coincide in this simplest case. By examination of some examples taken from the allotropes of the elements, it is also shown how the arithmetic criterion can be used to classify more complex crystals, such as monoatomic 4-lattices. This gives a group-theoretical framework for distinguishing structures when the space-group classification fails to do so, and Fischer & Koch's criterion, as presented in the literature, may not be immediately applied.

1. Introduction

1.1. Background

The problems posed by materials science, especially in the new field of active crystalline materials, require an ever more detailed modeling of the behavior of crystalline solids, with the associated phenomena of twinning and microstructure formation [see for instance Ball & James (1992, 2001), Luskin (1996), Müeller (1998), James (1999), James & Hane (2000), Pitteri & Zanzotto (2001) for reviews about recent activity on the modeling of such phenomena based on non-linear thermoelasticity theory].

Both in the theoretical and in the experimental work on crystalline materials, one must consider, besides simple lattices, also 'multilattices' [called 'ideal crystals' by Engel (1986), or 'multiregular point systems' by Dolbilin *et al.* (1998)]. These structures are triply periodic subsets of the tridimensional affine space constituted by unions of a finite number of translates of a given simple lattice, and can describe in full detail the atomic arrangements in crystalline materials with more than one atom in their translational unit cell. A multilattice is called an n-lattice when it is necessary to specify that n atoms are present in its unit cell; in this case, the multilattice is a union of n congruent interpenetrating simple lattices.

As pointed out by Ericksen (1970, 1977, 1980), a central question in the modeling of crystal mechanics from the standpoint of non-linear elasticity is writing an appropriate constitutive equation for the energy of the crystalline substance. To this end, and in order to determine the correct location of the energy wells and to keep a proper track of the symmetry changes occurring in lattices that undergo solid-state phase transformations, the 'arithmetic symmetry' of deformable crystals should be investigated.

For simple lattices (1-lattices), the notion of arithmetic symmetry is classical, going back to the earlier decades of this century; according to this point of view, the classification of 1-lattice structures is based on the conjugacy properties of the representations of their symmetry groups as subgroups of the arithmetic group $GL(3,\mathbb{Z})$.[1] The main reason for formulating the arithmetic criterion for simple-lattice symmetry is that it describes these structures in a more precise way than the orthogonal framework, as it determines also all the inequivalent centerings of 1-lattices, subdividing the latter into the classical 14 Bravais types.[2] In the same way, the group $GL(2,\mathbb{Z})$ is the basis for studying the arithmetic symmetry of planar simple lattices (1-nets), which are subdivided into five arithmetic types, and so on for any dimensions; see for instance Schwarzenberger (1972), Engel (1986), Sternberg (1994), Michel (1995).

Only recently an arithmetic framework has been proposed for investigating the symmetry of multilattices: see Pitteri & Zanzotto (1998, 2001). This notion originated from earlier work on the invariance for the energy functions of non-linearly elastic crystalline materials by Ericksen (1977), Parry (1978) and Pitteri (1985).

[1] $GL(3,\mathbb{Z})$ denotes the group of invertible 3×3 matrices with integral entries (as usual, in this paper we denote by $\mathbb{Z}$ and $\mathbb{R}$ the sets of integral and real numbers, respectively).
[2] Pitteri & Zanzotto (1996) discuss the relation between the arithmetic classification of simple lattices and the earlier criterion actually stated by Bravais (1850).

The arithmetic criterion for multilattices extends in a natural way the classical ideas mentioned above regarding simple lattices: as for the latter, the classification is based on the conjugacy properties of the symmetry groups of multilattices within suitable arithmetic groups.[3] Such groups generalize the role played by $GL(3, \mathbb{Z})$ for simple lattices, as recalled above. This method allows one to produce a detailed classification of crystal structures: given $n \geq 1$, one can establish all the essentially distinct structures with n points in their unit cell. For $n > 1$, the arithmetic classification is finer than the space-group classification [see Proposition 5 in Pitteri & Zanzotto (1998)]. One can therefore also identify all the distinct n-lattice structures that share the same space group.[4] We notice that the literature seems lacking on this point. Well known empirical classifications of crystal structures, such as the *Strukturberichte* (1913–1940), give structure lists, for instance under the heading of their space group, without any criterion to help identify the possibilities that are theoretically available. This lack is even more evident in structure lists given under the heading of the 'Pearson symbols' (see Villars & Calvert, 1991); the latter give a coarse indication of the feature of a crystal by indicating its Bravais type and the number of atoms in its conventional cell. The arithmetic criterion is the theoretical tool that allows one to identify all the distinct structures falling under the heading of each Pearson symbol.

1.2. Results of this paper

The study of the arithmetic symmetry of multilattices is in its early stages [see the aforementioned literature, and also Adeleke (1999) and Ericksen (1999)]. In Fadda & Zanzotto (2000), we have made a first systematic investigation of the simplest non-trivial case, showing that the monoatomic 2-nets (*i.e.* monoatomic 2-lattices in two dimensions) are subdivided into five distinct arithmetic types. In this paper, we illustrate the three-dimensional (3D) case.

(*a*) We show how the systematic analysis of the arithmetic symmetry of multilattices can be performed for monoatomic 2-lattices, of which we give the complete classification into distinct arithmetic types [see Table 1 as a summary; see Table 2 in Fadda & Zanzotto (2001) for a representation of their periodic cells]. This involves establishing all the conjugacy classes of the symmetry groups of 2-lattices within the arithmetic group $\Gamma_{3,1}$ defined in formulae (15)–(16) below [we recall that the role of $\Gamma_{3,1}$ for 2-lattices is completely analogous to that of $GL(3, \mathbb{Z})$ for 1-lattices]. To reach this goal, we indicate in §3 a procedure that allows us to minimize the required computations by making suitable use of the information given in *International Tables for Crystallography* (1996).[5] We find that there exist 29 distinct arithmetic types of monoatomic 2-lattices in 3D. As for the general case, also here we obtain a finer classification than the one based on space-group symmetry, as there are cases of distinct 2-lattice types that share their space group (see Table 1).[6] The 29 distinct types include all the 2-lattice structures reported in the literature for the elemental crystals; among these are the five *Strukturberichte* that are monoatomic 2-lattices plus a recently proposed 2-lattice structure of Si and also two other 2-lattice structures for which an identification in the *Strukturberichte* is not available (see Table 1 and §4 for more details and references). The arithmetic method gives to the empirical classifications of crystalline structures and to the search of new ones a group-theoretical basis.[7]

(*b*) We also discuss in §5 some examples of monoatomic 4-lattices, taken from nature, in order to show how the arithmetic criterion operates with more complex structures.

1.3. Relation to the classification of crystallographic orbits by Fischer & Koch (Koch & Fischer, 1975; Fischer & Koch, 1996)

We recall that any monoatomic 2-lattice is a 'regular point system' in the 3D affine space, *i.e.* it is a set of points constituted by a single crystallographic orbit.[8]

Now, there exists in the literature a well established criterion for the classification of crystallographic orbits, proposed by Fischer & Koch (Koch & Fischer, 1975; Fischer & Koch, 1996); see also Hermann (1935) and Engel (1986). This criterion considers two orbits as equivalent when their site-symmetry groups are conjugate in the affine normalizer of the

[3] These arithmetic groups arise from the analysis of the general indeterminacy in the choice of the multilattice descriptors (see Pitteri, 1985). In the case of deformable simple lattices, the descriptors are the vectors forming the lattice basis, which is determined up to a transformation in $GL(3, \mathbb{Z})$, whence the role of the latter group in the study of simple-lattice symmetry. For multilattices, one also considers the shift vectors giving the positions of the further simple lattices constituting the multilattice (or, equivalently, of the further points in the unit cell), so that more general arithmetic groups must be considered [see for instance formulae (16) or (32) below]. The arithmetic criterion presented by Pitteri & Zanzotto (1998) can be generalized in a straightforward way also to classify 'polyatomic' crystal structures constituted by atoms belonging to a finite number of distinct atomic species. Here, we confine our attention to 'monoatomic' crystals, whose points are all physically indistinguishable.

[4] This happens much in the same way in which the classical arithmetic criterion for 1-lattices allows one to determine the three distinct cubic centerings P, F, I that pertain to the same cubic holohedry.

[5] Appendix *B* shows through an example how such computations are actually carried out.

[6] We recall that for simple lattices these two classifications are equivalent (see for instance Janssen, 1973, p. 120).

[7] Also the description of the symmetry hierarchies that exist among the 29 different types of 3D monoatomic 2-lattices, and the ensuing account of all the possibilities for symmetry breaking in these structures, constitute interesting knowledge for modeling phase transitions in crystalline materials; see Fadda & Zanzotto (2001) for detailed information on the symmetry groups of 2-lattices and their inclusion relations up to $\Gamma_{3,1}$-conjugacy (partial ordering of the 29 conjugacy classes).

[8] 'Regular point systems' is the term used in the literature for the special multilattices on which the space-group action is transitive, so that they are constituted by a single orbit [see Hilbert & Cohn-Vossen (1932), Engel (1986), Dolbilin *et al.* (1998)]. In general, however, a multilattice is not a single crystallographic orbit, but a union of finitely many orbits with the same translational invariance, and does not coincide with a single orbit even when all of its atoms belong to a single species. See §5 for more details, and for examples taken from the allotropic structures of the elements. As recalled above, general multilattices are also termed 'multiregular point systems' (Dolbilin *et al.*, 1998), or 'ideal crystals' (Engel, 1986, p. 2), when it is useful to stress the fact that they are not single orbits. It is well known that, besides 3D periodicity, the characteristic feature of a regular point system is that it 'looks the same' if seen from every one of its points (see Engel, 1986). This is not true for multiregular point systems, which 'look different' in finitely many ways when seen from their own points.

orbits' stabilizers. The corresponding classes of equivalent orbits are called 'lattice complexes' by Fischer & Koch, or 'orbit types' by Engel. A referee pointed out to us that an explicit count based on Fischer & Koch's method gives the same 29 types of monoatomic 2-lattices as the arithmetic method discussed here; therefore the two criteria turn out, *a posteriori*, to be equivalent for these simplest regular point systems.[9] As, *a priori*, the two classification principles involve groups of a rather different nature, the equivalence of the two classifications gives a remarkable link between the arithmetic framework and the classification based on lattice complexes, which is a subject classically studied in crystallography. One conjectures that the two criteria be actually equivalent for all the single-orbit structures, but at present we can offer no general conclusion about this question. It should be stressed, however, that the method by Fischer & Koch originated as a classification of (single) orbits, and it is not obvious how to extend it to more complex crystal structures; the arithmetic criterion, on the other hand, classifies general crystals. The examples of 4-lattices discussed in §5 show that this method gives a group-theoretical foothold for classifying periodic structures when the space-group classification fails to do so, and also the method by Fischer & Koch appears inadequate (at least as currently presented in the literature). This is one main reason for pursuing the investigation of the arithmetic framework for multilattice symmetry, which, moreover, seems readily amenable to computerized calculation procedures.[10]

2. Three-dimensional 2-lattices

As mentioned in the *Introduction*, one goal of this paper is to illustrate how to perform the systematic analysis of the arithmetic symmetry of multilattices in a manageable case, that is, for monoatomic 2-lattices. In order to keep the treatment self-contained, we recall some of the notions discussed by Pitteri & Zanzotto (1998) and Fadda & Zanzotto (2000), for brevity referred to hereafter as I and II, where further details can be found.

2.1. Descriptors and configuration spaces of 2-lattices

We use the traditional Grassmann notation for the points and translation vectors in the three-dimensional real affine space $\mathbb{A}^3$, whose origin is denoted by O.

A 2-lattice is an infinite and discrete subset $\mathcal{M}$ of points in $\mathbb{A}^3$, coinciding with the union of two 'affine simple lattices' (also called 1-lattices),

$$\mathcal{M} = \mathcal{M}(\mathbf{e}_a, \mathbf{p}) = \{O + \mathcal{L}(\mathbf{e}_a)\} \bigcup \{O + \mathbf{p} + \mathcal{L}(\mathbf{e}_a)\}. \quad (1)$$

Here $\mathcal{L}(\mathbf{e}_a)$ denotes a simple vector lattice in the translation space $\mathbb{R}^3$ of $\mathbb{A}^3$, generated by the basis $\mathbf{e}_a$, $a = 1, 2, 3$,

$$\mathcal{L}(\mathbf{e}_a) = \{\mathbf{v} \in \mathbb{R}^3 \,:\, \mathbf{v} = v^a \mathbf{e}_a,\ v^a \in \mathbb{Z}\}. \quad (2)$$

In (2) and hereafter, the summation convention over repeated indices will be understood.

Given a 2-lattice $\mathcal{M}$ in $\mathbb{A}^3$, in this paper the origin O is always chosen on a point of $\mathcal{M}$, as is implicit in (1). The vector lattice $\mathcal{L}(\mathbf{e}_a)$ appearing in (2) is called the *skeletal* lattice of $\mathcal{M}$, which gives the 3D periodicity of the 2-lattice $\mathcal{M}$; the basis $\mathbf{e}_a$ and the corresponding unit cell are called the skeletal basis and unit cell of $\mathcal{M}$. The vector

$$\mathbf{p} = p^a \mathbf{e}_a \quad (3)$$

in (1) is called the 'shift vector' or the 'shift' of $\mathcal{M}$: it gives the separation of the two simple lattices constituting $\mathcal{M}$. We call the vectors $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{p})$ the *descriptors* of $\mathcal{M}$. They satisfy the conditions

$$\mathbf{e}_1 \cdot \mathbf{e}_2 \times \mathbf{e}_3 \neq 0 \quad \text{and} \quad \mathbf{p} \neq l^a \mathbf{e}_a, \quad \text{for} \quad l^a \in \mathbb{Z},\ a = 1, 2, 3, \quad (4)$$

which guarantee that the two simple lattices constituting $\mathcal{M}$ are three-dimensional and not coincident. We often denote the 2-lattice descriptors by $\boldsymbol{\varepsilon}_\sigma$, $\sigma = 1, 2, 3, 4$,

$$\boldsymbol{\varepsilon}_a = \mathbf{e}_a, \quad a = 1, 2, 3, \quad \text{and} \quad \boldsymbol{\varepsilon}_4 = \mathbf{p}, \quad (5)$$

and, accordingly, in (1) we write $\mathcal{M} = \mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$.

The set of all 4-tuples of vectors of $\mathbb{R}^4$ satisfying conditions (4) is denoted by $\mathcal{D}_{3,1}$, and is called the space of descriptors, or the *configuration space* of 3D 2-lattices. One studies the structure of this space in order to study the kinematics of deformable 2-lattices.

Let $\mathcal{Q}_4$ denote the ten-dimensional vector space of all symmetric 4×4 real matrices; it is useful to extend to multilattices the usual notion of lattice metric (or 'Gram matrix'), and define the space $\mathcal{Q}_{3,1} \subset \mathcal{Q}_4$ of the *2-lattice metrics* K such that

$$K = (K_{\sigma\tau}), \quad K_{\tau\sigma} = K_{\sigma\tau} = \boldsymbol{\varepsilon}_\sigma \cdot \boldsymbol{\varepsilon}_\tau \quad \text{for} \quad \boldsymbol{\varepsilon}_\sigma \in \mathcal{D}_{3,1} \quad (6)$$

($\sigma, \tau = 1, 2, 3, 4$), where $\boldsymbol{\varepsilon}_\sigma$ satisfy conditions (3)–(5). An element $K \in \mathcal{Q}_{3,1}$ is a 4×4 symmetric matrix which is only positive semi-definite because the vectors $\boldsymbol{\varepsilon}_\sigma$ are not linearly independent in $\mathbb{R}^3$. However, not all the symmetric positive semi-definite matrices belong to $\mathcal{Q}_{3,1}$ because, by definition, $\boldsymbol{\varepsilon}_\sigma$ in (6) must also satisfy conditions (3)–(5). If we define the usual dual basis

$$\mathbf{e}^a = K^{ab} \mathbf{e}_b \quad (K^{ab} K_{bc} = \delta^a_c) \quad (7)$$

of $\mathbf{e}_a$, and express the shift $\mathbf{p}$ as [see (3)]

$$p = p_a \mathbf{e}^a = p^a \mathbf{e}_a, \quad (8)$$

we see that the explicit form of a 2-lattice metric $K \in Q_{3,1}$ defined in (6) is the following:

[9] We remark that here we classify monoatomic 2-lattices independently of Fischer & Koch's principle: our procedure is not a new way of retrieving their results. Only *a posteriori*, through a comparison of the explicit list of the distinct types obtained from the two methods, does one find that they are equivalent for the specific case of monoatomic 2-lattices.

[10] To summarize, the method by Fischer & Koch classifies, by definition, structures that are regular point systems, while the arithmetic criterion classifies any multiregular point systems. It is an open question whether these two independent criteria coincide for regular point systems. This paper shows that the two classifications do coincide for regular point systems with two points in their unit cell.

$$(K_{\sigma\tau}) = (K_{\tau\sigma}) = \left(\begin{array}{c|c} K_{ab} & K_{a4} = p_a = K_{ab}p^b \\ \hline K_{a4} & K_{44} = K_{ab}p^a p^b = p_a p^a \end{array}\right), \quad (9)$$

where, by (4), $p^1,\ p^2, p^3$ are not simultaneously in $\mathbb{Z}$. Clearly, $K_{ab} = \mathbf{e}_a \cdot \mathbf{e}_b$ ($a,\ b = 1, 2, 3$) is but the metric of the skeletal lattice $\mathcal{L}(\mathbf{e}_a)$. Also, by (3), (7), (8), $K_{44} = \|\mathbf{p}\|^2$ in (9) is a rational function of the nine other independent entries of K; thus the space $\mathcal{Q}_{3,1}$ is a nine-dimensional non-linear submanifold of the ten-dimensional vector space $\mathcal{Q}_4$.

It is not difficult to see that, for any two sets of descriptors $\boldsymbol{\varepsilon}_\sigma$ and $\boldsymbol{\varepsilon}'_\sigma$ as in (4)–(6), we have

$$K' = K \quad \Leftrightarrow \quad \boldsymbol{\varepsilon}'_\sigma = \mathbf{Q}\boldsymbol{\varepsilon}_\sigma \quad \text{for some} \quad \mathbf{Q} \in O(3). \quad (10)$$

Since we are often interested in properties that are independent of the orientation of a multilattice in $\mathbb{A}^3$, then owing to (10), also the space of 2-lattice metrics $\mathcal{Q}_{3,1}$ is referred to as the 'configuration space' of 3D 2-lattices.

Remark. The 2-lattices considered so far are, implicitly, 'monoatomic', as mentioned in footnote **3**, in that all their points are physically indistinguishable. However, the considerations above all extend to the 'diatomic' case, in which the two simple lattices constituting the 2-lattice in (1) are made of atoms belonging to two different species. The only change necessary in what follows is that, in the diatomic case, the variable α defined in formula (16) below can only have the value 1, rather than ± 1 as in the monoatomic case. See also point (5) in §4 below and §8 in II for further comments on the classification of diatomic lattices.

2.2. Essential descriptors of monoatomic 2-lattices

Certain descriptors $\boldsymbol{\varepsilon}_\sigma$ of monoatomic 2-lattices actually give a 1-lattice in $\mathbb{A}^3$ (see for instance Fig. 1 in I). Such $\boldsymbol{\varepsilon}_\sigma$ are called *non-essential* descriptors of 1-lattices, and will be avoided hereafter as they give rise to various problems [see Ericksen (1998) and Pitteri & Zanzotto (2001) for further details]. This does not hamper our systematic investigation of the arithmetic types of monoatomic 2-lattices, for no actual 2-lattice is missed if only essential descriptors are considered. Explicitly, in the configuration space $\mathcal{D}_{3,1}$, the non-essential descriptors are as follows:

$$(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{p}) \in \mathcal{D}_{3,1} \text{ is non-essential} \Leftrightarrow \mathbf{p} = \tfrac{1}{2}\beta^a \mathbf{e}_a + \mathbf{t}, \quad (11)$$

where $\mathbf{t} \in \mathcal{L}(\mathbf{e}_a)$ and the numbers β^a are

$$\text{either } (1, 1, 1) \text{ or a permutation of } (1, 1, 0) \text{ or } (1, 0, 0) \quad (12)$$

[also recall conditions $(4)_2$ on the shift $\mathbf{p}$].

In our analysis, we confine ourselves to the portions of the configuration spaces of 2-lattices that only contain essential descriptors not satisfying (11)–(12), thus generating monoatomic 2-lattices which are *not* 1-lattices. Explicitly, we consider

$$\mathcal{D}^{\text{ess}}_{3,1} = \left\{(\mathbf{e}_a, \mathbf{p}) \in \mathcal{D}_{3,1} \,:\, \mathbf{p} \neq \tfrac{1}{2}\beta^a \mathbf{e}_a + \mathbf{t},\ \ \beta^a \text{ as in (12)}\right\} \subset \mathcal{D}_{3,1}, \quad (13)$$

and

$$\mathcal{Q}^{\text{ess}}_{3,1} = \left\{K \in \mathcal{Q}_{3,1} \,:\, K_{\sigma\tau} = \boldsymbol{\varepsilon}_\sigma \cdot \boldsymbol{\varepsilon}_\tau,\ \boldsymbol{\varepsilon}_\sigma \in \mathcal{D}^{\text{ess}}_{3,1}\right\} \subset \mathcal{Q}_{3,1}. \quad (14)$$

For brevity, also the spaces $\mathcal{D}^{\text{ess}}_{3,1}$ and $\mathcal{Q}^{\text{ess}}_{3,1}$ are referred to as the 'configuration spaces' of 2-lattices.

2.3. The global symmetry group of monoatomic 2-lattices and its action on the configuration spaces

As discussed in I and by Pitteri & Zanzotto (2001), the group of operations describing the general indeterminacy in the choice of multilattice descriptors is the basis for the study of their arithmetic classification; this generalizes the classical procedure used for simple lattices. The indeterminacy in the choice of the essential descriptors of 2-lattices leads to considering the following arithmetic 'global symmetry' group (see Pitteri, 1985),

$$\Gamma_{3,1} < GL(4, \mathbb{Z}), \quad (15)$$

constituted by the unimodular integral 4×4 matrices with the following structure: for $a, b = 1, 2, 3$,

$$\mu \in \Gamma_{3,1} \Leftrightarrow \mu^\tau_\sigma = \left(\begin{array}{ccc|c} & m^b_a & & l^1 \\ & & & l^2 \\ & & & l^3 \\ \hline 0 & 0 & 0 & \alpha \end{array}\right), \quad (16)$$

where (m^b_a) is any matrix in $GL(3, \mathbb{Z})$, $l^b \in \mathbb{Z}$, and $\alpha = \pm 1$ (recall the *Remark* at the end of §2.2).[11]

The structure of the matrices $\mu \in \Gamma_{3,1}$ is justified by Proposition 3 in I, which we recall here for the 2-lattice case:

Proposition 1. Let $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$ be a monoatomic 2-lattice in an essential description. Then $\bar{\boldsymbol{\varepsilon}}_\sigma$ are new essential descriptors for $\mathcal{M}$ up to a translation [that is, $\mathcal{M}(\bar{\boldsymbol{\varepsilon}}_\sigma) = \mathcal{M}(\boldsymbol{\varepsilon}_\sigma) + \mathbf{t}, \mathbf{t} \in \mathbb{R}^3$] if and only if there exists a matrix $\mu \in \Gamma_{3,1}$ such that

$$\bar{\boldsymbol{\varepsilon}}_\sigma = \mu^\tau_\sigma \boldsymbol{\varepsilon}_\tau, \quad \mu \in \Gamma_{3,1}, \quad (17)$$

The matrix $\mu \in \Gamma_{3,1}$ determines uniquely the new descriptors $\bar{\boldsymbol{\varepsilon}}_\sigma$ and *vice versa*.[12]

Owing to (16) and (17), the new lattice basis and shift are given explicitly by

$$\bar{\mathbf{e}}_a = m^b_a \mathbf{e}_b, \qquad \bar{\mathbf{p}} = \alpha\,\mathbf{p} + l^a \mathbf{e}_a, \quad (18)$$

where $(m^b_a) \in GL(3, \mathbb{Z})$, $l^a \in \mathbb{Z}$ and $\alpha = \pm 1$.

Proposition 1 shows that the essential descriptors $\boldsymbol{\varepsilon}_\sigma \in \mathcal{D}^{\text{ess}}_{3,1}$ of a 2-lattice transform by means of a matrix in $\Gamma_{3,1}$, and that the changes of essential descriptors are in a one-to-one correspondence with such matrices. For this reason, we refer

[11] For more general multilattices, with n atoms in their unit cells, the relevant group is a subgroup of $GL(n + 2, \mathbb{Z})$; see I or §5 below.

[12] Since the vectors $\boldsymbol{\varepsilon}_\sigma$, $\sigma = 1, 2, 3, 4$, are not linearly independent, there are infinitely many 4×4 matrices relating them to the vectors $\bar{\boldsymbol{\varepsilon}}_\sigma$. Proposition 1 states that, when $\boldsymbol{\varepsilon}_\sigma$ and $\bar{\boldsymbol{\varepsilon}}_\sigma$ are essential, there is always one and only one such matrix in the group $\Gamma_{3,1}$.

to $\Gamma_{3,1}$ as the global symmetry group of monoatomic 2-lattices in 3D.

A change of descriptors as in (17) induces, in obvious notation, the following transformation of the multilattice metric K in (6),

$$\bar{K} = \mu^T K \mu, \tag{19}$$

where, in general, $\bar{K} \neq K$.[13] Formulae (17) and (19) give natural actions of the group $\Gamma_{3,1}$ on the configuration spaces $\mathcal{D}^{\rm ess}_{3,1}$ and $\mathcal{Q}^{\rm ess}_{3,1}$; for instance, the orbit of a given $K \in \mathcal{Q}^{\rm ess}_{3,1}$ under $\Gamma_{3,1}$ is the set

$$\left\{\mu^T K \mu,\, \mu \in \Gamma_{3,1}\right\} \subset \mathcal{Q}^{\rm ess}_{3,1}. \tag{20}$$

Based on these actions the arithmetic symmetry of 2-lattices is studied; regarding this, we explicitly recall that the action (19) of $\Gamma_{3,1}$ on $\mathcal{Q}^{\rm ess}_{3,1}$ generalizes to 2-lattices the usual action

$$C \mapsto m^T C m, \quad C \in \mathcal{C}^+(\mathcal{Q}_3), \quad m \in GL(3,\mathbb{Z}), \tag{21}$$

considered in crystallography for classifying the arithmetic symmetry of *simple* lattices (that is, 1-lattices). In (21), the symbol $\mathcal{C}^+(\mathcal{Q}_3)$ indicates the set (a cone) of 3×3 positive definite symmetric matrices (1-lattice metrics).

2.4. Lattice groups, point groups and arithmetic types of 2-lattices

As for 1-lattices, the arithmetic classification of 2-lattice symmetry is based on the analysis of the subgroups of $\Gamma_{3,1}$ that act *isometrically* on some 2-lattice [or, equivalently, that stabilize some 2-lattice metric under the action (19)], and that are maximal for this property. Therefore, the main focus in what follows is establishing the conjugacy properties of the subgroups of matrices $\mu \in \Gamma_{3,1}$ for which the equation

$$\mu^T K \mu = K \tag{22}$$

holds for some $K \in \mathcal{Q}^{\rm ess}_{3,1}$; as we shall see, such groups are necessarily finite.

To be precise, let $\boldsymbol{\varepsilon}_\sigma \in \mathcal{D}^{\rm ess}_{3,1}$ with metric $K \in \mathcal{Q}^{\rm ess}_{3,1}$ be given; we define the *lattice group* $\Lambda(\boldsymbol{\varepsilon}_\sigma)$ of the 2-lattice $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$,

$$\Lambda(\boldsymbol{\varepsilon}_\sigma) < \Gamma_{3,1} < GL(4,\mathbb{Z}), \tag{23}$$

as the subgroup of all the integral matrices $\mu \in \Gamma_{3,1}$ such that

$$\begin{aligned}\Lambda(\boldsymbol{\varepsilon}_\sigma) &= \left\{\mu \in \Gamma_{3,1} \,:\, \mu^\tau_\sigma \boldsymbol{\varepsilon}_\tau = \mathbf{Q}\boldsymbol{\varepsilon}_\sigma,\ \mathbf{Q} \in O(3)\right\} \\ &= \left\{\mu \in \Gamma_{3,1} \,:\, \mu^T K \mu = K\right\} \\ &= \Lambda(K).\end{aligned} \tag{24}$$

By (10), for $\boldsymbol{\varepsilon}_\sigma \in \mathcal{D}^{\rm ess}_{3,1}$ with metric K, the following holds:

$$\mu^T K \mu = K \quad \Leftrightarrow \quad \mu^\tau_\sigma \boldsymbol{\varepsilon}_\tau = \mathbf{Q}\boldsymbol{\varepsilon}_\sigma \quad \text{for some} \quad \mathbf{Q} \in O(3). \tag{25}$$

Thus, $(24)_2$ above holds, and the lattice group $\Lambda(\boldsymbol{\varepsilon}_\sigma)$ is also denoted $\Lambda(K)$ as in $(24)_3$, for it depends only on the metric K of the descriptors $\boldsymbol{\varepsilon}_\sigma$. This also means that, given any $\boldsymbol{\varepsilon}_\sigma \in \mathcal{D}^{\rm ess}_{3,1}$,

$$\Lambda(\mathbf{Q}\boldsymbol{\varepsilon}_\sigma) = \boldsymbol{\Lambda}(\boldsymbol{\varepsilon}_\sigma) \quad \text{for all} \quad \mathbf{Q} \in O(3), \tag{26}$$

that is, the lattice group is independent of the orientation of the 2-lattice in $\mathbb{A}^3$.

By (24), under a change of descriptors $\bar{\boldsymbol{\varepsilon}}_\sigma = \mu^\tau_\sigma \boldsymbol{\varepsilon}_\tau$ for the 2-lattice $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$ as in (17), the lattice group transforms as follows:

$$\Lambda(\mu^\tau_\sigma \boldsymbol{\varepsilon}_\tau) = \mu^{-1}\Lambda(\boldsymbol{\varepsilon}_\sigma)\mu \quad \text{for all} \quad \mu \in \Gamma_{3,1}. \tag{27}$$

Proposition 1 and formula (27) state that any given 2-lattice $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$ determines an entire *conjugacy class* of lattice groups in $\Gamma_{3,1}$. This is completely analogous to the case of 1-lattices and, as for the latter, we define two 2-lattices $\mathcal{M}$ and $\mathcal{M}'$ to be of the same *arithmetic type* when their lattice groups are $\Gamma_{3,1}$-conjugate. We also say that two metrics K and K' (or two sets of descriptors $\boldsymbol{\varepsilon}_\sigma$ and $\boldsymbol{\varepsilon}'_\sigma$) are of the same arithmetic type when their lattice groups are conjugate in $\Gamma_{3,1}$. This generates a subdivision of $\mathcal{Q}^{\rm ess}_{3,1}$ into equivalence classes [the 'strata' of the action (19)], which are called the arithmetic types within $\mathcal{Q}^{\rm ess}_{3,1}$ (analogously for $\mathcal{D}^{\rm ess}_{3,1}$). We shall thus determine and study the properties of all the conjugacy classes of lattice groups in $\Gamma_{3,1}$ in order to obtain a description of the 'arithmetic symmetry types' of 2-lattices in 3D. An analog of the subdivision into Bravais types that is classical for 3D simple lattices is produced in this way.[14]

To find the lattice groups in $\Gamma_{3,1}$, it will be more convenient to analyze, rather than (22), the equations

$$\mathbf{Q}\mathbf{e}_a = m^b_a \mathbf{e}_b, \qquad \mathbf{Q}\mathbf{p} = \alpha\,\mathbf{p} + l^a \mathbf{e}_a \tag{28}$$

for $(\mathbf{e}_a, \mathbf{p}) \in \mathcal{D}^{\rm ess}_{3,1}$, $\mathbf{Q} \in O(3)$, $\alpha = \pm 1$, $l^a \in \mathbb{Z}$. By (5), (6), (16), (18) and (25), conditions (28) are equivalent to (22).

Given a 2-lattice $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$, with $\boldsymbol{\varepsilon}_\sigma = (\mathbf{e}_a, \mathbf{p})$, the operations $\mathbf{Q} \in O(3)$ that solve $(28)_1$ for some $\mathbf{e}_a$ and $m \in GL(3,\mathbb{Z})$ belong, by definition, to the (holohedral) point group $P(\mathbf{e}_a)$ of the skeletal lattice $\mathcal{L}(\mathbf{e}_a)$; the skeletal lattice group $L(\mathbf{e}_a)$ collects the corresponding matrices $m \in GL(3,\mathbb{Z})$ (see I). The operations $\mathbf{Q} \in O(3)$ satisfying *both* the equations in (28) belong by definition to the point group $P(\boldsymbol{\varepsilon}_\sigma)$ of the 2-lattice $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$. In general, the skeletal point group $P(\mathbf{e}_a)$ is thus larger than the multilattice point group $P(\boldsymbol{\varepsilon}_\sigma)$, as is well known and, as is easily seen since the operations in $P(\boldsymbol{\varepsilon}_\sigma)$, must also solve equation $(28)_2$ (see also §2.5).

We recall (see I) that the lattice group $\Lambda(\boldsymbol{\varepsilon}_\sigma)$ is isomorphic to the point group $P(\boldsymbol{\varepsilon}_\sigma)$ of $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$, and is thus necessarily finite. However, $\Lambda(\boldsymbol{\varepsilon}_\sigma)$ carries more information than $P(\boldsymbol{\varepsilon}_\sigma)$: indeed, unlike with the point group, given the group of matrices $\Lambda(\boldsymbol{\varepsilon}_\sigma)$ it is possible to reconstruct uniquely the space group of $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$ (see Proposition 5 in I). This, together with the example in Appendix *A* of I, shows that the arithmetic symmetry of multilattices gives in general a finer classification than their space-group symmetry.

[13] As usual, μ^T denotes the transpose of any matrix μ.

[14] The classical 14 Bravais types in three dimensions, recalled in the *Introduction*, are indeed obtained by considering the conjugacy classes of lattice groups of simple lattices ('arithmetic holohedries') within $GL(3,\mathbb{Z})$.

2.5. The Bravais type of a multilattice; excess skeletal symmetry

Given a 2-lattice $\mathcal{M}$, its lattice group $\Lambda < \Gamma_{3,1}$ determines a group $C_\Lambda < GL(3,\mathbb{Z})$, which is the subgroup of $GL(3,\mathbb{Z})$ containing the matrices m in the upper left corner of the matrices $\mu \in \Lambda$ [see formula (16)]. The group C_Λ determines the *arithmetic class* of $\mathcal{M}$ (and of Λ); this in turn determines uniquely a minimal lattice group L_Λ containing C_Λ.[15] The group L_Λ selects a Bravais lattice type, which we define to be 'the Bravais type' of $\mathcal{M}$ and of its lattice group Λ.[16] It is important to remark that some of the 2-lattices whose lattice group is Λ may have skeletal lattice (2) whose lattice group $L' < GL(3,\mathbb{Z})$ is *larger* than L_Λ. However, this does not increase the multilattice symmetry Λ, and for this reason in these cases we speak of 'excess skeletal symmetry'. It can be seen that excess skeletal symmetry occurs only on lower-dimensional submanifolds of $I(\Lambda)$ which are *not* themselves fixed sets of any lattice group Λ' larger than Λ.[17] These submanifolds often appear in the solutions of equation $(28)_2$, and one must be aware of the fact that they do not contribute to the description of the arithmetic types in the configuration spaces of multilattices; see Appendix *B*4 for an example.

3. Some lemmas useful in the analysis of 2-lattices

In this section, we give some results that establish a rapid procedure for determining the arithmetic types of monoatomic 2-lattices (see Appendix *A* for proofs).

We are interested in describing 'enough' (but not 'too many') groups of solutions to equation (22) for suitable metrics K in $\mathcal{Q}^{\rm ess}_{3,1}$, or, equivalently, 'enough' solutions to equations (25) or (28) for suitable $\boldsymbol{\varepsilon}_\sigma \in \mathcal{D}^{\rm ess}_{3,1}$, with $\mathbf{Q} \in O(3)$ and $\mu \in \Gamma_{3,1}$, that is, with $\alpha = \pm 1$, $m \in GL(3,\mathbb{Z})$, $l^a \in \mathbb{Z}$. In fact, in order to establish the arithmetic types in $\mathcal{D}^{\rm ess}_{3,1}$ or $\mathcal{Q}^{\rm ess}_{3,1}$, we only need to determine enough solutions of (28) so as to expose all the equivalence classes of lattice groups in $\Gamma_{3,1}$. Lemmas 2 and 3 below tell us explicitly which $(\mathbf{e}_a, \mathbf{p})$ need to be tested in (28) in order to obtain the necessary information; all other $\boldsymbol{\varepsilon}_\sigma \in \mathcal{D}^{\rm ess}_{3,1}$ produce conjugate lattice groups that do not affect the determination of the arithmetic types.

The following lemma cuts in half the lattice group computations deriving from equations (28). As $-1 \equiv {\rm diag}(-1,-1,-1,-1) \in \Gamma_{3,1}$, necessarily all monoatomic 2-lattices are centrosymmetric, and since -1 trivially solves equation (22) for all $K \in \mathcal{Q}^{\rm ess}_{3,1}$, we have:

Lemma 1. The lattice groups (24) of monoatomic 2-lattices all contain the matrix $-1 \in \Gamma_{3,1}$. Thus for all $K \in \mathcal{Q}^{\rm ess}_{3,1}$, it follows that

$$\Lambda(K) = \Lambda^+(K) \cup -\Lambda^+(K), \tag{29}$$

where $\Lambda^+(K)$ is the subgroup of matrices μ in $\Lambda(K)$ such that $\alpha = 1$ [see (16)].

Because of this special property of 2-lattices, we only need to determine explicitly the matrices in the subgroup $\Lambda^+(K)$ of any lattice group, that is, we need to check (25) or $(28)_2$ only for $\alpha = 1$.[18] Any solution $(\mathbf{Q}, l^a)$ of $(28)_2$ found for a given $\mathbf{p}$ and $\alpha = 1$ then generates another solution $(-\mathbf{Q}, -l^a)$ for the same $\mathbf{p}$ and $\alpha = -1$ [notice that, given $\mathbf{p}$, $\mathbf{Q}$ solves $(28)_2$ if and only if $-\mathbf{Q}$ does].

Lemma 2. Let a basis $\mathbf{e}_a$ be given; let $\boldsymbol{\varepsilon}_\sigma = (\tilde{\mathbf{e}}_a, \mathbf{p})$ and the matrices $\mu \in \Lambda(\tilde{\mathbf{e}}_a, \mathbf{p})$ be any solution of (28), and suppose that $\tilde{\mathbf{e}}_a = \tilde{m}^b_a \mathbf{e}_b$ for some $\tilde{m} \in GL(3,\mathbb{Z})$, *i.e.* let $\mathbf{e}_a$ and $\tilde{\mathbf{e}}_a$ give the same skeletal lattice. Then the descriptors $(\tilde{\mathbf{e}}_a, \mathbf{p})$ and $(\mathbf{e}_a, \mathbf{p})$ generate the same 2-lattice in $\mathbb{A}^3$ up to a translation, so that the lattice groups $\Lambda(\tilde{\mathbf{e}}_a, \mathbf{p})$ and $\Lambda(\mathbf{e}_a, \mathbf{p})$ are $\Gamma_{3,1}$-conjugate.

This lemma and the independence (26) of the lattice group from the orientation of a multilattice tell us that in order to determine the arithmetic types in $\mathcal{D}^{\rm ess}_{3,1}$ we only need to test equation (28) for descriptors $\boldsymbol{\varepsilon}_\sigma = (\mathbf{e}_a, \mathbf{p})$ such that $\mathbf{e}_a$ belongs to a pre-fixed set of 14 bases generating the skeletal lattices of the 14 distinct Bravais types. When possible, the bases chosen in our computations coincide with the 'conventional' ones used in *International Tables for Crystallography* (1996).[19]

Once a basis $\mathbf{e}_a$ is chosen for the skeletal type of the 2-lattice that is being investigated, equation $(28)_1$ is solved through classical computations that produce the group of integral matrices leaving the skeletal simple lattice invariant. This gives the skeletal lattice group $L(\mathbf{e}_a)$ (see the end of §2.4) and, correspondingly, the group of orthogonal operations constituting the skeletal point group $P(\mathbf{e}_a)$ [see below formula (28) and the example in formula (49)]. As these groups are known, one then checks equation $(28)_2$ for $\alpha = 1$ and $\mathbf{Q} \in P(\mathbf{e}_a)$.

In principle, given a basis $\mathbf{e}_a$, one should still check in equation $(28)_2$ descriptors $(\mathbf{e}_a, \mathbf{p})$ with a shift vector $\mathbf{p}$ variable in an unbounded subset of $\mathbb{R}^3$, *i.e.* for all $\mathbf{p}$ except for the exclusions in (13). However, the fact that we only need to determine the lattice groups up to $\Gamma_{3,1}$-conjugacy restricts the descriptors $\boldsymbol{\varepsilon}_\sigma$ that need to be considered to the $\boldsymbol{\varepsilon}_\sigma = (\mathbf{e}_a, \mathbf{p})$

[15] Unlike with 1-lattices, multilattices can realize non-holohedral lattice groups and point groups, that is, it can be $C_\Lambda \not\leq L_\Lambda$ (see for instance type number 25 in Table 1).

[16] In *International Tables for Crystallography* (1996), this definition is given directly for the space groups; as our lattice group Λ determines the space group, our definition is equivalent.

[17] These submanifolds of $I(\Lambda)$ are not fixed sets in $\mathcal{Q}^{\rm ess}_{3,1}$ but their projections on the subspace $\langle K_{11}, K_{12}, \ldots, K_{33}\rangle \simeq \mathcal{C}^+(\mathcal{Q}_3)$ are fixed sets for the simple-lattice action (21). As recalled in II, there is the prejudice that, physically, excess skeletal symmetry should not be a stable feature of a multilattice (see for instance Landau & Lifshitz, 1959, §130).

[18] We notice that if an operation $\mathbf{Q}$ of the point group $P(\boldsymbol{\varepsilon}_\sigma)$ corresponds, through equation (25) or (28), to a matrix $\mu \in \Lambda^+(\boldsymbol{\varepsilon}_\sigma)$, then, with the choice made in (1) for the origin O, the operation $(\mathbf{Q}|\mathbf{0})$ belongs to the space group $\mathcal{S}[\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)]$ of the 2-lattice $\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)$. However, the operation $-\mathbf{Q}$, corresponding to the matrix $-\mu \in -\Lambda^+(\boldsymbol{\varepsilon}_\sigma)$, gives the affine operation $(-\mathbf{Q}|\mathbf{p}) \in \mathcal{S}[\mathcal{M}(\boldsymbol{\varepsilon}_\sigma)]$, which involves also a translation $\mathbf{p}$. For instance, the fact that 2-lattices are always centrosymmetric means that in their space groups there is always the operation $(-\mathbf{1}|\mathbf{p})$.

[19] For the centered types of skeletal lattices, *International Tables for Crystallography* (1996) utilize a conventional non-unit cell that is not suitable for the computations related to equation (28), which need an actual skeletal basis.

whose $\mathbf{p}$ varies only in a *bounded* domain in $\mathbb{R}^3$. This is due to the following lemma [recall the definition (2) of $\mathcal{L}(\mathbf{e}_a)$]:

Lemma 3. Given any $(\mathbf{e}_a, \tilde{\mathbf{p}}) \in \mathcal{D}^{\rm ess}_{3,1}$, there exists a bounded domain $\mathcal{A}(\mathbf{e}_a) \subset \mathbb{R}^3$ such that

$$\tilde{\mathbf{p}} = \mathbf{Q}\,\mathbf{p} + \mathbf{t}, \tag{30}$$

where $\mathbf{p} \in \mathcal{A}(\mathbf{e}_a)$, $\mathbf{Q} \in P(\mathbf{e}_a)$ and $\mathbf{t} \in \mathcal{L}(\mathbf{e}_a)$; the lattice group $\Lambda(\mathbf{e}_a, \tilde{\mathbf{p}})$ is $\Gamma_{3,1}$-conjugate to the lattice group $\Lambda(\mathbf{e}_a, \mathbf{p})$. The domain $\mathcal{A}(\mathbf{e}_a)$ can be chosen to be the 'asymmetric unit' of the (unique) space group that is symmorphic and realizes the holohedry $P(\mathbf{e}_a)$.[20]

To summarize, Lemmas 2 and 3 tell us that, in order to find the $\Gamma_{3,1}$-conjugacy classes of the lattice groups arising from equations (28), one only needs to consider the lattice groups obtained from the analysis of (28) for descriptors $\boldsymbol{\varepsilon}_\sigma = (\mathbf{e}_a, \mathbf{p})$ such that: (*a*) the basis $\mathbf{e}_a$ is any given basis for one of the 14 types of Bravais lattices; (*b*) the shift $\mathbf{p}$ is in the asymmetric unit $\mathcal{A}(\mathbf{e}_a)$ of the holohedral symmorphic space group related to the basis $\mathbf{e}_a$. The lattice groups of any descriptors not satisfying properties (*a*) and (*b*) are necessarily conjugate to some lattice group of descriptors that do, and consequently the former do not add any information for the purposes of determining the distinct arithmetic types of 2-lattices.

Owing to the next two propositions, we shall be able to utilize some further information contained in *International Tables for Crystallography* (1996):

Lemma 4. Given a basis $\mathbf{e}_a$ and a shift vector $\mathbf{p} \in \mathcal{A}(\mathbf{e}_a)$, the descriptors $\boldsymbol{\varepsilon}_\sigma = (\mathbf{e}_a, \mathbf{p})$ that solve $(28)_2$ for $\mathbf{Q} \in P(\mathbf{e}_a)$, $l^a \in \mathbb{Z}$ and $\alpha = 1$, are those for which $\mathbf{p}$ belongs to a 'special Wyckoff position' in $\mathcal{A}(\mathbf{e}_a)$ whose site-symmetry contains $\mathbf{Q}$.

Indeed, by definition, from the Wyckoff positions listed in *International Tables for Crystallography* (1996), one only obtains the elements of $\Lambda^+(\mathbf{e}_a, \mathbf{p})$. To $\Lambda^+(\mathbf{e}_a, \mathbf{p})$ we must then add all the elements of $-\Lambda^+(\mathbf{e}_a, \mathbf{p})$, as indicated by Lemma 1, to obtain the full lattice group of $(\mathbf{e}_a, \mathbf{p})$.

Now, given a basis $\mathbf{e}_a$ and the solutions $m \in L(\mathbf{e}_a)$ to equation $(28)_1$, we want to establish which lattice groups in $\Lambda < \Gamma_{3,1}$, if any, have the Bravais type of $\mathbf{e}_a$, according to the definition given in §2.5. For many $\mathbf{p} \in \mathcal{A}(\mathbf{e}_a)$, the solutions $\mathbf{Q}$ obtained from Lemma 4 are actually too few, that is, they give a (non-holohedral) point group that pertains to a holohedry smaller than $P(\mathbf{e}_a)$.[21] The following corollary makes this more precise, by indicating which special Wyckoff positions $\mathbf{p}$ give lattice groups $\Lambda(\mathbf{e}_a, \mathbf{p})$ whose Bravais type is exactly that of $\mathbf{e}_a$:

Corollary 1. Let a basis $\mathbf{e}_a$ (and thus a Bravais type) be given, and let $\boldsymbol{\varepsilon}_\sigma = (\mathbf{e}_a, \mathbf{p}) \in \mathcal{D}^{\rm ess}_{3,1}$, with $\mathbf{p} \in \mathcal{A}(\mathbf{e}_a)$ and such that the exclusions in (13) hold. The lattice groups $\Lambda(\mathbf{e}_a, \mathbf{p})$ whose Bravais type is that of $\mathbf{e}_a$ are given by the solutions to $(28)_2$ derived[22] from the special Wyckoff positions in $\mathcal{A}(\mathbf{e}_a)$ whose site-symmetry group has the following properties: either

(*a*) it has index 2 in $P(\mathbf{e}_a)$ and it does not contain $-\mathbf{1}$; or

(*b*) it has index 4 in $P(\mathbf{e}_a)$, it does not contain $-\mathbf{1}$, and it realizes, with $-\mathbf{1}$, a non-holohedral Laue group in $P(\mathbf{e}_a)$.[23]

In Appendix *B*, we consider an explicit example of how the results above are used in the determination of the arithmetic types of 2-lattices with a body-centered orthorhombic skeletal type. We recall, as in footnote **19**, that, for the centered skeletal types, *International Tables for Crystallography* (1996) utilize conventional cells that are not of unit volume. In these cases, the listed 'multiplicity' of a special Wyckoff position does not coincide with the index of its site-symmetry group within the point group, but is a multiple of the index through a factor f that depends on the volume of the conventional cell ($f = 2, 2, 4$, for base-, body- and face-centered lattices, respectively).

4. The 29 arithmetic types of monoatomic 2-lattices

The analysis of the solutions to equations (28) based on the results of the previous section shows that there exist 29 conjugacy classes of lattice groups in $\Gamma_{3,1}$, and thus 29 distinct monoatomic 2-lattice types. In Table 1, we give the Bravais type, the space group and the position of the extra atom in the unit cell, for each of the 29 2-lattice types, indicating also any *Strukturberichte* and examples of real materials known to assume these crystal structures. We refer to Fadda & Zanzotto (2001) for the illustration of their cells.

Some comments may be useful regarding the above result.

(1) From Table 1, one can easily establish the number of free parameters pertaining to each 2-lattice type, a generic change of which does not affect the arithmetic symmetry. This allows one to derive the sets of 'symmetry-preserving deformations' that are possible for each type.

(2) Given a simple lattice, at each point of which is placed an atom, there may or may not correspondingly exist (a number of) distinct types of monoatomic 2-lattices. These correspond to all the inequivalent ways of putting an extra atom in the unit cell of the given simple lattice. For instance, there are four 2-lattice types, numbered (25) to (28) in Table 1, that have hexagonal Bravais type; types number (26)–(28) originate from three inequivalent ways of placing extra hexagonal nets of points in a hexagonal 1-lattice so as to maintain a sixfold axis [type (27), for the correct 'c/a ratio', gives the well known h.c.p. structure]. The 2-lattice type

[20] This is the space group of the affine 1-lattice $O + \mathcal{L}(\mathbf{e}_a)$, whose point group is isomorphic to the holohedry $P(\mathbf{e}_a)$ (see §2.4). Of course there are 14 such groups (one for each Bravais type) with their corresponding asymmetric units, indicated explicitly in *International Tables for Crystallography* (1996). That the domain $\mathcal{A}(\mathbf{e}_a)$ in this lemma is bounded comes from the fact that $\mathcal{A}(\mathbf{e}_a)$ is a special case of a 'fundamental domain' for a space-group action on $\mathbb{R}^3$. See Appendix *B* for an example.

[21] Indeed, only 'a few' of the positions $\mathbf{p}$ in $A(\mathbf{e}_a)$ give the correct Bravais type (see Corollary 1 below). The other positions produce smaller lattice groups in $\Gamma_{3,1}$, for which $\mathbf{e}_a$ is a cell having excess symmetry; such positions are consequently not relevant. An example is given in Appendix *B*4.

[22] Recall the comment below Lemma 4.

[23] Hence, in the cubic case the site symmetry must contain four threefold operations; in the tetragonal case, it must contain a fourfold operation; in the hexagonal case it must either contain a sixfold operation or a threefold operation; in the rhombohedral case, it must contain a threefold operation. Alternative (*a*) in Corollary 1 gives the holohedral 2-lattices; alternative (*b*) gives the non-holohedral 2-lattices, and only occurs once; see point (2) in §4.

number 25, on the other hand, is produced by placing the extra hexagonal net within the original lattice in such a way that the sixfold axis is no longer present in the resulting structure. This 2-lattice type is non-holohedral, as it realizes the class $\bar{3}m$ in the holohedry $6/m\,2/m\,2/m$; it is a 2-lattice of trigonal class with a hexagonal Bravais type. This is the only non-holohedral type among the 29, falling into case (*b*) of Corollary 1, applied to the Wyckoff position 4(*h*) of the space group $P\,6/m\,2/m\,2/m$. We show the hexagonal cells of these four 2-lattice types in Fig. 1. Another example worth mentioning is, for instance, the 2-lattice type number (29), which is the only one that has cubic symmetry. The skeleton is face-centered cubic with the extra atom placed at coordinate $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ in the conventional f.c.c. cell; the further atomic positions in the conventional cell, which are obtained, as usual, through the face-centering vectors, are $(\frac{1}{4},\frac{3}{4},\frac{3}{4})$, $(\frac{3}{4},\frac{3}{4},\frac{1}{4})$ and $(\frac{3}{4},\frac{1}{4},\frac{3}{4})$. The resulting monoatomic 2-lattice gives the structure of diamond, well known in crystallography. For the two other cubic Bravais types (primitive and body-centered), no 2-lattice type exists. Indeed, no shift vectors can solve equation $(28)_2$ with cubic lattice groups in $\Gamma_{3,1}$: any 2-lattice with a primitive or a body-centered cubic skeleton exhibits excess skeletal symmetry.

(3) About 270 crystalline allotropes of the elements have been reported in the literature (see Table 1 for some references). Not all the 29 distinct 2-lattice types that we list are observed in nature (the same is true for the 14 Bravais types of simple lattices, only five of which are actually observed in the elements). Our list does, however, include all the eight 2-lattice crystal structures observed in the elements so far. These are given by the five *Strukturberichte* that are monoatomic 2-lattices,[24] plus two other 2-lattice configurations not included in the *Strukturberichte* (observed in Pu, O and Bi); the 2-lattice structure proposed by Boyer *et al.* (1991) as a low-energy metastable form of Si, named 'bct5' (body-centered tetragonal with a fivefold coordination), is also accounted for (see Table 1 for details and references).

(4) Relevant information for the theory of phase transitions in complex crystalline structures is obtained from the knowledge of the symmetry hierarchies (group–subgroup relations and partial ordering of the conjugacy classes in $\Gamma_{3,1}$), giving all the possibilities for symmetry breaking and transformation twinning that exist for monoatomic 2-lattices. We establish this in Fadda & Zanzotto (2001); the analogous information for 1-lattices can be found in Zanzotto (1996) or Pitteri & Zanzotto (2001). There is also the problem of 'merging' the descriptions of the kinematics of deformable 2-lattices with that of 1-lattices, which we have kept distinct so far by considering only the 'essential part' $\mathcal{D}^{\rm ess}_{3,1}$ of the space $\mathcal{D}_{3,1}$ (see §2.2).[25]

(5) The results obtained in this paper about the arithmetic types of monoatomic 2-lattices in 3D carry through to the *diatomic* case, provided we only consider matrices μ with $\alpha = 1$, rather than $\alpha = \pm 1$, in (15)–(16) and in all the ensuing lattice groups. Remark, however, that this is not sufficient to classify completely the arithmetic types of diatomic 2-lattices. The reason is that the 'non-essential' positions of the shift **p** when $\boldsymbol{\varepsilon}_\sigma \in \mathcal{D}_{3,1}\backslash\mathcal{D}^{\rm ess}_{3,1}$ cannot be excluded in the diatomic case, as they give rise to admissible diatomic 2-lattices, which also need an appropriate analysis.

5. Examples of monoatomic 4-lattices

The previous analysis regards the simplest case of monoatomic 2-lattices, for which we give the complete arithmetic classification. A systematic study of more complex structures proves computationally challenging, although in principle the procedure in its broad lines is the same as the one for 2-lattices. In this section, we give some examples to show how the arithmetic criterion is applied to 4-lattices. This is especially interesting because *n*-lattices, unlike 2-lattices, are not in general constituted by a single crystallographic orbit (they are multiregular point systems and not regular point systems in the affine space – see footnote **8**). This case shows how the arithmetic criterion treats structures that cannot immediately be analyzed by means of the lattice complexes by Fischer & Koch (Koch & Fischer, 1975; Fischer & Koch, 1996) (recall §1.3).

We refer to I for the notation and general concepts regarding the arithmetic symmetry of *n*-lattices. The reader can derive most of such notions from those given in §2 for the case $n = 2$, by extending the number of shift vectors to three. This is because, as in (1), we conventionally assume a lattice point to coincide with the origin of the affine space, so that three vectors are needed to give the positions of the three further points in the unit cell of a 4-lattice. So, for the latter, the multilattice descriptors in (5) are given by the vectors $\boldsymbol{\varepsilon}_\sigma$, $\sigma = 1, \ldots, 6$,

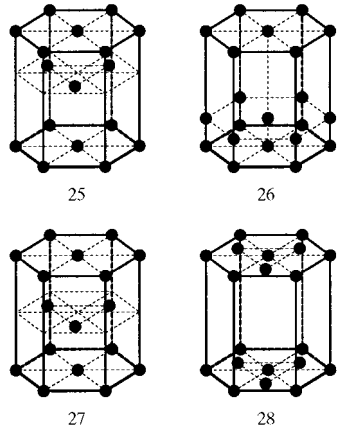

Figure 1
The four arithmetic types of monoatomic 2-lattices with hexagonal Bravais type. The numbering is as in Table 1. Type number 27 gives the h.c.p. structure (*A*3).

[24] Out of the roughly one hundred *Strukturberichte* usually considered (see *Strukturberichte*, 1913–1940), 27 are monoatomic and, among the latter, six are 1-lattices and five, which are all included in our list of 29, are 2-lattices. The latter comprise for instance the well known structures of α-U, of diamond, of the h.c.p. metals *etc.*; see Table 1.

[25] This is an interesting point because, as is well known, many crystalline materials undergo phase transitions from 1- to 2-lattice structures and *vice versa*, such as the h.c.p. $\leftrightarrow$ b.c.c. or h.c.p. $\leftrightarrow$ f.c.c. transitions (see for instance Nishiyama *et al.*, 1978).

Table 1
The 29 arithmetic types of monoatomic 2-lattices in three dimensions.

Examples of elemental crystals are taken from Donohue (1982), *CRC Handbook of Chemistry and Physics* (2000), Pearson (1958), Smithells (1949), Villars & Calvert (1991) and Boyer *et al.* (1991). Representation of the cells and a description of the lattice groups and their inclusion relations are given in Fadda & Zanzotto (2001).

Bravais type	No.	Coordinates of the shift vector **p** in the conventional cell used in *International Tables for Crystallography* (1996)	Space group	Examples and *Strukturberichte*
Triclinic	1	x, y, z	$P\bar{1}$	
Primitive monoclinic	2	$x, \frac{1}{2}, z$	$P12_1/m1$	
	3	$x, 0, z$	$P12/m1$	
	4	$0, y, \frac{1}{2}$	$P12/c1$	
	5	$0, y, 0$	$P12/m1$	
Base-centered monoclinic	6	$x, 0, z$	$C12/m1$	α-O, β-Bi
	7	$0, y, \frac{1}{2}$	$C12/c1$	
	8	$0, y, 0$	$C12/m1$	
Primitive orthorhombic	9	$\frac{1}{2}, \frac{1}{2}, z$	$P2_1/m2_1/m2/n$	
	10	$\frac{1}{2}, 0, z$	$P2_1/m2/m2/a$	
	11	$0, 0, z$	$P2/m2/m2/m$	
Base-centered orthorhombic	12	$0, \frac{1}{2}, z$	$C2/m2/m2/a$	
	13	$0, 0, z$	$C2/m2/m2/m$	
	14	$0, y, \frac{1}{2}$	$C2/m2/c2_1/m$	α-U, α'-Ce, γ-Am, α'-Tb, α'-Dy; $A20$
	15	$0, y, 0$	$C2/m2/m2/m$	
Face-centered orthorhombic	16	$0, 0, z$	$F2/m2/m2/m$	
	17	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$F2/d2/d2/d$	γ-Pu
Body-centered orthorhombic	18	$0, \frac{1}{2}, z$	$I2_1/m2_1/m2_1/a$	
	19	$0, 0, z$	$I2/m2/m2/m$	
Primitive tetragonal	20	$\frac{1}{2}, \frac{1}{2}, z$	$P4/n2_1/m2/m$	
	21	$0, 0, z$	$P4/m2/m2/m$	
Body-centered tetragonal	22	$0, \frac{1}{2}, \frac{1}{4}$	$I4_1/a2/m2/d$	β-Sn, β-Si, β-Ge; $A5$
	23	$0, 0, z$	$I4/m2/m2/m$	bct5 Si
Rhombohedral	24	x, x, x	$R\bar{3}2/m$	C-rh. graphite, α-As, α-Bi, α-Sb, β-O; $A7$
Hexagonal	25	$\frac{2}{3}, \frac{1}{3}, z$	$P\bar{3}2/m1$	
	26	$0, 0, z$	$P6/m2/m2/m$	
	27	$\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$	$P6_3/m2/m2/c$	α-Mg, α-Ti, α-Zn, *etc.*; A3 (h.c.p.)
	28	$\frac{2}{3}, \frac{1}{3}, 0$	$P6/m2/m2/m$	
Face-centered cubic	29	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$F4_1/d\bar{3}2/m$	C-diamond, α-Sn, α-Si, α-Ge, β'-Se; $A4$

$$\boldsymbol{\varepsilon}_a = \mathbf{e}_a, \;\; a = 1, 2, 3, \quad \text{and} \quad \boldsymbol{\varepsilon}_{3+i} = \mathbf{p}_i, \;\; i = 1, 2, 3. \tag{31}$$

A main point that needs to be specified, for a general n, regards the structure of the arithmetic group that is at the basis of the classification criterion, which is given in (16) for $n = 2$. For 4-lattices, this group, which is denoted by $\Gamma_{3,3}$, is the subgroup of $GL(6, \mathbb{Z})$ constituted by the unimodular integral 6×6 matrices having the following structure (see I, or Pitteri, 1985): for $a, b, i, j = 1, 2, 3$,

$$\mu \in \Gamma_{3,3} \Leftrightarrow (\mu_\sigma^\tau) = \left(\begin{array}{c|c} m_a^b & l_i^b \\ \hline 0 & \alpha_i^j \end{array}\right), \tag{32}$$

where (m_a^b) is any matrix in $GL(3, \mathbb{Z})$, l_i^b are arbitrary integers and $\alpha = (\alpha_i^j)$ is a 3×3 matrix belonging to the finite non-commutative group of matrices generated by the permutation matrices[26] of the set $\{1, 2, 3\}$ and by the three 3×3 matrices obtained from the identity by replacing one of its rows by a row of -1's, for instance,

$$\begin{pmatrix} -1 & -1 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{33}$$

etc. The submatrices α_i^j in (32) generated in this way form a representation, by means of 24 suitable 3×3 matrices, of the group S_4 of the permutations of four objects. Any such matrix

[26] The $\nu \times \nu$ permutation matrix α of a permutationf of $\{1, \ldots, \nu\}$ is defined as usual by $\alpha_i^j r_j = r_{f(i)}$ for any numbers $r_1, \ldots, r_\nu$; so the entries of the matrix α_i^j are all 0, except in the $f(i)$th row of the ith column where they are 1.

α_i^j is either a permutation matrix or a permutation matrix, one of whose rows is substituted by a row of -1's.

Now, let us consider some examples of 4-lattice structures. In the appropriate range of temperature and pressure, the following three 4-lattices, described respectively by three sets of descriptors $\tilde{\boldsymbol{\varepsilon}}_\sigma$, $\hat{\boldsymbol{\varepsilon}}_\sigma$ and $\bar{\boldsymbol{\varepsilon}}_\sigma$, $\sigma = 1, \ldots, 6$, are observed, respectively, the first two in C, and the third one in La [see for instance Donohue (1982), where also figures can be found].

(a) Hexagonal diamond structure:[27] $\tilde{\boldsymbol{\varepsilon}}_\sigma = (\mathbf{e}_a, \tilde{\mathbf{p}}_i)$, with

$$\tilde{\mathbf{p}}_1 = \left(\tfrac{1}{3}\tfrac{2}{3}\tfrac{1}{2}\right), \quad \tilde{\mathbf{p}}_2 = \left(\tfrac{1}{3}\tfrac{2}{3}z\right), \quad \tilde{\mathbf{p}}_3 = \left(00z+\tfrac{1}{2}\right). \tag{34}$$

(b) Hexagonal graphite structure ($A9$): $\hat{\boldsymbol{\varepsilon}}_\sigma = (\mathbf{e}_a, \hat{\mathbf{p}}_i)$, with

$$\hat{\mathbf{p}}_1 = \left(00\tfrac{1}{2}\right), \quad \hat{\mathbf{p}}_2 = \left(\tfrac{2}{3}\tfrac{1}{3}0\right), \quad \hat{\mathbf{p}}_3 = \left(\tfrac{1}{3}\tfrac{2}{3}\tfrac{1}{2}\right). \tag{35}$$

(c) α-La structure ($A3'$): $\bar{\boldsymbol{\varepsilon}}_\sigma = (\mathbf{e}_a, \bar{\mathbf{p}}_i)$, with

$$\bar{\mathbf{p}}_1 = \left(00\tfrac{1}{2}\right), \quad \bar{\mathbf{p}}_2 = \left(\tfrac{1}{3}\tfrac{2}{3}\tfrac{1}{4}\right), \quad \bar{\mathbf{p}}_3 = \left(\tfrac{2}{3}\tfrac{1}{3}\tfrac{3}{4}\right). \tag{36}$$

In all the above structures, the three shift vectors $\mathbf{p}_i$ are given by means of their coordinates with respect to a standard hexagonal basis $\mathbf{e}_a$, with $\mathbf{e}_3$ parallel to the sixfold axis and orthogonal to the plane of $\mathbf{e}_1$ and $\mathbf{e}_2$, which are spaced $2\pi/3$ apart. These three hexagonal 4-lattices share the *same* space group $P6_3/mmc$ and the hexagonal holohedry $6/mmm$ (which, incidentally, are the space group and holohedry of the h.c.p. structure).

Now, structure (a) is a single orbit, belonging to the lattice complex that derives from the Wyckoff position $4(f)$ of the space group $P6_3/mmc$. Structure (b) does not belong to any lattice complex, and indeed is the union of two crystallographic orbits, obtained from the Wyckoff positions $2(b)$ and $2(d)$ of $P6_3/mmc$. Structure (c), too, does not belong to any lattice complex; it is again obtained as the union of two orbits, $2(a)$ and $2(c)$, of the group $P6_3/mmc$ (see Donohue, 1982, for further details).

It is not immediately clear how the existing classification criteria are to be applied to the above three structures. Fischer & Koch's list of lattice complexes is only meant to capture configuration (a). The other two structures are unions of two orbits (multiregular point systems), and therefore are not in the list of lattice complexes; each constituent orbit does appear in that list, but there is no accepted criterion in the literature to say when two unions of orbits are to be considered 'essentially' identical (or distinct). Some factors intervene to complicate the matter when lattice complexes are used in the attempt to investigate these structures. For instance, it can be seen that the orbits $2(a)$ and $2(b)$ of $P6_3/mmc$ belong to the same lattice complex with space group $P6/mmm$, while $2(c)$ and $2(d)$ belong to the same lattice complex pertaining to $P6_3/mmc$.[28] So the two distinct 4-lattices (b) and (c) are obtained respectively as unions of the same two structures (with distinct space groups) in different relative positions. It is not immediately obvious to see how the classification of orbits in lattice complexes will produce a classification of multiregular point systems.

The arithmetic criterion, on the other hand, gives a straightforward group-theoretical basis for treating the above three structures on the same footing, and to check in which way they are 'essentially' different. Indeed, the 4-lattices (a), (b) and (c) above are found to have symmetry groups belonging to distinct conjugacy classes of the arithmetic group $\Gamma_{3,3}$ defined in (32).[29]

In order to show this, we consider the lattice groups $\Lambda(\tilde{\boldsymbol{\varepsilon}})$, $\Lambda(\hat{\boldsymbol{\varepsilon}})$ and $\Lambda(\bar{\boldsymbol{\varepsilon}})$, of the 4-lattices above; these are the finite subgroups of $\Gamma_{3,3}$ obtained by solving equations (25) or (28) generalized to the case $n = 4$ [see also equations (45) or (47) in I],

$$\mathbf{Q}\mathbf{e}_a = m_a^b \mathbf{e}_b, \quad \mathbf{Q}\mathbf{p}_i = \alpha_i^j \mathbf{p}_j + l_i^a \mathbf{e}_a. \tag{37}$$

To check that the three resulting lattice groups (which are all isomorphic to the hexagonal holohedry $6/mmm$) are *not* conjugate in $\Gamma_{3,3}$, it is not necessary to list all their elements; it is enough to give the matrices μ as in (32) that correspond, through equation (37) considered for the sets of descriptors (34), (35) and (36), to the central inversion $\bar{1}$ and to the sixfold operation 6^+ belonging to the hexagonal holohedry $6/mmm$. Indeed, if the lattice groups were conjugate in $\Gamma_{3,3}$, the μ representatives of $\bar{1}$ would necessarily correspond to each other in the conjugacy, and likewise for the μ representatives of 6^+ (with the same matrix in $\Gamma_{3,3}$ to perform the conjugacy). A calculation based on (37) gives, in obvious notation, the matrices $\tilde{\mu}_{\bar{1}}$, $\hat{\mu}_{\bar{1}}$, $\bar{\mu}_{\bar{1}}$ and $\tilde{\mu}_{6^+}$, $\hat{\mu}_{6^+}$, $\bar{\mu}_{6^+}$, which all belong to $\Gamma_{3,3}$, as follows:

$$\tilde{\mu}_{\bar{1}} = \left(\begin{array}{ccc|ccc} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 & 0 & -1 \\ \hline & & & 0 & 0 & -1 \\ & 0 & & -1 & -1 & -1 \\ & & & 1 & 0 & 0 \end{array}\right), \tag{38}$$

$$\hat{\mu}_{\bar{1}} = \left(\begin{array}{ccc|ccc} -1 & 0 & 0 & 0 & -1 & -1 \\ 0 & -1 & 0 & 0 & -1 & -1 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ \hline & & & -1 & -1 & -1 \\ & 0 & & 0 & 0 & 1 \\ & & & 0 & 1 & 0 \end{array}\right), \tag{39}$$

[27] In the literature, it is not customary to describe the structures (a) and (b) with the origin on a lattice point as we do. The coordinates of the four atoms in their conventional cell are usually given as follows: $(\frac{1}{3}\frac{2}{3}z)$ $(\frac{2}{3}\frac{1}{3}z+\frac{1}{2})$ $(\frac{1}{3}\frac{2}{3}\bar{z})$ $(\frac{1}{3}\frac{2}{3}\bar{z}+\frac{1}{2})$ for structure (a); $(00\frac{1}{4})$ $(00\frac{3}{4})$ $(\frac{2}{3}\frac{1}{3}\frac{1}{4})$ $(\frac{1}{3}\frac{2}{3}\frac{3}{4})$ for structure (b).

[28] The orbits $2(a)$ and $2(b)$ of $P6_3/mmc$ actually give the same primitive hexagonal 1-lattice, while $2(c)$ and $2(d)$ give the same 2-lattice (the h.c.p. structure). We notice, however, that $2(a)$ and $2(b)$ do not belong to the same Wyckoff set of $P6_3/mmc$; they only are equivalent when considered in the same lattice complex of $P6/mmm$.

[29] This happens in the same way in which, for instance, the primitive face-centered and body-centered cubic structures are said to belong to distinct 1-lattice (Bravais) types, because their symmetry groups determine distinct 'arithmetic' conjugacy classes in $GL(3,\mathbb{Z})$. Exactly as the arithmetic criterion produces the 14 Bravais types of 1-lattices (and the 29 types of 2-lattices in Table 1), it can also produce all the distinct types of 4-lattices that are possible, and not only the three considered here.

$$\bar{\mu}_{\bar{1}} = \left(\begin{array}{ccc|ccc} -1 & 0 & 0 & 0 & -1 & -1 \\ 0 & -1 & 0 & 0 & -1 & -1 \\ 0 & 0 & -1 & -1 & -1 & -1 \\ \hline & & & 1 & 0 & 0 \\ & 0 & & 0 & 0 & 1 \\ & & & 0 & 1 & 0 \end{array}\right), \quad (40)$$

$$\tilde{\mu}_{6^+} = \left(\begin{array}{ccc|ccc} 1 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & -1 & 1 & 0 & 1 \\ \hline & & & -1 & -1 & -1 \\ & 0 & & 0 & 0 & 1 \\ & & & 0 & 1 & 0 \end{array}\right), \quad (41)$$

$$\hat{\mu}_{6^+} = \left(\begin{array}{ccc|ccc} 1 & -1 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 \\ \hline & & & -1 & -1 & -1 \\ & 0 & & 0 & 0 & 1 \\ & & & 0 & 1 & 0 \end{array}\right), \quad (42)$$

$$\bar{\mu}_{6^+} = \left(\begin{array}{ccc|ccc} 1 & -1 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 \\ \hline & & & -1 & -1 & -1 \\ & 0 & & 0 & 0 & 1 \\ & & & 0 & 1 & 0 \end{array}\right). \quad (43)$$

Now, it can be verified that imposing the necessary conditions for conjugacy of the two groups $\Lambda(\bar{\boldsymbol{\varepsilon}})$ and $\Lambda(\hat{\boldsymbol{\varepsilon}})$,

$$\bar{\mu}_{6^+}\mu = \mu\hat{\mu}_{6^+}, \quad \bar{\mu}_{\bar{1}}\mu = \mu\hat{\mu}_{\bar{1}}, \quad (44)$$

with $\mu \in \Gamma_{3,3}$, leads to a contradiction: no such μ can do the job. Likewise with the conjugacy conditions for the two lattice groups $\Lambda(\hat{\boldsymbol{\varepsilon}})$ and $\Lambda(\tilde{\boldsymbol{\varepsilon}})$, or with the two groups $\Lambda(\tilde{\boldsymbol{\varepsilon}})$ and $\Lambda(\bar{\boldsymbol{\varepsilon}})$. Therefore, $\Lambda(\bar{\boldsymbol{\varepsilon}})$, $\Lambda(\hat{\boldsymbol{\varepsilon}})$ and $\Lambda(\tilde{\boldsymbol{\varepsilon}})$ belong to three distinct conjugacy classes in $\Gamma_{3,3}$, and for this reason the three structures (*a*), (*b*) and (*c*) above belong to three distinct arithmetic types of 4-lattices.[30]

6. Conclusions

An arithmetic criterion was proposed in I for studying multilattice symmetry: it arose in earlier works on phase transitions in crystalline solids as the natural tool for describing the symmetry properties and symmetry changes that can occur in deformable crystals, and for determining the correct invariance of their constitutive functions [see, for instance, the literature quoted in §1.1, and also James (1987), Bhattacharya *et al.* (1993) and Ericksen (1997, 1998, 1999)]. This method also allows for a detailed classification of crystal structures with any number of atoms in their unit cell.

In this paper, we have investigated systematically the arithmetic symmetry of multilattices in the simplest case, that is, tridimensional monoatomic 2-lattices, determining their 29 distinct arithmetic types. This contributes to our understanding of the kinematics of complex crystalline materials, and helps establish a comprehensive background for the precise modeling of their behavior. The analysis can be adapted to the case of general n-lattice structures with $n > 2$.

Like 1-lattices, monoatomic 2-lattices are all constituted by a single crystallographic orbit (they are regular point systems in the affine space – see footnote **8**), and are therefore classified also by the well known criterion by Fischer & Koch (Koch & Fischer, 1975; Fischer & Koch, 1996); see also Hermann (1935) and §8.5 in Engel (1986). We find that the latter classification and our own coincide, that is, the same 29 types of monoatomic 2-lattices are identified by the two independent methods.[31] We conjecture that the two classification criteria are indeed equivalent for all regular point systems. Our work proves, *a posteriori*, that such equivalence holds at least for monoatomic 2-lattices.

Regardless of this, we remark that only a minority of crystal structures in nature are constituted by a single crystallographic orbit [see the examples of 4-lattices in §5; see also Donohue (1982) and Smithells (1949)]. There is thus a need for a general classification criterion. As explained in §5, it is not immediately clear how the classification by Fischer & Koch can be extended to general n-lattices (multiregular point systems). The arithmetic criterion described in I, on the other hand, is by its very definition applicable to any crystal structure, not only to single orbits, nor only to monoatomic ones. If the above conjecture is valid and there is equivalence of the two criteria for all regular point systems, then the arithmetic criterion constitutes a generalization to multiregular point systems of the well established criterion for single orbits given by Fischer & Koch.[32]

APPENDIX *A*
Some proofs

A1. Proof of Lemma 2

The descriptors $(\mathbf{e}, \mathbf{p})$ and $(\tilde{\mathbf{e}}, \mathbf{p})$ in the statement of Lemma 2 generate (possibly up to an inessential translation) the same 2-lattice because $\mathcal{L}(\mathbf{e}_a) = \mathcal{L}(\tilde{\mathbf{e}}_a)$ and, thus, by (1), $\mathcal{M}(\mathbf{e}_a, \mathbf{p}) = \mathcal{M}(\tilde{\mathbf{e}}_a, \mathbf{p})$; hence, by Proposition 1, $\Lambda(\mathbf{e}_a, \mathbf{p})$ and $\Lambda(\tilde{\mathbf{e}}_a, \mathbf{p})$ are conjugate.

A2. Proof of Lemma 3

Given a skeletal basis $\mathbf{e}_a$, formula (30) states the defining property of the 'asymmetric unit', here denoted by $\mathcal{A}(\mathbf{e}_a)$, of

[30] Other examples are possible, for instance with 3-lattices; see Proposition 5 in I.

[31] This means that the two criteria distinguish in the same manner the 2-lattice structures that are 'essentially' different from a physical point a view, that is, which have different nearest-neighbor relations *etc.*, grouping together only the 2-lattices whose atomic landscape around each of their lattice points is essentially the same. This is what happens, for instance, with the *A*-, *B*- or *C*-centerings in base-centered orthorhombic 1-lattices; such centerings are indeed 'essentially' the same and are equivalent for both classification principles when applied to 1-lattice structures.

[32] Fischer & Koch (Koch & Fischer, 1975; Fischer & Koch, 1996) determine 402 types of regular point systems (lattice complexes). As single orbits have a maximal number of atoms in their unit translational cells, there is a *finite number* of distinct types of regular point systems, also in the arithmetic sense. This is not the case for multiregular point systems (multilattices), because, at least mathematically, the latter can have any given number of points in their unit cell.

the symmorphic holohedral space group of the simple skeletal lattice $\mathcal{L}(\mathbf{e}_a)$ (see *International Tables for Crystallography*, 1996). Thus, for any $(\mathbf{e}_a, \mathbf{p})$ and $(\mathbf{e}_a, \tilde{\mathbf{p}})$ as in (30), since $\mathcal{L}(\mathbf{Q}\mathbf{e}_a) = \mathcal{L}(\mathbf{e}_a)$ by the definition of $P(\mathbf{e}_a)$, one has, from (1),

$$\begin{aligned}\mathbf{Q}\mathcal{M}(\mathbf{e}_a, \mathbf{p}) &= \mathcal{M}(\mathbf{Q}\mathbf{e}_a, \mathbf{Q}\mathbf{p}) = \mathcal{M}(\mathbf{e}_a, \mathbf{Q}\mathbf{p}) \\ &= \mathcal{M}(\mathbf{e}_a, \mathbf{Q}\mathbf{p} + \mathbf{t}) = \mathcal{M}(\mathbf{e}_a, \tilde{\mathbf{p}}),\end{aligned} \tag{45}$$

hence $\Lambda(\mathbf{e}_a, \tilde{\mathbf{p}})$ and $\Lambda(\mathbf{e}_a, \mathbf{p})$ are $\Gamma_{3,1}$-conjugate by Proposition 1 and equation (27).

A3. Proof of Lemma 4

The statement in this lemma is true by the very definition of a special Wyckoff position in *International Tables for Crystallography* (1996), Vol. A; in this case, given the simple lattice $\mathcal{L}(\mathbf{e}_a)$ and its symmorphic space group, a vector $\mathbf{p} \in \mathcal{A}(\mathbf{e}_a)$ gives a special Wyckoff position with $\mathbf{Q} \in P(\mathbf{e}_a)$ in its site-symmetry group if $\mathbf{Q}$ is such that $\mathbf{Q}\mathbf{p}$ and $\mathbf{p}$ differ by a vector in $\mathcal{L}(\mathbf{e}_a)$, as required by $(28)_2$ for $\alpha = 1$.

A4. Proof of Corollary 1

By Lemma 4, checking the special Wyckoff positions in $\mathcal{A}(\mathbf{e}_a)$ gives solutions of $(28)_2$ for $\alpha = 1$. Now, if $-\mathbf{1}$ solves $(28)_2$ for some $(\mathbf{e}_a, \mathbf{p})$ and $\alpha = 1$, then $-\mathbf{p} = \mathbf{p} + l^a\,\mathbf{e}_a$, so that necessarily $\mathbf{p}$ violates the exclusions (13). Therefore no special Wyckoff position with a site-symmetry group containing $-\mathbf{1}$ can give allowed $\mathbf{p}$'s, the latter thus being positions in $\mathcal{A}(\mathbf{e}_a)$ with site-symmetry groups of index at least 2 within the point group.

Furthermore, by Lemma 1, we conclude that the point groups of monoatomic 2-lattices always contain $-\mathbf{1}$, that is, only Laue groups can be realized as point groups of monoatomic 2-lattice structures. As is well known, among the eleven Laue point groups, seven are holohedral and four are non-holohedral. The holohedral case is realized when the lattice group Λ of the 2-lattice has elements μ whose matrices m in (16) form the full lattice group $L(\mathbf{e}_a)$ of the given skeletal basis $\mathbf{e}_a$ [that is, the corresponding elements $\mathbf{Q}$ solving $(28)_2$ form the full skeletal holohedry $P(\mathbf{e}_a)$]. In this case, by considering $(28)_2$ for $\alpha = 1$, we obtain a group of index exactly 2 in $P(\mathbf{e}_a)$; for this reason, for any holohedral 2-lattices, we must only consider the special Wyckoff positions as in case (*a*).

There is also the possibility that a 2-lattice be non-holohedral; we must then check for cases in which $(28)_2$ is not solved by all the elements $\mathbf{Q}$ in $P(\mathbf{e}_a)$. As the non-holohedral Laue groups are all of index 2 in their own holohedries, we obtain the index condition in case (*b*) of Corollary 1. Then the rest of the possibilities must be checked as mentioned in footnote **20**. It results that only for the symmorphic hexagonal holohedral space group $P6/m2/m2/m$ does one find a Wyckoff position $4(h)$ whose site symmetry is a non-holohedral trigonal subgroup $3m$ (of index 4); this gives the 2-lattice type number 25, whose Laue point group is $\bar{3}m$.

APPENDIX *B*
Example: computation of the arithmetic types of monoatomic 2-lattices with base-centered orthorhombic skeleton

Here we give an explicit example of how the results in Table 1 are obtained, by determining explicitly the distinct arithmetic types of monoatomic 2-lattices whose skeleton is of the base-centered orthorhombic Bravais type. Four distinct types of 2-lattices arise with this skeleton, two of which share the same space group.

B1. Skeletal basis, asymmetric unit and solutions to equations $(28)_1$

Let $\mathbf{i}, \mathbf{j}, \mathbf{k}$ be an orthonormal basis, and let the base-centered orthorhombic basis $\mathbf{e}_a$ be given by

$$\mathbf{e}_1 = \tfrac{1}{2}(a\mathbf{i} + b\mathbf{j}), \quad \mathbf{e}_2 = \tfrac{1}{2}(-a\mathbf{i} + b\mathbf{j}), \quad \mathbf{e}_3 = c\mathbf{k}, \tag{46}$$

for some positive numbers a, b, c. The conventional cell basis is $\mathbf{a} = a\mathbf{i}, \mathbf{b} = b\mathbf{j}, \mathbf{c} = c\mathbf{k}$. Our goal is the analysis of the solutions $(\mathbf{e}_a, \mathbf{p})$ of equations (28) when the skeletal basis $\mathbf{e}_a$ is as above, and the shift

$$\mathbf{p} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c} \tag{47}$$

belongs to the asymmetric unit $\mathcal{A}(\mathbf{e}_a)$ given by

$$\begin{aligned}\mathcal{A}(\mathbf{e}_a) = \Big\{\mathbf{p} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c} : \\ 0 \le x \le \tfrac{1}{4}, 0 \le y \le \tfrac{1}{2}, 0 \le z \le \tfrac{1}{2}\Big\},\end{aligned} \tag{48}$$

which, from Lemma 3, is taken from the holohedral symmorphic space group $C2/m2/m2/m$ corresponding to the Bravais type of $\mathbf{e}_a$ (see *International Tables for Crystallography*, 1996). Also recall the exclusions (13) for the non-essential descriptors [notice that the latter are expressed in terms of the actual lattice basis in (46) rather than the conventional cell basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$].

The solutions to equations $(28)_1$ are well known and give the following skeletal point group $P(\mathbf{e}_a)$ and lattice group $L(\mathbf{e}_a)$ with eight elements,

$$\begin{aligned}P(\mathbf{e}_a) &= \big\{\pm\mathbf{1}, \pm\mathbf{Q}^{\pi}_{\mathbf{i}}, \pm\mathbf{Q}^{\pi}_{\mathbf{j}}, \pm\mathbf{Q}^{\pi}_{\mathbf{k}}\big\}, \\ L(\mathbf{e}_a) &= \left\{\pm 1, \pm\begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},\right. \\ &\qquad \left. \pm\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \pm\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right\},\end{aligned} \tag{49}$$

where $\mathbf{Q}^{\omega}_{\mathbf{v}}$ denotes the counter-clockwise rotation of angle ω about the direction $\mathbf{v}$.

B2. Solutions to equations $(28)_2$ for $\alpha = 1$ and resulting lattice groups

Among the solutions of $(28)_1$ listed in (49), we must now select those that also satisfy $(28)_2$ for $l^a \in \mathbb{Z}$ and (some) $\mathbf{p} \in \mathcal{A}(\mathbf{e}_a)$ in (48). By Corollary 1, we only need to check the

special Wyckoff positions for the space group $C2/m2/m2/m$ that satisfy conditions (a) or (b) in the statement. In this case, only case (a) is relevant because, as is well known, no non-holohedral Laue subgroups are contained within the orthorhombic holohedry *mmm* represented by the groups $P(\mathbf{e}_a)$ and $L(\mathbf{e}_a)$ in (49). As the conventional cell in this case has volume 2, we only need to check the special Wyckoff positions of $C2/m2/m2/m$ whose listed multiplicity is 4.[33] All the Wyckoff positions of this space group, except for 4(e) and 4(f), meet the requirements of the lemmas and corollary in §3; taking Lemma 1 into account, such positions give the following orthorhombic subgroups of $\Gamma_{3,1}$:

$$\Lambda_{oC,4l}(\mathbf{e},\mathbf{p}) = \left\{ \pm 1, \pm \left(\begin{array}{cccc} -1 & 0 & 0 & -1 \\ 0 & -1 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \pm \left(\begin{array}{cccc} 0 & -1 & 0 & -1 \\ -1 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \pm \left(\begin{array}{cccc} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right) \right\},$$

$$\Lambda_{oC,4k}(\mathbf{e},\mathbf{p}) = \left\{ \pm 1, \pm \left(\begin{array}{cccc} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \pm \left(\begin{array}{cccc} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \pm \left(\begin{array}{cccc} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right) \right\},$$

$$\Lambda_{oC,4j}(\mathbf{e},\mathbf{p}) = \left\{ \pm 1, \pm \left(\begin{array}{cccc} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \pm \left(\begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \pm \left(\begin{array}{cccc} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right) \right\},$$

$$\Lambda_{oC,4i}(\mathbf{e},\mathbf{p}) = \left\{ \pm 1, \pm \left(\begin{array}{cccc} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \pm \left(\begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \pm \left(\begin{array}{cccc} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right) \right\},$$

$$\Lambda_{oC,4h}(\mathbf{e},\mathbf{p}) = \left\{ \pm 1, \pm \left(\begin{array}{cccc} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \pm \left(\begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \pm \left(\begin{array}{cccc} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right) \right\},$$

$$\Lambda_{oC,4g}(\mathbf{e},\mathbf{p}) = \left\{ \pm 1, \pm \left(\begin{array}{cccc} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \pm \left(\begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \pm \left(\begin{array}{cccc} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right) \right\}.$$

B3. Conjugacy classes of lattice groups and distinct arithmetic types

Now, in order to establish the distinct arithmetic types of monoatomic 2-lattices with a base-centered orthorhombic skeleton, we need to study the $\Gamma_{3,1}$-conjugacy properties of the six lattice groups found above. First of all, we notice that the groups $\Lambda_{oC,4j}$ and $\Lambda_{oC,4h}$ are $\Gamma_{3,1}$-conjugate through the matrix

$$\mu_1 = \left(\begin{array}{cccc} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right), \qquad (50)$$

and that, similarly, $\Lambda_{oC,4i}$ and $\Lambda_{oC,4g}$ are also conjugate through μ_1. So we need no longer consider the groups $\Lambda_{oC,4h}$ and $\Lambda_{oC,4g}$. One can then proceed by using Proposition 5 in I, which implies that 2-lattices with non-isomorphic space groups cannot have $\Gamma_{3,1}$-conjugate lattice groups, while, on the contrary, lattices with $\Gamma_{3,1}$-conjugate lattice groups necessarily have isomorphic space groups. In our case, we find the following:

(a) 2-lattices with lattice group $\Lambda_{oC,4j}$ have space group $C2/m2/c2_1/m$;

(b) 2-lattices with lattice group $\Lambda_{oC,4i}$ have space group $C2/m2/m2/m$;

(c) 2-lattices with lattice group $\Lambda_{oC,4k}$ have space group $C2/m2/m2/m$;

(d) 2-lattices with lattice group $\Lambda_{oC,4l}$ have space group $C2/m2/m2/a$.

By the aforementioned proposition, we conclude that the 2-lattices belonging to cases (a), (b)–(c) and (d) have lattice groups that are not conjugate in $\Gamma_{3,1}$, leaving the possibility that the lattice groups $\Lambda_{oC,4k}$ and $\Lambda_{oC,4i}$ [cases (b) and (c)] may be conjugate. A direct check on their conjugacy conditions shows that they are not $\Gamma_{3,1}$-conjugate. This establishes the existence of four distinct conjugacy classes of base-centered orthorhombic lattice groups in $\Gamma_{3,1}$, whose representatives are the groups mentioned in (a)–(d) above. Thus there exist four distinct arithmetic types of monoatomic 2-lattices with a base-

[33] As remarked at the end of §3, for centered lattices the multiplicity of a special Wyckoff position given in *International Tables for Crystallography* (1996) is a multiple of the index of the site-symmetry group; in this base-centered case, the multiplicative factor is 2.

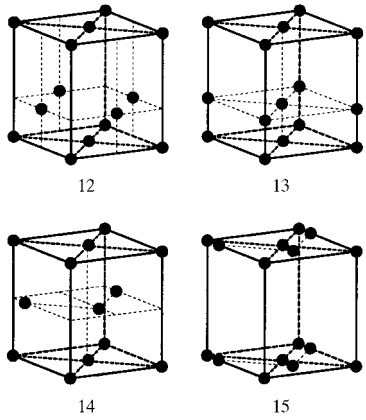

Figure 2
The four arithmetic types of monoatomic 2-lattices with base-centered orthorhombic Bravais type, obtained through the computations indicated in Appendix *B*. The numbering is as in Table 1. Type number 14 is the structure of α-U ($A20$).

centered orthorhombic skeleton [see the types numbered (12)–(15) in Table 1; type (14) gives the well known structure of α-U]. Fig. 2 represents the conventional cells of these 2-lattice types.

As the distinct types (13) and (15) [cases (*b*) and (*c*) above] share their space group, we have an instance here in which the arithmetic criterion for the classification of multilattice symmetry is finer than the one given by the space groups. The different arrangement of the atoms in the cells of structures (13) and (15) is not captured by the space-group class.

B4. An example of Wyckoff position giving excess skeletal symmetry

Here we give an example of how the higher-multiplicity Wyckoff positions not included in cases (*a*) or (*b*) of Corollary 1 lead to non-generic 2-lattices with excess skeletal symmetry. We consider the Wyckoff position denoted $8(p)$ for the same space group $C2/m2/m2/m$; this position has multiplicity 8 in the conventional double cell, *i.e.* its site-symmetry group has index 4 in $P(\mathbf{e}_a)$. The corresponding lattice group is

$$\Lambda(\mathbf{e}_a, \mathbf{p}) = \left\{ \pm 1, \pm \left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array} \right) \right\}, \qquad (51)$$

where $\mathbf{p} = (xy0)$ in the conventional cell. This is a primitive monoclinic lattice group whose generic 2-lattice belongs to type (3) in Table 1. The relation $\|\mathbf{e}_1\| = \|\mathbf{e}_2\|$ that is satisfied by the base-centered orthorhombic basis $\mathbf{e}_a$ in (46) is not enough to increase to orthorhombic the symmetry of this 2-lattice, and merely gives a case of excess (*i.e.* orthorhombic) skeletal symmetry for a primitive monoclinic 2-lattice.[34]

[34] Notice that, as explained in §3, we are using the information contained in the list of Wyckoff positions of a space group (in this case $C2/m2/m2/m$) only to find rapidly the solutions $\mathbf{p}$ to equation $(28)_2$, given $\mathbf{e}_a$ in (46). In general, the subdivision into Wyckoff sets of these Wyckoff positions is not related to the final subdivision into arithmetic types of the 2-lattices resulting from these solutions.

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