Ces différentes formules nous ont permis de dénombrer les sous-groupes isomorphes de $\Gamma(P1)$ et $\Gamma(p1)$ pour tous les indices comprise entre 2 et 30 (Tableaux 2 et 3).

III. Liste de sous-groupes

Dans le Tableau 4 figurent les sous-groupes isomorphes de $\Gamma(P1)$ pour tous les indices compris entre 2 et 7. Chaque sous-groupe est identifié par un numéro suivi (entre parenthèses) par les mailles, éventuellement confondues, qui correspondent aux matrices de passage $\mathbf{T}^{\mathrm{I}}$ à $\mathbf{T}^{\mathrm{VI}}$; ces mailles élémentaires sont exprimées en fonction de la maille élémentaire (**A**,**B**,**C**)

Tableau 5. *Sous-groupes isomorphes de* $\Gamma(p1)$ *pour tous les indices compris entre* 2 *et* 7

Indice 2
[1(2**A**,**B**); 2(**A**,2**B**)]; [3(2**A**, **B** + **A**)(**A** + **B**, 2**B**)].

Indice 3
[1(3**A**,**B**); 2(**A**,3**B**)]; [3(3**A**, **B** + **A**)(**A** + **B**, 3**B**)]; [4(3**A**, **B** − **A**) (**A** − **B**, 3**B**)].

Indice 4
[1(4**A**,**B**); 2(**A**,4**B**)]; [3(4**A**, **B** + **A**)(**A** + **B**, 4**B**)]; [4(4**A**, **B** − **A**) (**A** − **B**, 4**B**)]; [5(4**A**, **B** + 2**A**)(2**A** + **B**, 2**B**); 6(**A** + 2**B**, 4**B**) (2**A**, 2**B** + **A**)]; [7(2**A**, 2**B**)].

Indice 5
[1(5**A**,**B**); 2(**A**,5**B**)]; [3(5**A**, **B** + **A**)(**A** + **B**, 5**B**)]; [4(5**A**, **B** − **A**) (**A** − **B**, 5**B**)]; [5(5**A**, **B** + 2**A**)(**A** − 2**B**, 5**B**); 6(5**A**, **B** − 2**A**) (**A** + 2**B**, 5**B**)].

Indice 6
[1(6**A**, **B**); 2(**A**,6**B**)]; 3(6**A**, **B** + **A**)(**A** + **B**, 6**B**)]; [4(6**A**, **B** − **A**) (**A** − **B**, 6**B**)]; [5(6**A**, **B** + 2**A**)(2**A** + **B**, 3**B**); 6(**A** + 2**B**, 6**B**) (3**A**, 2**B** + **A**)]; [7(6**A**, **B** − 2**A**)(2**A** − **B**, 3**B**); 8(**A** − 2**B**. 6**B**) (3**A**, 2**B** − **A**)]; [9(6**A**, **B** + 3**A**)(3**A** + **B**, 2**B**); 10(**A** + 3**B**, 6**B**) (2**A**, 3**B** + **A**)]; [11(3**A**, 2**B**); 12(2**A**, 3**B**)].

Indice 7
[1(7**A**,**B**); 2(**A**,7**B**)]; [3(7**A**, **B** + **A**)(**A** + **B**, 7**B**)]; [4(7**A**, **B** − **A**) (**A** − **B**, 7**B**)]; [5(7**A**, **B** + 2**A**)(**A** − 3**B**, 7**B**); 6(7**A**, **B** − 3**A**) (**A** + 2**B**, 7**B**)]; [7(7**A**, **B** − 2**A**)(**A** + 3**B**, 7**B**); 8(7**A**, **B** + 3**A**) (**A** − 2**B**, 7**B**)].

de $\Gamma(P1)$. Les sous-groupes dont les mailles élémentaires présentent des analogies (échange des rôles des vecteurs **A**, **B**, **C**) ont été regroupés entre crochets. Pour chacun des indices 2, 3, 5, 6, 7, les sous-groupes sont équivalents par les automorphismes de $\Gamma(P1)$ et ne forment donc qu'une seule classe. Pour l'indice 4, les 28 premiers sous-groupes forment une classe d'équivalence, les 7 derniers une autre classe (Billiet. 1979). D'une manière analogue, le Tableau 5 donne les sous-groupes isomorphes de $\Gamma(p1)$ pour tous les indices compris entre 2 et 7. Les sous-groupes ne forment qu'une seule classe par rapport aux automorphismes de $\Gamma(p1)$ pour chacun des indices 2, 3, 5, 6, 7. Pour l'indice 4, les 6 premiers sous-groupes forment une classe, le dernier sous-groupe forme une seconde classe à lui seul.

Il convient de remarquer que les mailles conventionnelles des sous-groupes isomorphes de $\Gamma(P\bar{1})$ sont données par les mêmes matrices que celles des sous-groupes isomorphes de $\Gamma(P1)$, c'est-à-dire par le Tableau 4, l'origine des sous-groupes $\gamma(P\bar{1})$ étant placée en ($k_1/2$, $k_2/2$, $k_3/2$; k_i entier) par rapport au repère conventionnel de $\Gamma(P1)$ (Sayari & Billiet, 1977). D'une façon analogue, les sous-groupes isomorphes de $\Gamma(p2)$ sont données par le Tableau 5, l'origine étant placée en ($k_1/2$, $k_2/2$; k_i entier) (Sayari, Billiet & Zarrouk, 1978).

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A Perturbation Stable Cell Comparison Technique*

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Abstract

A modified method of describing lattices (or, equivalently, unit cells) is described. In the proposed parameterization, there is no discontinuous measure of agreement such as is found in studies of reduced cells. Although the Niggli reduced cell is uniquely defined for every lattice, the angles of the reduced cell may vary wildly with minor lattice distortions. It is proposed that lattices be described by the sets of seven parameters consisting of reduced-cell edge lengths, the lengths of edges of the reduced cell of the reciprocal lattice, and the reduced-cell volume.

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Introduction

Recently we were asked to consider the properties of lattices for a practical problem. We were invited to prepare a computer program capable of searching the data in the *Determinative Tables* (Donnay & Ondik, 1973) to find matches to measured unit cells. Among the design criteria was the specification that the search should find *all* cells closely related to the measured one. This includes cells for which the symmetry has been misidentified or for which a slightly different form or symmetry has been reported, or for which the symmetry or cell parameters have been modified by substitution of one atom type for another. The data base contains approximately 50 000 compounds. This large number would make it impractical to search among all of the related lattice types since this would mean that several or many searches would be required for each cell. Searches on reduced-cell lengths and volume only would put together cells which were not really related to one another; a four-parameter specification of cells which require six parameters cannot be unique. In order to deal with this problem, we were led to the study of reduced cells and the consideration of the various invariants of lattices.

Let a 'lattice' be defined as a collection of points, each of which is reachable from any of the others by an integral combination of three given vectors. It should be noted that lattices contain identical points, and we shall therefore be concerned only with metric properties and not structural or diffraction properties. When we discuss symmetry, we will use only the 'metric symmetry' of the lattice. The literature contains several 'reduced cells' for standard presentation of lattices (Niggli, 1928; Delaunay, 1933; Buerger, 1957). A 'Buerger reduced cell' of a lattice is a set of three lengths (a,b,c) and three angles (α,β,γ) such that vectors **a**,**b**,**c** with lengths a,b,c respectively, with angle γ between **a** and **b**, α between **b** and **c**, and β between **c** and **a**, yield the original lattice, and such that there exist no three shorter vectors which will do so. That is, a,b,c are the lengths of the three shortest non-coplanar vectors in the lattice. However, there may be as many as five alternate sets of angles, hence five Buerger reduced cells (Gruber, 1973). If there are alternate sets of angles, one such Buerger reduced cell may be selected as the reference cell by such criteria as the standardized presentation of the off-diagonal terms of the matrix tensor (the Niggli reduced cell, see Mighell, Santoro & Donnay, 1969) or minimum total surface area of the cell (Gruber, 1978). Unfortunately, for each of these criteria, there are, in practice, cases in which very small changes in the lattice yield very large, discontinuous jumps in the reduced-cell angles. This occurs in spite of the fact that each of these latter two reduced cells is unique to its particular lattice. Such discontinuities are widely recognized among crystallographers and have been described: 'The special conditions commonly occur. They are essential, and they must be satisfied to avoid confusion. . . . Errors that frequently occur in reduction procedures are caused by: . . .(*b*) failure to consider the [effect of] experimental error on the scalars when applying the inequalities inherent in reduction . . .' (Mighell, 1976), and '. . . in some cases two reduced cells satisfying the convention may result . . .' (Lawton & Jacobson, 1965). It is important to note that the 'special' conditions (Mighell, Santoro & Donnay, 1969) in Niggli reduction are specified only for those cases in which multiple Buerger cells occur. Thus the occurrence of such cases depends partly upon the accuracy of experimental techniques. Further, since non-integer numbers computed by different paths usually differ slightly in the one or two least significant digits, the occurrence of 'special' conditions also depends inherently on computer accuracy, algorithms, path of computation, and a programmer's decision concerning when two numbers are to be considered equal. This state of affairs arises not from shortcomings in methods of selecting reference cells, but rather from the use of cell angles as parameters for cell comparison. We suggest an alternative set of lattice parameters $(a,b,c,a^{*\prime},b^{*\prime},c^{*\prime},V$, where each quantity refers to the parameter of the reduced cell in the appropriate space) which, by avoiding the use of cell angles, avoids the instabilities associated with previous approaches. In this formulation, approximately equal parameters will be found for lattices which approximate each other. We have not been able to prove the converse proposition which we state here as a theorem lacking proof.

Theorem: the set of reduced-cell lengths in real space, the reduced-cell lengths in reciprocal space, and the reduced-cell volume uniquely define the lattice.

A corollary is that any two lattices for which the seven parameters are nearly equal are closely related lattices. While we cannot prove this theorem, we present an algorithm by which all Buerger cells corresponding to a given set of parameters may be found. An extension of this approach for the identification of Bravais lattice type is also outlined.

Method

Choose a primitive cell within the lattice and perform Buerger reduction. Compute the cell reciprocal to a primitive cell, and reduce that reciprocal cell. Call the three reduced-cell lengths a,b,c and the reduced-reciprocal-cell edge lengths $a^{*\prime}$, $b^{*\prime},c^{*\prime}$, chosen so that $a \leq b \leq c$ and $a^{*\prime} \leq b^{*\prime} \leq c^{*\prime}$. Take these six numbers and the reduced-cell's volume, V, as the identifying parameters of the lattice. Although part of the relationship between the real and reciprocal lattices is lost upon reducing and upon putting each set of lengths in ascending order, these steps are necessary for stability under perturbation. Reduction is clearly necessary in each space for stable, identifiable results. Arbitrary

ordering is required; in many cases there is no clear relationship between the lengths in the two spaces. To attempt to maintain the relationship between the real and reciprocal axes would lead to instabilities similar to those found for angles. For lattices in which several Buerger reduced cells exist, the *sets* of lengths of the edges of these alternate cells are the same (Gruber, 1973). The same, of course, holds for the reciprocal lattice. The volume is required in the set of parameters. If it is not included, there are many regions in which different lattices can be found that agree in the six length parameters, but which differ in the relationship of the set of lengths in one space to the set of lengths in the other. Thus, for any given cell, our seven parameters are unambiguously defined. In the next section we demonstrate that they are stable under perturbation of the lattice.

It remains to specify a method for obtaining cell angles from our seven parameters. From the equation:

$$(V/abc)^2 = 1 - (\cos^2\alpha + \cos^2\beta + \cos^2\gamma) + 2\cos\alpha\cos\beta\cos\gamma,$$

with α and β regarded as given, there are up to two solutions for $\cos\gamma$. For each such solution, we may calculate a reciprocal cell. By reducing the reciprocal cell, we calculate parameters to compare with our given $a^{*\prime},b^{*\prime},c^{*\prime}$. Taking the sum of the squares of the fractional differences of each of these latter three parameters as a figure of merit, we need only perform a global minimization of that figure of merit on the two-dimensional α,β plane. Figs. 1(*a*) and 1(*b*) are contour plots of this figure of merit for the positive-square-root solutions for $\cos\gamma$ for the cell used as an example by Gruber (1973). The negative-square-root solution is the same mirrored at 90° in either α or β (however, the values of γ differ). The 20 minima correspond (after relabelings and chirality changes) to the five cells given by Gruber (1973).

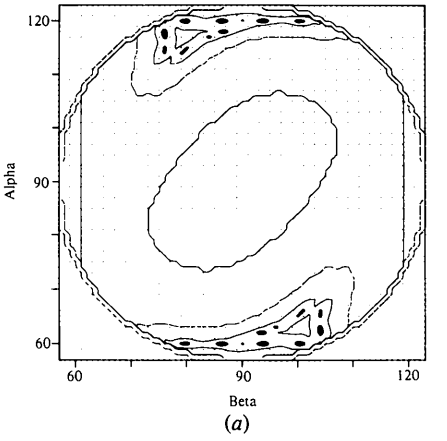
Perturbation stability and error propagation

We first recapitulate the standard error analysis for reduced-cell edges. Consider the effect of a perturbation of a given cell on the parameters to be used in matching. Given any primitive cell as input, its edge vectors **a**,**b**,**c** are related to the Buerger reduced cell of non-coplanar vectors of minimal lengths $\mathbf{a}_r,\mathbf{b}_r,\mathbf{c}_r$ by:

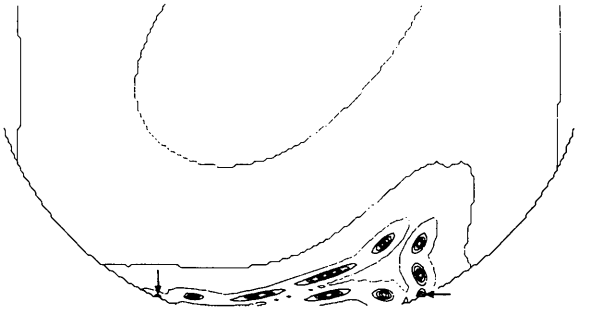
$$\begin{pmatrix}\mathbf{a}_r\\ \mathbf{b}_r\\ \mathbf{c}_r\end{pmatrix} = \mathsf{N}\begin{pmatrix}\mathbf{a}\\ \mathbf{b}\\ \mathbf{c}\end{pmatrix},$$

where N is an integer matrix whose determinant has an absolute value of 1. Errors in the original cell are also propagated by N. It should be noted that reduction may require N to have some rather large integers which would greatly inflate the propagated errors.

Now consider a reduced cell with known errors. Such a cell may well perturb to a non-reduced cell. However, as long as the perturbations are small, the reduced-cell edges of the perturbed cell will consist of some subset of the original unperturbed cell's edges and its various diagonals, and the new edge will be a diagonal of the unperturbed cell only when the diagonals are already equal or nearly equal in length to the edges. Thus, the worst case will be that in which the new edge is a linear combination of the original edges with at most unit weights. In such a case, the errors in the lengths of the original edges must be combined to



(*a*)



(*b*)

Fig. 1. A contour plot of the agreement function described in the text. This plot is for the positive-square-root solution for $\cos\gamma$. The cell is the case described in detail by Gruber (1973) (see Table 1). The constraint that the real cell be Buerger reduced has not been applied. In this case, the only effect of that constraint is to narrow the range of allowed $\cos\gamma$ to include only small regions near the Buerger reduced cells. Inclusion of that constraint obscures the picture. (*a*) Overview of the α,β plane in the region of interest. The areas in the corners do not admit real solutions of $\cos\gamma$. Twenty solutions occur in the figure. (*b*) Enlargement of the lower section of (*a*). Eight solutions are easily seen and the other two are indicated by arrows. Note that among the 40 solutions in the two branches of solutions for $\cos\gamma$, there are only the five correct cells described by Gruber (1973).

discover the error of the resulting edge. Assuming r.m.s. errors of approximately equal size, we might inflate each error by about the square root of three to insure good capture of neighboring cells.

We now consider the remaining parameters. Reduced reciprocal-cell edges admit the same analysis as above. Volume is not changed by reduction (except for computational imprecision) and changes smoothly with perturbations of edge lengths or cell angles. Thus, it remains to consider cell angles. Except for perturbation of edges to face or body diagonals, angles do admit a similar analysis. That exception is, however, fatal. A switch to a diagonal involves a discontinuous and possibly large change in angles. To understand this discontinuity, we consider in detail the conditions leading to such a switch. A reduced-cell edge will be the same length as a face diagonal if any of the following conditions are met:

$$\begin{aligned} |\cos\alpha| &= b/2c \\ |\cos\alpha| &= c/2b \\ |\cos\beta| &= a/2c \\ |\cos\beta| &= c/2a \\ |\cos\gamma| &= a/2b \\ |\cos\gamma| &= b/2a. \end{aligned}$$

A reduced-cell edge will be of the same length as a body diagonal if any of the following conditions is met:

$$\left.\begin{array}{c} -\cos\alpha/a - \cos\beta/b - \cos\gamma/c \\ \text{or} \\ -\cos\alpha/c - \cos\beta/b + \cos\gamma/c \\ \text{or} \\ \cos\alpha/a - \cos\beta/b + \cos\gamma/c \\ \text{or} \\ \cos\alpha/a + \cos\beta/b - \cos\gamma/c \end{array}\right] = \left[\begin{array}{c} (a^2 + b^2)/2abc \\ \text{or} \\ (b^2 + c^2)/2abc \\ \text{or} \\ (a^2 + c^2)/2abc \end{array}\right.$$

(12 equations in all). In considering error propagation of angles, one must consider approximate equality in each of the above 18 conditions. However, even exact equality is not unusual. If $\alpha = 60°$ and $\mathbf{b} = \mathbf{c}$, then $\mathbf{b} - \mathbf{c}$ may replace $\mathbf{c}$. Then if $\gamma \neq 90°$, the new β will be far from the original β. See, for example, the first two cases for cell '*B*' in Table 1. Other examples of the instabilities of reduced-cell angles are also included in Table 1. We note that when none of the above equalities is satisfied, there is only one Buerger reduced cell. When several of the equalities are satisfied, there are several Buerger reduced cells. In the latter case, slight perturbations can select any one of the Buerger reduced cells as the only Buerger reduced cell (it will be the Niggli reduced cell also). It should be noted that although any one of the Buerger reduced cells may become the only Buerger reduced cell, it may not be the one of the cells that was Niggli reduced. Similar problems arise with the equalities and inequalities in Niggli reduction criteria (Mighell, Santoro & Donnay, 1969).

Uses of the parameterization

Roof (1969) has compiled a table of general and special Niggli matrices for each of the 41 reduced-cell types. As useful as this table is, it requires searching among many conditions and extremely careful attention to the cell's standard deviations. A similar table might be constructed for our parameterization, but many of the centered cells would have even more representations

Table 1. *Reduced cells*

(*A*) The two nearly identical cells cited by Lawton & Jacobson (1965) which have differing Niggli reduced cell angles.

a (Å)	*b* (Å)	*c* (Å)	α(°)	β(°)	γ(°)
Reduced real (Niggli) cells					
6·490	10·358	10·359	60·520	71·750	71·761
6·490	10·360	10·360	108·254	108·246	107·223
Reduced reciprocal cells					
0·1130–	0·1130+	0·1653	101·079	101·097	115·909
0·1130–	0·1130+	0·1653	101·097	101·082	115·915

(*B*) Perturbations of the lattice described by Gruber (1973) which has five Buerger reduced cells. (1) The five Buerger reduced cells as listed by Gruber; in parts (2) and (3) the lengths of each of the Buerger reduced cells are modified as listed – for instance, in part (2)(*a*)(iii) the cell being reduced is $a = 2·05$, $b = 4·00$, $c = 4·10$ Å, $\alpha = 120·000$, $\beta = 93·583$, $\gamma = 104·483°$. In parts (*a*), (*b*), (*c*), (*d*), the reduced-cell parameters in the appropriate space are shown. In parts (*d*), *V* is the reduced-cell volume and '*r*' is the fractional difference (in per cent) between the length of '*c*' for a particular cell and the next shortest length in the lattice which is not a linear combination of '*a*' and '*b*'. When '*r*' is zero, there exist at least two Buerger reduced cells.

(1) Reduced (Buerger) cells

	a (Å)	*b* (Å)	*c* (Å)	α(°)	β(°)	γ(°)
(i)	2·00	4·00	4·00	60·000	79·200	75·517
(ii)	2·00	4·00	4·00	60·000	86·420	75·517
(iii)	2·00	4·00	4·00	120·000	93·583	104·483
(iv)	2·00	4·00	4·00	117·950	93·583	104·483
(v)	2·00	4·00	4·00	113·967	100·800	104·483

(2) (*a*) $a = 2·05$, $b = 4·00$, $c = 4·10$ Å

				(*b*)	α	β	γ
(i)	2·05	4·00	4·051	(i)	61·225	86·715	75·517
(ii)	2·05	4·00	4·051	(ii)	61·225	79·411	75·517
(iii)	2·05	4·00	4·051	(iii)	61·225	75·625	79·200
(iv)	2·05	4·00	4·060	(iv)	112·680	101·268	104·483
(v)	2·05	4·00	4·054	(v)	116·702	93·979	104·484

(*c*)	$a^{*\prime}$	$b^{*\prime}$	$c^{*\prime}$	(*d*)	*V* (Å^3)	*r* (%)
(i)	0·2824	0·2937	0·5052	(i)	28·12	1·2
(ii)	0·2824	0·2904	0·5052	(ii)	28·11	1·2
(iii)	0·2861	0·2865	0·5052	(iii)	28·11	0·2
(iv)	0·2824	0·2904	0·5071	(iv)	28·11	1·0
(v)	0·2824	0·2937	0·5066	(v)	28·11	1·1

(3) (*a*) $a = 1·95$, $b = 4·00$, $c = 4·10$ Å

				(*b*)	α	β	γ
(i)	1·95	3·99	4·051	(i)	117·055	93·284	103·778
(ii)	1·95	3·99	4·051	(ii)	113·142	100·588	103·778
(iii)	1·95	4·00	4·036	(iii)	113·117	103·530	100·800
(iv)	1·95	3·99	4·042	(iv)	61·403	80·122	76·223
(v)	1·95	3·99	4·049	(v)	61·348	87·433	76·224

(*c*)	$a^{*\prime}$	$b^{*\prime}$	$c^{*\prime}$	(*d*)	*V* (Å^3)	*r* (%)
(i)	0·2824	0·2936	0·5311	(i)	26·76	1·2
(ii)	0·2824	0·2902	0·5311	(ii)	26·76	1·2
(iii)	0·2861	0·2865	0·5311	(iii)	26·74	0·4
(iv)	0·2824	0·2902	0·5292	(iv)	26·76	1·4
(v)	0·2824	0·2936	0·5298	(v)	26·72	1·3

than in Roof's enumeration. Instead, we propose the following procedure which is applied directly to the non-triclinic Bravais lattice types. The process is repeated for each lattice type. The problem may be formulated as a least-squares process. The seven parameters defined above as indicative of a lattice are considered to be the data. The six real cell parameters of the Bravais lattice, $a,b,c,\alpha,\beta,\gamma$, are considered to be the independent variables with appropriate symmetry constraints for the particular lattice type. Either the least-squares matrix can be constructed for all six parameters of the Bravais lattice or only the necessary variables may be varied. In the former case, symmetry constraints must be applied. If appropriate weights are used in the least-squares process, then each result provides a measure in standard deviations of the difference between the cell of interest and the non-triclinic Bravais lattice in question:

$$d^2 = [\Delta a/\sigma(a)]^2 + [\Delta b/\sigma(b)]^2 + \ldots + [\Delta V/\sigma(V)]^2.$$

Minimizing d^2 gives the best cell of the specified type and a direct statistical measure of the difference from the input cell. It may be necessary to carry out a preliminary search on a grid in order to avoid false minima.

A second application is the comparison of two unit cells. As in the determination of Bravais lattice type, the distortion of one lattice with respect to another can be quantified. One could report an agreement factor computed as the square root of the sum of the squares of the differences of each of the seven parameters divided by the standard deviations. Some thought must be given to the covariance terms, since we are using seven parameters, and there may be fewer independent parameters defining a lattice. For example, the cubic lattices reduce to one parameter. Thus the measure given would overestimate the disagreement by about the square root of six.

Finally, Mighell (1976) suggested that data bases containing unit-cell information could be searched to identify unknown substances which happen to be crystalline. We have programmed our algorithm and used it to search the Cambridge Crystallographic Data Centre data base. The search is rapid and no false matches have been found. As an example, we searched using the cell parameters for the high-pressure form of benzene, $P2_1/c$, $a = 5{\cdot}417$, $b = 5{\cdot}376$, $c = 7{\cdot}532$ Å, $\beta = 110{\cdot}00°$. With up to 4% deviation in the seven parameters, three additional matches are found: high-pressure benzene, $P2_1/c$, $a = 5{\cdot}417$, $b = 5{\cdot}376$, $c = 7{\cdot}352$ (*sic*) Å; dimethyl sulfone, *Amma*, $a = 7{\cdot}36$, $b = 7{\cdot}36$, $c = 8{\cdot}00$ Å; dimethyl sulfone, *Cmcm*, $a = 7{\cdot}36$, $b = 8{\cdot}04$, $c = 7{\cdot}34$ Å. In many cases, fewer matches are found than would be found if only reduced-cell lengths and volume were searched. Two primitive triclinic cells from the *Determinative Tables* (Donnay & Ondik, 1973) are: $a = 7{\cdot}581$, $b = 7{\cdot}646$, $c = 7{\cdot}124$ Å, $\alpha = 106{\cdot}90$, $\beta = 100{\cdot}72$, $\gamma = 115{\cdot}12°$ and $a = 7{\cdot}604$, $b = 7{\cdot}649$, $c = 7{\cdot}109$ Å, $\alpha = 100{\cdot}52$, $\beta = 106{\cdot}78$, $\gamma = 115{\cdot}08°$. If the comparison is based only on the reduced-cell lengths and volumes, the maximum disagreement is 0·4% (in the volume). However, the largest disagreement in the full seven parameters is 1·1% (in $a^{*\prime}$). As expected, a number of test searches have not missed any compound which should be matched.

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