

Remarkable features in lattice-parameter ratios of crystals. I. Orthorhombic, tetragonal and hexagonal crystals

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The investigation of the lattice-parameter ratios of tetrahedral and hexagonal–rhombohedral inorganic compounds, as reported by Constant & Shlichta [(2003), *Acta Cryst. A* **59**, 281–282], has been extended to the structural data found for organic and metal-organic compounds (CSD), for bio-macromolecular crystals (PDB) and for inorganic materials (ICSD). In this first part of the series, the frequency distribution of orthorhombic, tetragonal and hexagonal crystals is presented. The results obtained confirm the existence of sharp peaks as a function of the ratios of lattice parameters and reveal additional exponential components, decaying for large and small values of these ratios. Practically all the important peaks occur at ratios which correspond to lattices having metric tensors with rational entries, the so-called integral lattices. The exponential component is interpreted as expressing a general statistical distribution which is valid for the generic crystal lattices, *i.e.* those normally considered. The exponential fraction dominates the peaked component in the organic and metal-organic cases, is less important for bio-macromolecular crystals and is much less important than the sharp peaks for inorganic crystals. Remarkable is the crystallographic relevance of the isometric hexagonal lattice, characterized by the axial ratio $c/a = 1$ and first observed in the molecular form of a protein. In the frequency distribution of 12 117 inorganic hexagonal crystals, the highest peak of 937 crystals occurs for $c = a$. In the hexagonal case of the bio-macromolecules the most important peak of 422 crystals is observed near the ideal h.c.p. (hexagonal closed packing) ratio of $(8/3)^{1/2}$.

1. Introduction

Axial-symmetric bio-macromolecules admit encasing forms with vertices belonging to lattices with typical axial ratios (Janner, 2001*a*, 2005*a,b,c*). These ratios imply that the lattices involved are *integral* and not *generic* ones. An *integral lattice* is characterized by the rational values of the scalar product of their lattice basis vectors, for a suitably chosen unit of length. This property is independent of the choice of lattice basis. In general, lattices belonging to a crystal system, or to a Bravais class, are not integral and in this case they are here denoted as *generic lattices*. Triggered by the intriguing crystallographic properties of bio-macromolecules, as mentioned above, one of the authors could assign integral lattices to most of the sharp peaks in the frequency distributions of hexagonal and tetragonal inorganic compounds, as reported by Constant & Shlichta (2003). Note that in three-dimensions only very few integral lattices are known to occur: (trivially) for cubic crystals, (less trivially) for ideal close-packed structures (like h.c.p.) and in the Frank's cubic hexagonal phases (Frank,

1965), as can be seen in the **B8** structure type (Lidin, 1998). In this paper, the analysis of Constant & Shlichta (2003) has been extended to include all lattice systems found in databases of inorganic, organic, metal-organic and bio-macromolecular crystals. Accordingly, lattice-parameter relations have been examined for the compounds of the Cambridge Structural Database (CSD), of the Inorganic Crystal Structure Database (ICSD) and of the Protein Data Bank (PDB), representing a total of *ca* 367 000 entries. At this level of generality, the problem represented by duplicated entries and of falsely assigned space groups has been considered of secondary importance and neglected.

The results obtained so far confirm the existence of sharp peaks as a function of the ratios of the lattice parameters, as reported by Constant & Shlichta (2003). The additional features observed are so specific for each of the three classes of compounds (CSD, ICSD and PDB), and for each of the five lattice systems, that a report requires more than one paper. The present one (denoted as part I) is restricted to the hexagonal, tetragonal and orthorhombic lattices, as presented in a poster at the ECM22 conference in Budapest (de Gelder & Janner, 2004). The discussion of the monoclinic and the

triclinic lattice distributions is postponed to part II (de Gelder & Janner, 2005).

2. Exponential behavior

2.1. Organic and metal-organic orthorhombic crystals

The exponential behavior is characteristic for the distribution of orthorhombic organic and metal-organic compounds of the Cambridge Structural Database. The peaked component is also present, but can be neglected. The number of compounds within each $\delta = 0.05$ range of parameter ratios represents a frequency distribution. This frequency is plotted as a function of the three possible axial ratios b/a , c/b and c/a for the lattice parameters of an ordered conventional cell with $a \leq b \leq c$ in Figs. 1, 2 and 3, respectively.

In Fig. 1 the distribution (b/a) shows a simple exponential decay from a maximum at $a = b$. Fig. 2 shows similar behavior in c/b , however, careful examination of the corresponding logarithmic plot shows that two slightly different exponential functions are involved, having a transition point at *ca* 1.75. The maxima at 1 correspond to pseudo-tetragonal lattices: one with axial ratios $c/a = c/b \geq 1$ and one with $a/b = a/c \leq 1$. The properties of these pseudo-tetragonal lattices are discussed later. In the c/a plot of Fig. 3 the maximum is not at the ratio 1. This ratio implies $a = b = c$ and thus a pseudo-

Frequency distribution of orthorhombic organic crystals

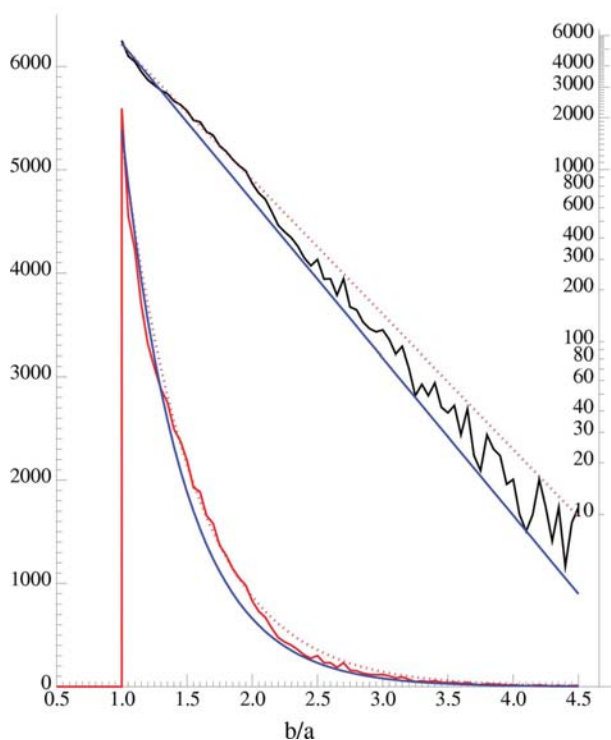


Figure 1 Frequency distributions within each $\delta = 0.05$ range of organic and metal-organic orthorhombic compounds as a function of b/a for the ordered lattice parameters $a \leq b \leq c$. For comparison, an exponential function with a decaying exponent of -2.1 is plotted starting from the maximal frequency value of 5595 at $b/a = 1$. The logarithm of these functions is also shown, together with the boundary for the small peaks which are considered as fluctuations around a statistical distribution of generic orthorhombic lattices. The total number of orthorhombic organic and metal-organic crystals from the CSD data is 58 207.

Frequency distribution of orthorhombic organic crystals

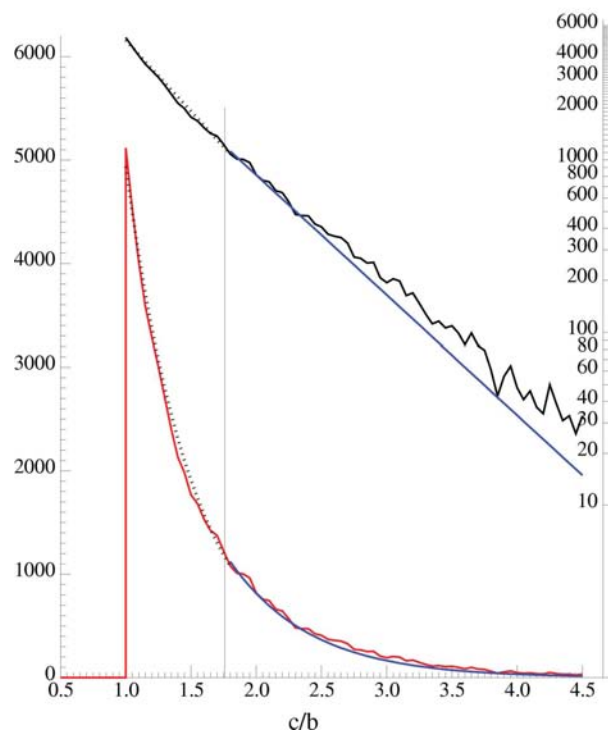


Figure 2 Frequency distribution of the same crystal set as in Fig. 1, plotted as a function of the lattice-parameter ratio c/b (for $a \leq b \leq c$ and $\delta = 0.05$). At $c/b = 1.75$ there is a transition from an exponential decaying function with an exponent of -1.9 (dotted line) to one with an exponent of -1.6 (full line). The logarithms of these functions are also shown.

cubic orthorhombic lattice: one deduces that, as one may expect, only a minor fraction of the pseudo-tetragonal lattices is also pseudo-cubic. The whole distribution can again be approximated by two exponential functions, but now with one increasing and one decreasing from a common maximum at ca 1.8. The two transition points (at 1.75 and at 1.8) practically coincide, within the coarse-grained approximation of $\delta = 0.05$ adopted for the frequency distributions. The three plots are not independent from each other because of the relation of $c/a = (c/b)(b/a)$. The corresponding probability densities are connected: each one can be expressed in terms of the other two (Parzer, 1960). The probabilistic analysis of this dependency lies beyond the aim of this work and is postponed to a subsequent paper. Peaks can be seen more clearly in Fig. 3 than in Figs. 1 and 2. This is due to the way the structural data have been clustered according to δ and represented. Anyhow, small peaks are very likely due to statistical fluctuations and not to relevant features of the structures.

2.2. Orthorhombic bio-macromolecular crystals

For the reasons given above, and to limit the number of figures, only frequency distributions as a function of c/b and c/a , respectively, are presented (Figs. 4 and 5). As in the organic and metal-organic case, the b/a distribution omitted is

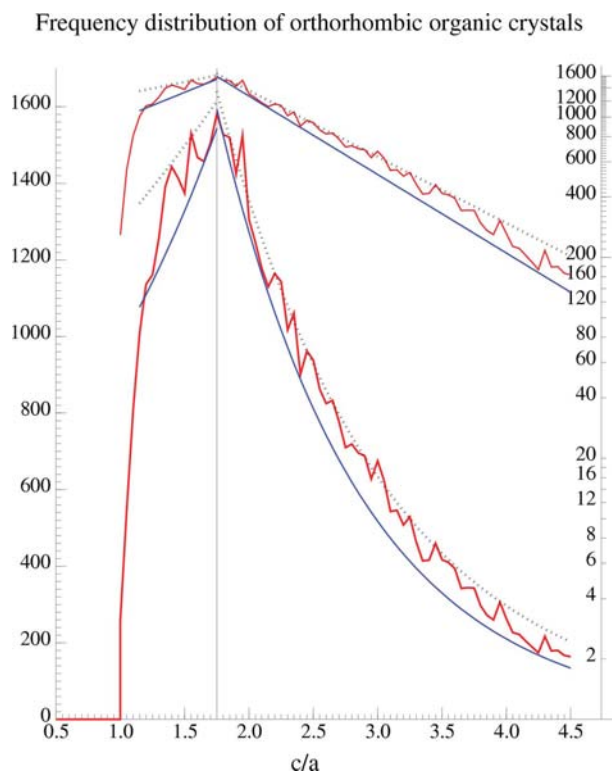


Figure 3 Frequency plot of orthorhombic organic and metal-organic compounds as a function of c/a (for $a \leq b \leq c$ and $\delta = 0.05$), together with the two exponential components 0.6 and -0.9 , respectively, and a transition point at $c/a = 1.8$. At the same value the maximal peak can be found, consisting of 1582 compounds from a total of 58 207 compounds in the CSD.

similar to the c/a one. For this class of compound the distributions have two components: an exponential component, similar to that observed in the previous subsection, and one consisting of more or less sharp peaks. A number of these peaks are not simply due to statistical fluctuations. For example, in Fig. 4, in addition to the peak at 1 which corresponds to pseudo-cubic lattices, two other important peaks can be identified: at $(3/4)(2)^{1/2}$ and at $2^{1/2}$, which can be associated with centered pseudo-tetragonal orthorhombic lattices, and a last one at $(8/3)^{1/2}$. Similar peaks at corresponding positions also occur in the plot as a function of b/a (not shown).

The assignment of integral lattices to the peaks occurring in Fig. 5 is more difficult. The general exponential behavior is similar to that observed in Fig. 3. Two exponential branches occur: one increasing and one decreasing as a function of c/a , with the transition point at 1.85, at about the same ratio as in the organic case.

2.3. Orthorhombic inorganic crystals

In the plots showing the abundance of orthorhombic inorganic crystals as a function of b/a , c/b and b/a , for $a \leq b \leq c$

Frequency distribution of orthorhombic pdb crystals

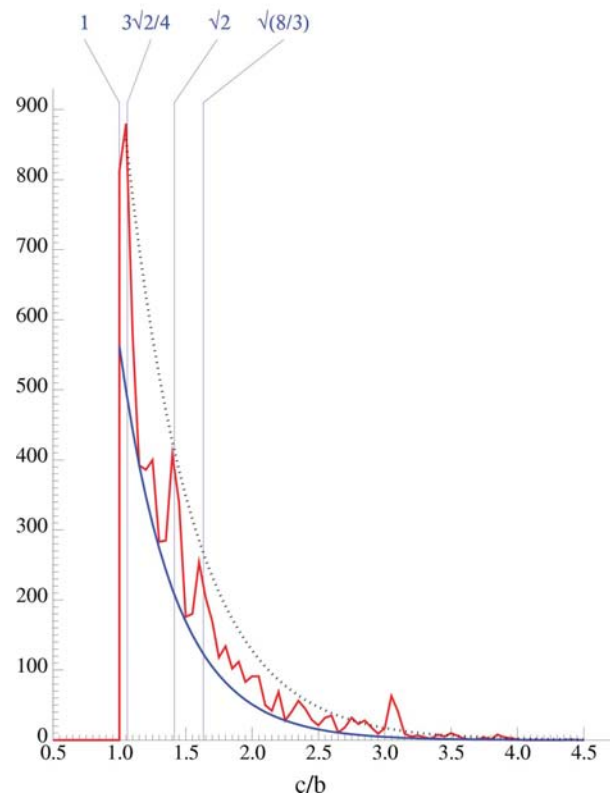


Figure 4 Frequency distribution of orthorhombic bio-macromolecular crystals as a function of c/b (for $a \leq b \leq c$ and $\delta = 0.05$), with a maximal peak of 880 compounds from a total number of 7279 PDB entries. The exponential component (with a decaying exponent -2.4) and the axial ratios of the integral lattices approximating a number of peaks in this distribution are shown. The dotted line follows the exponential decay (with an exponent of -2.0) of these peaks.

there is an exponential component similar but less pronounced than in the corresponding organic, metal-organic and bio-macromolecular distributions. The dominant feature is now represented by sharp peaks. The most important peaks correspond with the ratios of the integral lattices, as indicated in Figs. 6 and 7 for the c/b and the c/a distribution, respectively. The distribution as a function of b/a is similar to that for c/b and has been omitted.

3. Sharp peaks and integral lattices

As in the orthorhombic case, the exponential component of the hexagonal and tetragonal crystal lattices is more important for the organic and metal-organic compounds than for the inorganic materials and plays an intermediate role in the bio-macromolecular crystals. For the peaked component the situation is reversed. Sharp peaks occur in all the distributions of hexagonal and tetragonal crystals. While in the orthorhombic organic and metal-organic case the peaks are practically absent, it is the exponential component which becomes negligible for inorganic crystals.

There is another fundamental difference. The orthorhombic lattices could be ordered according to the value of the lattice parameters ($a \leq b \leq c$) and the ratios for the plots could be chosen to be ≥ 1 . In the hexagonal and tetragonal case there is a unique rotational axis of an order larger than 2 which is

conventionally chosen as the c axis. Therefore, there is only one axial c/a ratio, which can take values greater and smaller than 1. In a corresponding plot the value 1 subdivides the interval between the minimal and the maximal observed ratios $(c/a)_{\min}$ and $(c/a)_{\max}$ in an asymmetric way, even if the number of crystals belonging to the two sub-intervals are comparable. Clearly, by inversion the interval zero–one of finite length is transformed into one of infinite length. The consequence is that the plot of the number of compounds with axial ratios between c/a and $c/a + \delta$, for a fixed value of the coarse graining parameter δ (typically of the order 0.05), becomes deformed and compressed for c/a values smaller than 1. Also, the height and the resolution of the peaks can change. One could draw two pictures: one as a function of c/a and one for a/c , both for values equal to or greater than one. Then, however, the value 1 is duplicated and a comparison between the two plots is less direct than with a unique plot as a function of the logarithm of the axial ratio c/a , where $\ln(c/a) = -\ln(a/c)$. In doing so, the coarse-grained distribution adopted is given by the number of compounds with an axial ratio lying between $\ln(c/a)$ and $\ln(c/a) + \delta$ for a given value of δ . This is the type of plot adopted in this section.

Frequency distribution of orthorhombic pdb crystals

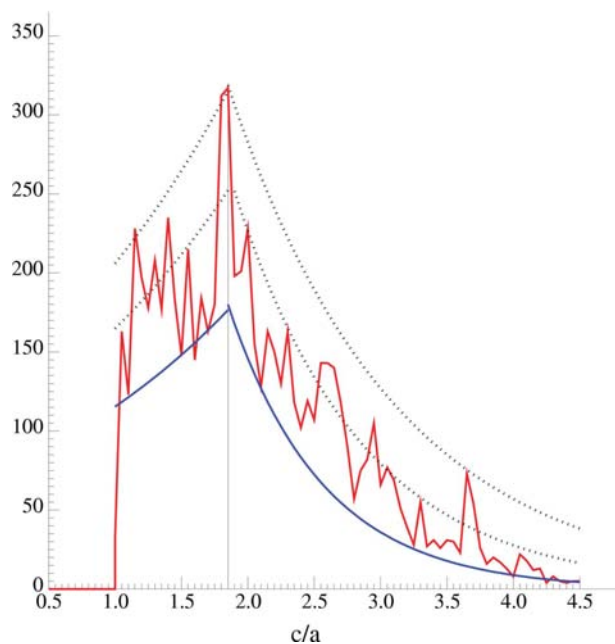


Figure 5
Peaked distribution of the same orthorhombic bio-macromolecular crystals as in Fig. 4, as a function of c/a (for $a \leq b \leq c$ and $\delta = 0.05$). The maximal peak, representing 317 compounds from a total of 7279 compounds of the PDB data, occurs at the transition point at 1.85 of the two exponential functions (with exponents 0.5 and -1.4 , respectively). The assignment of the peaks to the corresponding integral lattice values has been omitted.

Frequency distribution of orthorhombic inorganic crystals

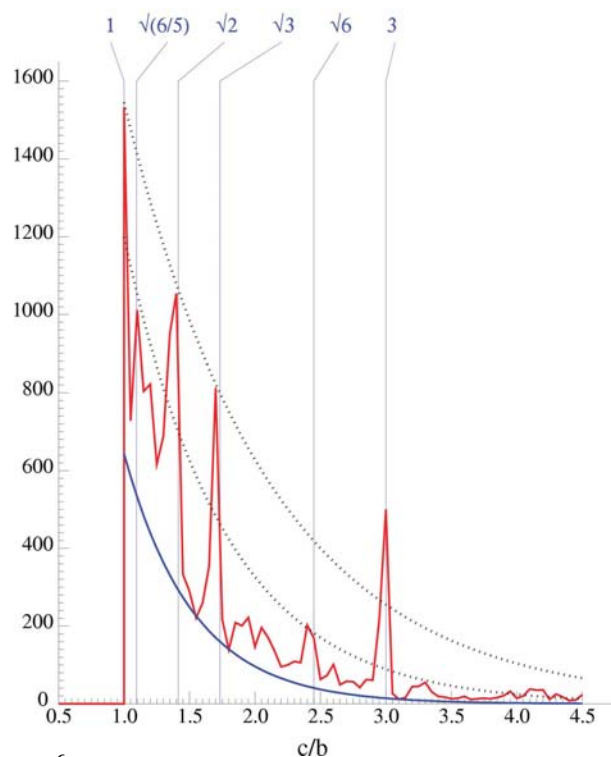


Figure 6
The exponential component of the frequency distribution of orthorhombic inorganic crystals taken from the ICSD data as a function of c/b (for $a \leq b \leq c$ and $\delta = 0.05$) is less important than in the previous cases. It is nevertheless indicated by an exponential decaying function (with an exponent of -1.9). The peaked component dominates the distribution and all the important peaks occur at ratios corresponding to integral lattices, as indicated. The maximum occurs at $c/b = 1$ and represents the pseudo-tetragonal lattice case consisting of 1533 crystals from a total number of 15 331 entries.

3.1. Hexagonal crystals

The distribution of hexagonal crystals is shown in Figs. 8, 9 and 10: for organic and metal-organic, for bio-macromolecular and for inorganic materials, respectively, as a function of $\ln(c/a)$ for $\delta = 0.05$, with c along the hexagonal axis. In all these cases sharp peaks are observed which correspond to axial ratios of integral lattices. Of course, the assignments indicated (for 14 different peaks in Fig. 8 and Fig. 10, and 11 in Fig. 9) are estimated and need not be correct.

There are, however, striking features which are very unlikely to be accidental. In particular, the most important peak in the inorganic crystal distribution occurs at $c = a$ and corresponds, therefore, to hexagonal isometric lattices. This is remarkable and fully unexpected, despite the fact that at the molecular level (not for the associated crystal) the isometric lattice case ($c = a$) clearly appears in the molecular forms of a number of axial-symmetric proteins for different rotational point-group symmetries (Janner, 2005*a,b,c*). Such a peak is absent in the hexagonal PDB crystal distribution (Fig. 9), except possibly as a center or as a superstructure of the isometric hexagonal case, with peaks at $\frac{1}{2}$, 2 and 3. In the organic and metal-organic crystals, the peak at $c = a$ is also

important (Fig. 8). As expected and as already observed by Constant & Shlichta (2003), the peak at $(8/3)^{1/2}$, which corresponds to the lattice of the h.c.p. structures, is a very important one for inorganic crystals. This peak is absent in the organic compounds. It is expected to play a role for bio-macromolecular crystals because of the globular structure of many proteins. Indeed, there is a dominant peak near this value. A better fit is obtained for $(5/2)^{1/2}$, but this assignment seems not to be structurally relevant. In any case, the nature of the crystals involved in this important peak has to be analyzed further.

The broad peak at $c/a = 0.9$ in the hexagonal plot of Constant & Shlichta (2003) does not appear in Fig. 10. Apparently, this is due to their fairly large value of 0.1 adopted for δ , together with the compression and deformation phenomena for the c/a values smaller than 1, as mentioned above.

3.2. Tetragonal crystals

The distribution of the tetragonal crystals as a function of $\ln(c/a)$ for c , the lattice parameter along the tetragonal axis, is similar to that of the hexagonal crystals. Characteristic is the fairly large number of sharp peaks. All the important peaks could be related to tetragonal integral lattices: 17 for the organic and metal-organic compounds (Fig. 11), 21 for the bio-

Frequency distribution of orthorhombic inorganic crystals

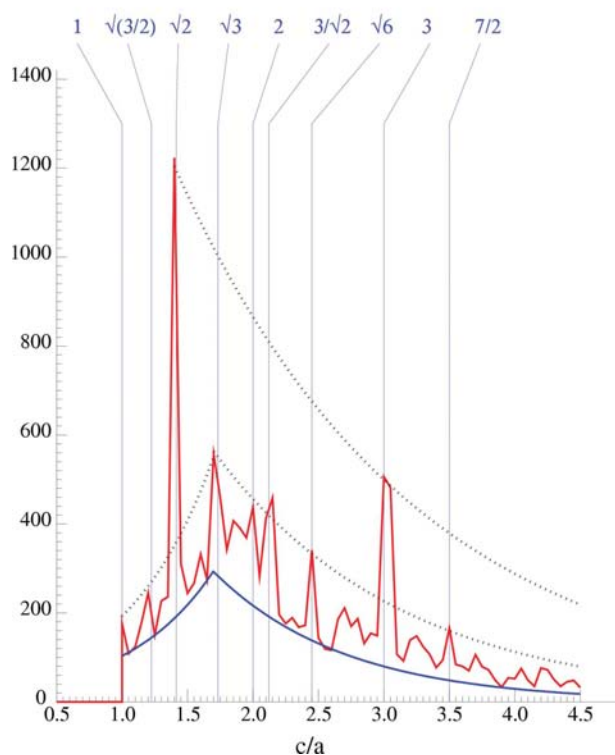


Figure 7

As in the previous figure, the peaked component of the frequency distribution of orthorhombic inorganic crystals plotted as a function of c/a (for $a \leq b \leq c$) is more important than the exponential part. This last part is indicated by two exponential functions, with exponents of 1.5 and -1.0 , respectively, and a transition point at $c/a = 1.75$. The dotted lines are also exponentials and limit the height of the nine peaks at ratios corresponding to integral lattices.

Frequency distribution of hexagonal organic crystals

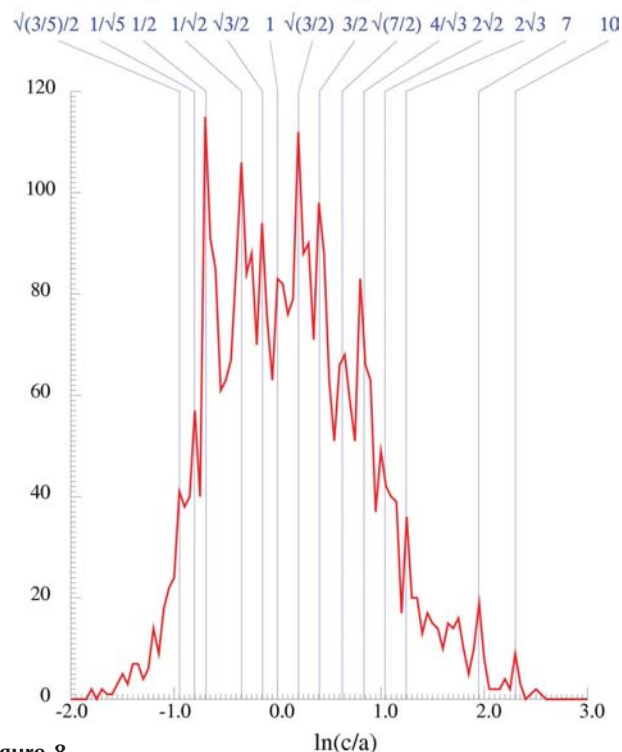


Figure 8

The frequency distribution of hexagonal organic and metal-organic crystals from the CSD (3425 entries, without those referred to as rhombohedral axes) is plotted as a function of $\ln(c/a)$ (for $\delta = 0.05$) with c along the hexagonal axis. All 14 more pronounced peaks of this distribution could be assigned to integral lattices with corresponding axial ratios, as indicated.

macromolecular ones (Fig. 12) and 15 for the inorganic crystals (Fig. 13). The isometric case $c = a$ occurs in this set as a pseudo-cubic tetragonal structure, possibly centered when the ratio c/a is equal to $\frac{1}{2}$, 2, 3, 5 and 9, as observed in the figures. Of note are the various combinations of $2^{1/2}$ and $3^{1/2}$ factors. As in the previous cases, a structural interpretation of these peaks, with or without considering the integral character of the lattice, is still missing.

4. Pseudo-symmetry

A structure is said to possess pseudo-symmetry when a non-negligible part of the atoms approximately satisfies a higher symmetry than that of the whole structure (Viterbo, 1992). The use of this concept, however, often depends on the context considered. In the present case, pseudo-symmetry arises when the lattice approximates one with a larger point-group symmetry than implied by the space group. In biomacromolecular crystals it very often happens that a protein does not have the same point-group symmetry as the space group. In biochemistry *non-crystallographic symmetry* is usually mentioned.

The frequency distributions presented here show that pseudo-symmetry plays a more important role in crystals than one would expect. For example, in all the orthorhombic crystals examined, the c/b and b/a distributions have an

exponential maximum at $c = a$ and $b = a$, respectively, implying that the corresponding lattices are tetragonal, in a coarse-grained approximation.

The phenomenon of sharp peaks at integral lattice positions can also be considered as pseudo-symmetry. Indeed, an integral lattice has a larger multimetric point-group symmetry than a generic lattice. Multimetric means that hyperbolic rotations leaving a lattice invariant are considered together with circular rotations (Janner, 1991, 1995, 2001*b*, 2004). There are cases, as for ice crystals, where the multimetric space group has the same point group as the lattice (Janner, 1997), but in general this needs not to be the case. In particular, it would be very surprising if the ca 1000 known crystals having an isometric hexagonal lattice (as shown in Fig. 10) were also invariant with respect to a multimetric space group with a corresponding point group of infinite order. Such a point group restricts the free real parameters, which may occur in Wyckoff positions, to appropriate rational values, and this is expected to occur only in special cases.

Experience shows that pseudo-symmetry is easily slightly broken. This symmetry-breaking is also observed in integral lattices, whose metrical relations are not implied by their Euclidean symmetry. Here is an example not based on

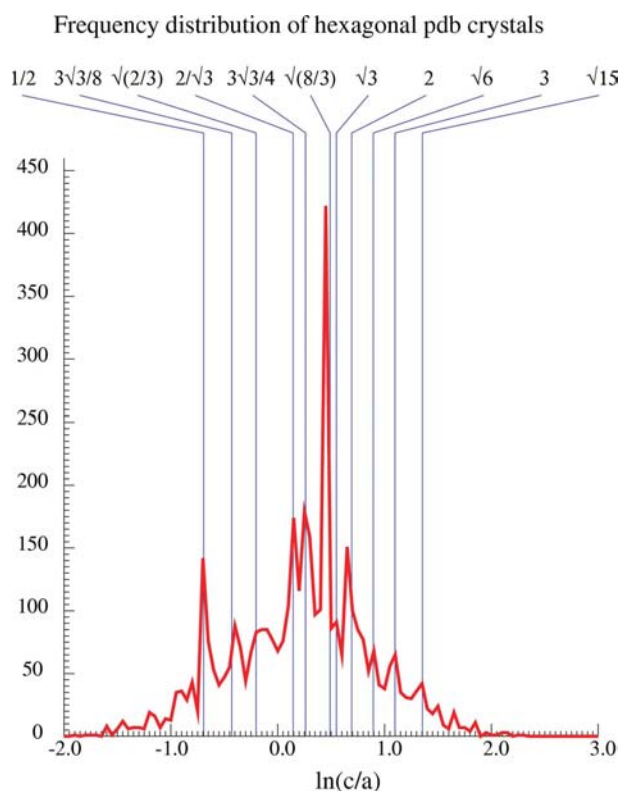


Figure 9 Similar plot to that in Fig. 8 for the hexagonal crystals of the PDB data (4090 entries and $\delta = 0.05$). The most important peak represents 422 crystals and occurs, as expected, near to the axial ratio $(8/3)^{1/2}$ of h.c.p. structures. The assignment $(5/2)^{1/2}$ is a better numerical fit, but structurally less relevant. The other peaks could also be related to integral lattices.

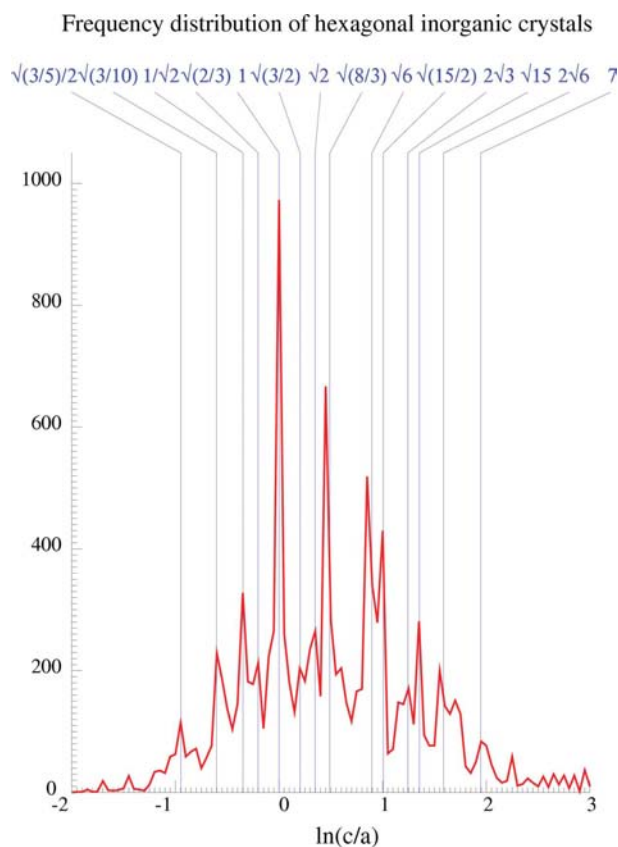


Figure 10 The frequency distribution of the 12 120 inorganic hexagonal crystals of the ICSD is plotted as a function of $\ln(c/a)$ for $\delta = 0.05$. Practically all sharp peaks (17) could be assigned to integral lattices. Remarkably, the largest peak, representing 973 crystals, occurs for $c = a$, which corresponds to the hexagonal isometric lattice case. The second important peak, labeled as $(8/3)^{1/2}$, corresponds to the lattices of ideal hexagonal close-packed structures.

multimetrical symmetry considerations. The ideal close-packed structures f.c.c. (face-centered cubic) and h.c.p. both have an integral lattice. Along the threefold axis, for an h.c.p. structure the axial ratio is $(8/3)^{1/2}$, as already pointed out; for the f.c.c. structure it is $3^{1/2}$. The axial ratio is exact in the cubic case and practically always approximate for h.c.p. structures.

4.1. Pseudo-tetragonal orthorhombic crystals

The frequency distribution of pseudo-tetragonal orthorhombic crystals can be compared either with that of other tetragonal crystals or with orthorhombic crystals. In the first case (and for ordered orthorhombic lattice parameters $a \leq b \leq c$) one should consider together the two cases $a = b$ and $b = c$. This corresponds to tetragonal axial ratios larger and smaller than 1, respectively, and one should adopt a plot in the logarithm of these ratios, as explained in §3. In the second case it is better to plot the frequency as a function of the ratios themselves and to restrict the considerations to one of the possible pseudo-tetragonal axes: a or c . This last alternative is adopted here because it allows an almost direct comparison with the orthorhombic distributions as a function of c/b (shown in Figs. 1, 4 and 6) and as a function of b/a (Figs. 3, 5

and 7), both of which contribute correspondingly to the pseudo-tetragonal plot $c/a \simeq c/b$ as $a \simeq b$. The equality sign has been avoided here to stress the point that the crystals contributing to a given ratio b/c satisfy the condition $b \leq a + \delta$ (here for $\delta = 0.05$). What is plotted is a coarse-grained distribution obtained by clustering the crystals within a given δ -range of c/m with $m = (a + b)/2$. The frequency distribution of the pseudo-tetragonal orthorhombic organic and metal-organic crystals (Fig. 14) shares the features shown in Figs. 2 and 4: a number of small peaks were added to a double exponential decay with a transition point at $c/b = 1.75$. This incidentally can be seen as an indication that the value 1.75 is not accidental, but has structural meaning. The maximum at $a = b = c$ corresponds to pseudo-cubic orthorhombic crystals.

Similar considerations apply to the frequency distribution of bio-molecular pseudo-tetragonal orthorhombic crystals. Now the peaks are more pronounced and can easily be assigned to integral lattices. There are two exponential components with a transition point at 1.75, as in the previous case. The largest peak does not occur at $c/a = c/b = 1$, but at the ratio $(\frac{2}{3})^{1/2}$, whose meaning is still hidden. Most impressive is the frequency distribution of the pseudo-tetragonal ortho-

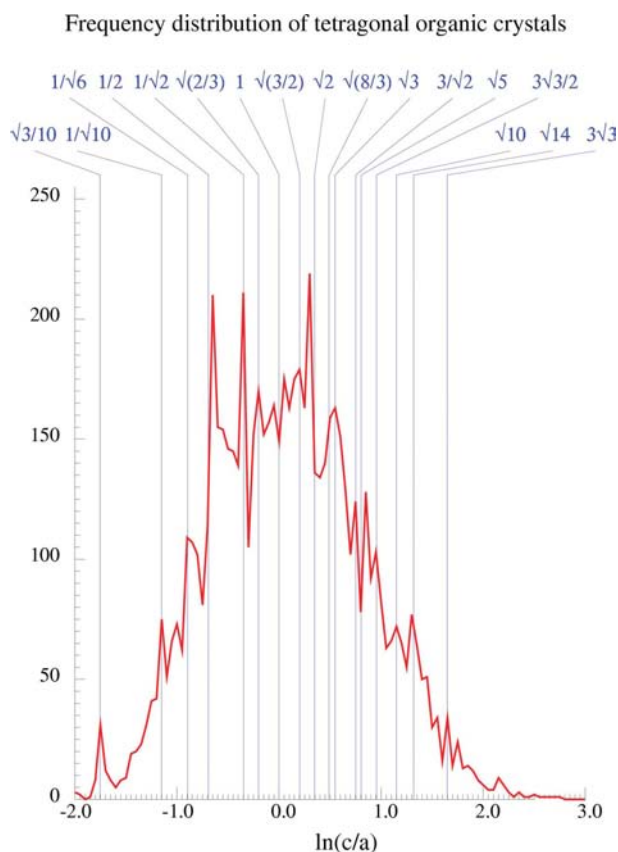


Figure 11
The large number of peaks (17) appearing in the frequency distribution of tetragonal organic and metal-organic crystals (6916 entries in the CSD) plotted as a function of $\ln(c/a)$, for $\delta = 0.05$, with c along the tetragonal axis, could be assigned to integral lattices, as indicated. There is also an important exponential component due to generic tetragonal lattices (not indicated).

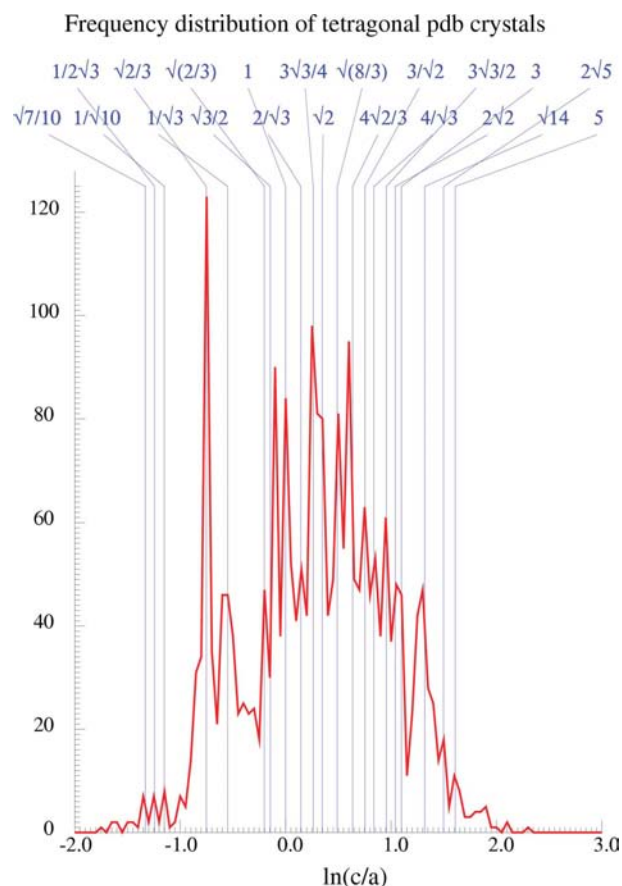


Figure 12
A surprisingly large number of sharp peaks (21) occurs in the frequency distribution of tetragonal bio-macromolecular crystals from PDB (2354 entries), as a function of $\ln(c/a)$, for $\delta = 0.05$. The largest peak is at the axial ratio $\frac{2^{1/2}}{3}$.

rhombic inorganic crystals (Fig. 15), with no exponential component and a distribution mainly restricted to only four sharp peaks at the ratio values 1 (pseudo-cubic), $2^{\frac{1}{2}}$, $6^{\frac{1}{2}}$ and 3.

5. Conclusions

The facts observed in the distribution of lattice-parameter ratios of hexagonal, tetragonal and orthorhombic crystal structures reported in the Cambridge Structural Database (CSD), in the Protein Data Bank (PDB) and in the Inorganic Crystal Structure Database (ICSD) can be summarized as follows:

(i) The crystal fraction showing that the exponential behavior, as a function of the lattice-parameter ratio, dominates in the organic and metal-organic compounds, is less important for bio-molecular crystals and is much less important for inorganic materials.

(ii) The importance of the peaked distribution follows the reverse order. It is most important in the inorganic case, much less in the organic and metal-organic crystals and is moderately important for bio-macromolecular crystals. Most of the important peaks can be assigned to integral lattices. There is a

general tendency towards the isometric case (with a ratio equal to 1).

(iii) Pseudo-symmetry plays a very important role. It is associated with lattices approximating one with a larger point-group symmetry than those implied by the space group of the crystals involved.

(iv) A structural basis for the properties mentioned above is still missing. Moreover, the mixed character of the peaks observed (exponential and integral) does not decide, without additional information, whether the lattice of a given crystal is generic or integral. The additional information can possibly be obtained for special cases: *e.g.* from the data reported in Fig. 1 for the exponential behavior and from those reported in Fig. 16 for the integral lattices. These situations represent, so to say, pure distributions, which could be the key for a structural analysis of the integral lattice phenomena.

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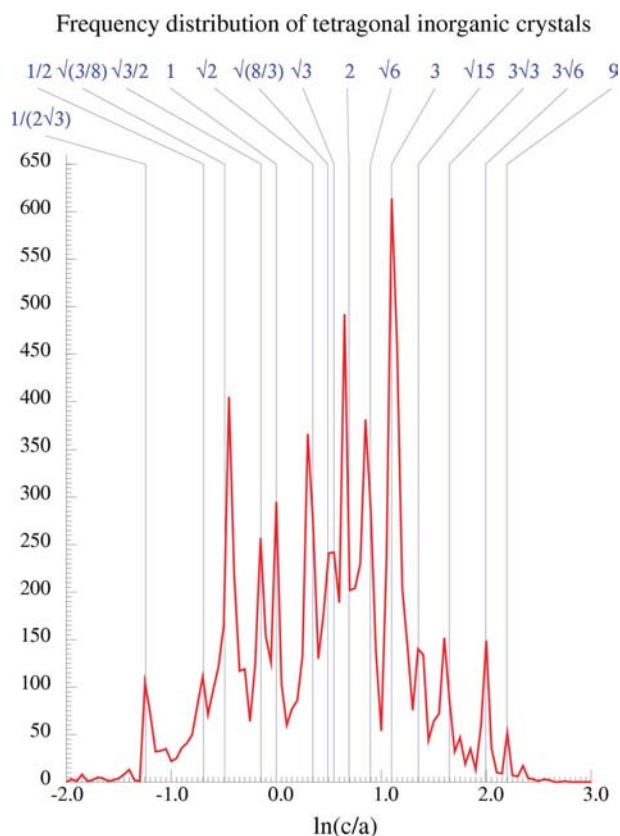


Figure 13
 The exponential component of the frequency distribution of tetragonal inorganic crystals of the ICSD data, with a total number of 10 031 entries, is plotted as a function of $\ln(c/a)$, for $\delta = 0.05$. The integral lattices corresponding to all these peaks are indicated by their axial ratio, as in the previous figures. The peak at 0.0 (axial ratio 1) corresponds to pseudo-cubic tetragonal crystals. The largest peak (axial ratio 3) and that labeled by 2 can be considered to be the tetragonal centering of a cubic lattice.

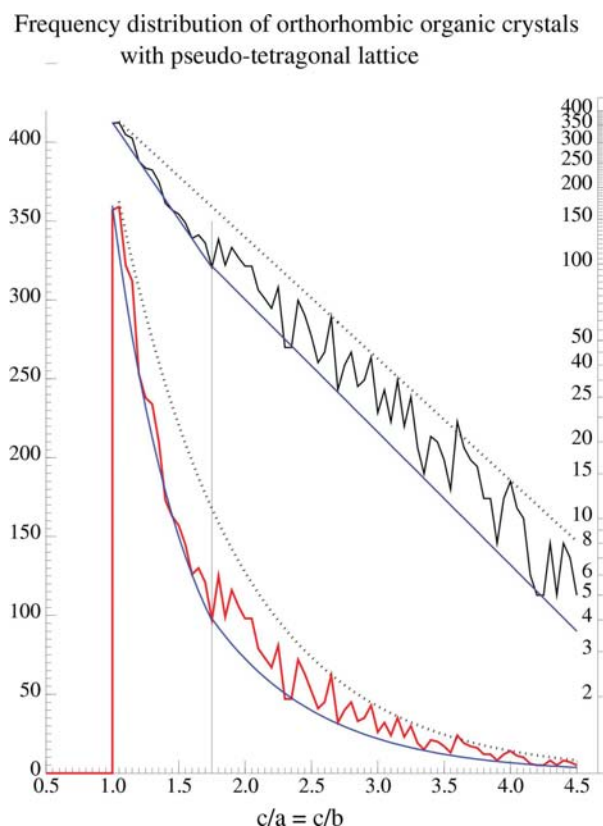


Figure 14
 Frequency distribution of the orthorhombic organic and metal-organic crystals belonging to the pseudo-tetragonal peak at $b/a = 1$ of Fig. 1. Here all the crystals with lattice-parameter values $b \leq a + \delta$ for $\delta = 0.05$ and $a \leq b \leq c$ (representing 5595 entries) have been plotted as a function of $2c/(a + b)$. There is a transition point at 1.75 from one exponential function with an exponent of -1.75 to one with an exponent of -1.2 . The dotted line limiting the peaks has an exponent of -1.1 . The logarithm of these various functions is also shown.

Frequency distribution of orthorhombic pdb crystals with pseudo-tetragonal lattice

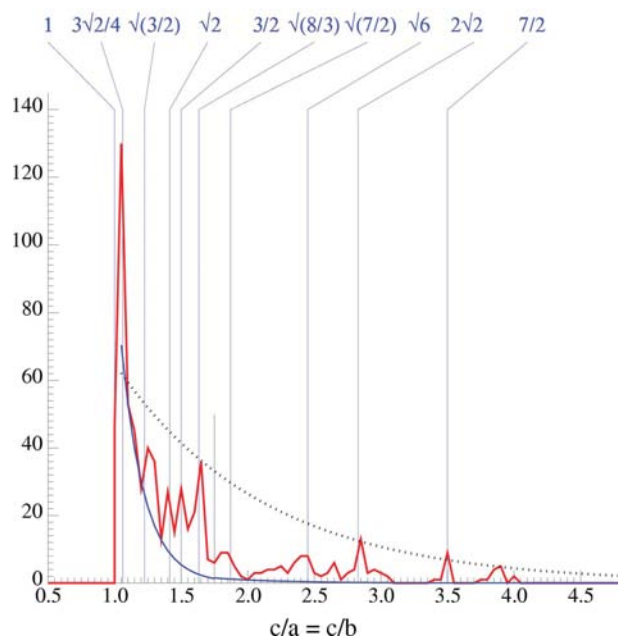


Figure 15
The peaked distribution of the pseudo-tetragonal PDB crystals (selected as in the previous case and representing 692 crystals) has a number of peaks at axial ratios of tetragonal integral lattices. There is also an exponential component involving two exponential functions, with exponents -1.6 and -0.9 , respectively, and a transition point at 1.75 , as indicated.

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Frequency distribution of orthorhombic inorganic crystals with pseudo-tetragonal lattice

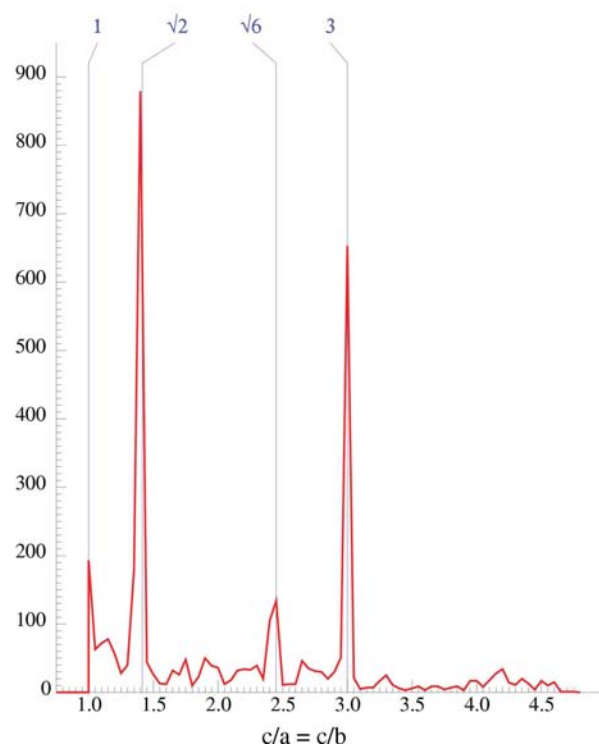


Figure 16
The frequency distribution of orthorhombic inorganic crystals having pseudo-tetragonal lattices, selected and plotted as in Fig. 14 (4095 entries), is practically concentrated over only four peaks at 1 , $2^{1/2}$, $6^{1/2}$ and 3 . It is a *pure* integral lattice distribution with no exponential component and thus practically no generic tetragonal lattices.

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