We can write $Q = \frac{1}{2}(Q+Q^*) + \frac{1}{2}(Q-Q^*)$, where the first two terms on the right constitute its real, and the last two its imaginary part. Both $G(R)$ and $G'(R)/2\pi i$ have Hermitian symmetry, since they are Fourier transforms of the real functions $\varrho(u)$ and $u\varrho(u)$, repectively. Consequently

$$Q = \frac{1}{2}\int_0^\infty G(-R)\,\frac{G'(R)}{2\pi i}\,\mathrm{d}R + \frac{1}{2}\int_0^\infty G(R)\,\frac{G'(-R)}{2\pi i}\,\mathrm{d}R$$

$$+ \frac{1}{2}\int_0^\infty [G(-R)G'(R)/2\pi i - G(R)G'(-R)/2\pi i]\mathrm{d}R$$

$$= -\frac{1}{2}\int_0^{-\infty} G(S)\,\frac{G'(-S)}{2\pi i}\,\mathrm{d}S$$

$$+ \frac{1}{2}\int_0^\infty G(R)\,\frac{G'(-R)}{2\pi i}\,\mathrm{d}R + \frac{1}{4\pi i}\int_0^\infty \frac{\mathrm{d}}{\mathrm{d}R}$$

$$\times\, [G(-R)G(R)]\mathrm{d}R$$

$$= \frac{1}{2}\int_{-\infty}^\infty G(R)\,\frac{G'(-R)}{2\pi i}\,\mathrm{d}R - \frac{i}{4\pi}[|G(R)|^2]_{R=0}^{R=\infty}$$

$$= \frac{1}{2}\int_{-\infty}^\infty G(R)\,\frac{G'(-R)}{2\pi i}\,\exp(-2\pi iRx)\mathrm{d}r|_{x=0}$$

$$+ iG^2(0)/4\pi ,$$

since $|G(\infty)|^2 = 0$.

By the convolution theorem, the integral is the convolution of the transforms of $G(R)$ and of $G'(R)/2\pi i$, i.e.

$$Q = \frac{1}{2}\int_{-\infty}^\infty \varrho(u)\,(u-x)\varrho(u-x)\mathrm{d}u|_{x=0} + iG^2(0)/4\pi .$$

$$\therefore\ Q = \frac{1}{2}\int_{-\infty}^\infty u\varrho^2(u)\mathrm{d}u + (i/4\pi)[\int_{-\infty}^\infty \varrho(u)\mathrm{d}u]^2.$$

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The Relation between Reduced and Conventional Unit Cells for Centred Monoclinic Lattices

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It is known that 13 among the 44 types of (Niggli) reduced cells correspond to centred monoclinic lattices. For these 13 types, the connexion is given between the reduced cell and a conventional cell. For centred lattices of monoclinic and orthorhombic symmetry, we describe the shape of the conventional cell for the different types of reduced cell. Errors are corrected in the section on Reduced Cells of the International Tables for X-ray Crystallography [Vol. I (1969), Birmingham: Kynoch Press].

Introduction

In 1928, Niggli described a unique choice of 'reduced' cell among the infinitely many different primitive cells

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by which a given lattice can be described. Such a unique choice makes it possible to list the lattice parameters in a standard way also in the case of monoclinic and triclinic crystals. Niggli showed how the Bravais class can be read off the reduced cell, and described the connexion between the reduced cell and a (generally not primitive) conventional cell that respects the lattice symme-

try. However, he did not give a method for passing from an arbitrary cell to the reduced cell. An important step in this direction was achieved by Buerger (1957, 1960), and the method was completed by Santoro & Mighell (1970). A concise account of the reduction procedure was given by Gruber (1973).

The third edition of Vol. 1 of *International Tables for X-ray Crystallography* contains an article on reduced cells by Mighell, Santoro & Donnay (1969). A number of errors in this article have been corrected by Mighell, Santoro & Donnay (1971) and by Parthé & Hornstra (1973). The article includes a useful table summarizing and extending Niggli's results for the 44 cases of reduced cell that can be distinguished. Two types of error remain in the table. In seven of the thirteen cases of centred monoclinic lattice, the transformations from the reduced to a conventional cell are not consistent with the stated conventions. The relations between the dimensions of a conventional cell given for centred lattices of orthorhombic and monoclinic symmetry are not always given correctly. These shortcomings have motivated the investigations reported in this paper.

Reduced cells

A basis of the lattice A is a set of three lattice vectors $\hat{a}$, $\hat{b}$, $\hat{c}$ such that each lattice vector has the form $n_1\hat{a}+n_2\hat{b}+n_3\hat{c}$, where the n_i are integers. Each basis determines a matrix

$$\begin{pmatrix} \hat{a}.\hat{a} & \hat{b}.\hat{b} & \hat{c}.\hat{c} \\ \hat{b}.\hat{c} & \hat{a}.\hat{c} & \hat{a}.\hat{b} \end{pmatrix}.$$

Among the matrices associated with the infinitely many different bases that can be chosen for a given lattice

A, there is always one and only one matrix that satisfies the conditions given by Niggli (1928). The reader may find these conditions also, *e.g.*, in Table 5.1.2.1 of Mighell, Santoro & Donnay (1969) (where the sign for the absolute value is missing in three places) or in Santoro & Mighell (1970).

A parallelepiped with edges given by the vectors of a basis forms a primitive cell of the lattice. If the matrix of the basis satisfies the Niggli conditions, the matrix, the cell, and the basis will be called 'reduced'. Depending on the values of $\hat{a}.\hat{a}$, $\hat{b}.\hat{b}$, $\hat{c}.\hat{c}$, $\hat{b}.\hat{c}$, $\hat{a}.\hat{c}$, and $\hat{a}.\hat{b}$, one can distinguish 44 different forms of reduced matrices. For each of these forms, Niggli has given the Bravais class of the lattice and he has discussed the relations between the reduced cell and a conventional cell.

Centred monoclinic lattices

Mighell, Santoro & Donnay (1969), to whom we shall refer as MSD, use for primitive monoclinic lattices a conventional cell determined by a right-handed system of lattice vectors **a**, **b**, **c** with the following properties: **b** has the direction of the twofold symmetry axis, **a** is the shortest vector perpendicular to **b**, and **c** is the shortest vector perpendicular to **b** that makes an obtuse angle with **a**. These conditions can be expressed as

$$\mathbf{a}.\mathbf{b}=\mathbf{b}.\mathbf{c}=0<-2\mathbf{a}.\mathbf{c}\le a^2\le c^2, \tag{1}$$

where a denotes the length of **a**. We can divide the centred monoclinic lattices into C lattices, A lattices, and I lattices according to whether they are obtained from the cell (1) by centring the $(\mathbf{a},\mathbf{b})$ face (C), centring the $(\mathbf{b},\mathbf{c})$ face (A) or by body centring (I).

Table 1. *The shortest three non-coplanar vectors and the corresponding right-handed reduced basis*

Lattice	Lengths of the shortest three non-coplanar vectors			Reduced basis				Number
	Shortest	Second	Third	$\hat{a}$	$\hat{b}$	$\hat{c}$		
C	a	c	d	$\mathbf{a}$	$-\mathbf{c}$	$\mathbf{d}^+$		28
	a	d	c	$-\mathbf{a}$	$-\mathbf{d}^+$	$\mathbf{c}$		29
	b	d	c	$-\mathbf{b}$	$\mathbf{d}^+$	$\mathbf{c}$		39
	d	d	c	$\left\{\begin{array}{l}\mathbf{d}^+ \\ -\mathbf{d}^+\end{array}\right.$	$\begin{array}{l}\mathbf{d}^- \\ -\mathbf{d}^-\end{array}$	$\begin{array}{l}-\mathbf{c} \\ -\mathbf{c}\end{array}$	if $a>b$ if $a<b$	10 14
A	a	b	e	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{e}^-$		41
	a	c	e	$\mathbf{a}$	$-\mathbf{c}$	$-\mathbf{e}^-$		30
	a	e	e	$\left\{\begin{array}{l}-\mathbf{a} \\ -\mathbf{a}\end{array}\right.$	$\begin{array}{l}\mathbf{e}^- \\ -\mathbf{e}^-\end{array}$	$\begin{array}{l}\mathbf{e}^+ \\ -\mathbf{e}^+\end{array}$	if $c>b$ if $c<b$	20 25
	b	a	e	$-\mathbf{b}$	$-\mathbf{a}$	$-\mathbf{e}^-$		37
	b	e	a	$\mathbf{b}$	$\mathbf{e}^-$	$\mathbf{a}$		39
	e	e	a	$\left\{\begin{array}{l}\mathbf{e}^- \\ -\mathbf{e}^-\end{array}\right.$	$\begin{array}{l}\mathbf{e}^+ \\ -\mathbf{e}^+\end{array}$	$\begin{array}{l}-\mathbf{a} \\ -\mathbf{a}\end{array}$	if $c>b$ if $c<b$	10 14
I	a	b	f	$-\mathbf{a}$	$-\mathbf{b}$	$\mathbf{f}^+$		41
	a	c	f	$\mathbf{a}$	$\mathbf{c}$	$-\mathbf{f}^+$		43
	a	f	f	$\left\{\begin{array}{l}\mathbf{a} \\ \mathbf{a}\end{array}\right.$	$\begin{array}{l}\mathbf{f}^+ \\ -\mathbf{f}^+\end{array}$	$\begin{array}{l}\mathbf{f}^- \\ -\mathbf{f}^-\end{array}$	if $(a+c)^2>b^2$ if $(a+c)^2<b^2$	20 25
	b	a	f	$\mathbf{b}$	$\mathbf{a}$	$-\mathbf{f}^+$		37
	b	f	a	$-\mathbf{b}$	$\mathbf{f}^+$	$-\mathbf{a}$		39
	b	f	g	$\mathbf{b}$	$\mathbf{f}^+$	$\mathbf{g}^+$		27
	f	f	a	$\left\{\begin{array}{l}\mathbf{f}^+ \\ -\mathbf{f}^+\end{array}\right.$	$\begin{array}{l}\mathbf{f}^- \\ -\mathbf{f}^-\end{array}$	$\begin{array}{l}\mathbf{a} \\ \mathbf{a}\end{array}$	if $(a+c)^2>b^2$ if $(a+c)^2<b^2$	10 14
	f	f	g	$-\mathbf{f}^+$	$\mathbf{f}^-$	$\mathbf{g}^+$		17

A reduced basis consists of the shortest three vectors of the lattice that do not lie in a plane. Candidates for basis vectors are therefore $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ and $\mathbf{d}^{\pm} = \frac{1}{2}(\mathbf{a} \pm \mathbf{b})$ for C lattices, $\mathbf{e}^{\pm} = \frac{1}{2}(\mathbf{c} \pm \mathbf{b})$ for A lattices, $\mathbf{f}^{\pm} = \frac{1}{2}(\mathbf{a} \pm \mathbf{b} + \mathbf{c})$ and $\mathbf{g}^{\pm} = \frac{1}{2}(\mathbf{a} \pm \mathbf{b} - \mathbf{c})$ for I lattices. Taking into account that

$$d \equiv d^{\pm} = \frac{1}{2}(a^2 + b^2)^{1/2} < a \quad \text{or} \quad < b ,$$
$$e \equiv e^{\pm} = \frac{1}{2}(b^2 + c^2)^{1/2} < b \quad \text{or} \quad < c ,$$
$$f \equiv f^{\pm} = \frac{1}{2}(a^2 + b^2 + c^2 + 2\mathbf{a} \cdot \mathbf{c})^{1/2} < g$$
$$\equiv g^{\pm} = \frac{1}{2}(a^2 + b^2 + c^2 - 2\mathbf{a} \cdot \mathbf{c})^{1/2}, \quad f < b \quad \text{or} \quad < c$$
$$g < b \quad \text{or} \quad < c ,$$

we are left with the possibilities listed in Table 1.

Among the 44 different types of reduced cell, 13 correspond to centred monoclinic lattices. In MSD these 13 types carry the numbers 10, 14, 17, 20, 25, 27, 28, 29, 30, 37, 39, 41, and 43. These numbers are given in the last column of Table 1. We see that among the 13 cases of centred monoclinic lattice there are six that consist of one type of lattice exclusively: 28 and 29 are C lattices, 30 A lattices, 17, 27, and 43 I lattices. The conditions under which each of the remaining seven cases is a C, A, or I lattice follow from equation (1) and are given in Table 2.

We can do without A-centred cells if we do not require $a \le c$ for the C-centred cell, $i.e.$: we can introduce a new conventional cell $\mathbf{a}_1$, $\mathbf{b}_1$, $\mathbf{c}_1$ for A lattices:

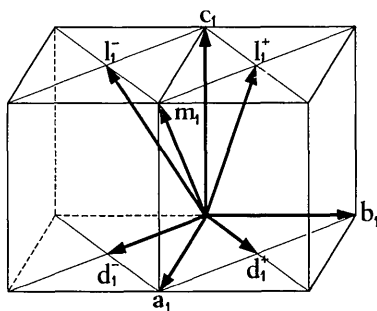$$\mathbf{a}_1 = \mathbf{c}, \quad \mathbf{b}_1 = -\mathbf{b}, \quad \mathbf{c}_1 = \mathbf{a},$$

Fig. 1. The new conventional cell for I lattices.

whence

$$\mathbf{a} = \mathbf{c}_1, \quad \mathbf{b} = -\mathbf{b}_1, \quad \mathbf{c} = \mathbf{a}_1, \quad \mathbf{e}^{\pm} = \frac{1}{2}(\mathbf{a}_1 \mp \mathbf{b}_1) = \mathbf{d}_1^{\mp} .$$

From equation (1) we obtain then for A lattices

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{b}_1 \cdot \mathbf{c}_1 = 0 < -2\mathbf{a}_1 \cdot \mathbf{c}_1 \le c_1^2 \le a_1^2 . \qquad (2)$$

MSD state in the footnote to their Table 5.1.3.1 that they have adopted this choice for the conventional cell. Following Niggli (1928), MSD consider an I-centred cell for 17, 27, and 43 and a C-centred cell otherwise. However, our Table 1 shows that for the MSD choice of the conventional cell, both kinds of centring come into play for 10, 14, 20, 25, 37, 39, and 41.

We do not want to consider different kinds of centring for a single type of reduced cell and we want to follow MSD as closely as possible. This can be done by choosing for I lattices a new conventional cell (Fig. 1) defined by vectors

$$\mathbf{a}_1 = \mathbf{a} + \mathbf{c}, \quad \mathbf{b}_1 = \mathbf{b}, \quad \mathbf{c}_1 = -\mathbf{a},$$

whence

$$\mathbf{a} = -\mathbf{c}_1, \quad \mathbf{b} = \mathbf{b}_1, \quad \mathbf{c} = \mathbf{a}_1 + \mathbf{c}_1 \equiv \mathbf{m}_1 ,$$

$$\mathbf{f}^{\pm} = \frac{1}{2}(\mathbf{a}_1 \pm \mathbf{b}_1) = \mathbf{d}_1^{\pm} , \quad \mathbf{g}^{\pm} = -(\mathbf{c}_1 + \mathbf{d}_1^{\mp}) \equiv -\mathbf{l}_1^{\mp} .$$

Table 3. *Connexion between reduced and C centred conventional cell for the cases* 17, 27 *and* 43

Number	Transformation from reduced cell to conventional cell	Dimensions of conventional cell
17	$\overline{1}10/\overline{1}\overline{1}0/101$	$a_1 = [2(2\hat{a}^2 - \|\hat{\mathbf{b}} \cdot \hat{\mathbf{c}}\| - \|\hat{\mathbf{a}} \cdot \hat{\mathbf{c}}\|)]^{1/2}$ $b_1 = [2(\|\hat{\mathbf{b}} \cdot \hat{\mathbf{c}}\| + \|\hat{\mathbf{a}} \cdot \hat{\mathbf{c}}\|)]^{1/2}$ $c_1 = [\hat{a}^2 + \hat{c}^2 - 2\|\hat{\mathbf{a}} \cdot \hat{\mathbf{c}}\|]^{1/2}$ $\cos \beta_1 = 2(\|\hat{\mathbf{a}} \cdot \hat{\mathbf{c}}\| - \hat{a}^2)/a_1 \cdot c_1$
27	$1\overline{2}0/\overline{1}00/01\overline{1}$	$a_1 = [4\hat{b}^2 - \hat{a}^2]^{1/2}$ $b_1 = \hat{a}$ $c_1 = [\hat{b}^2 + \hat{c}^2 - 2\hat{\mathbf{b}} \cdot \hat{\mathbf{c}}]^{1/2}$ $\cos \beta_1 = 2(\hat{\mathbf{b}} \cdot \hat{\mathbf{c}} - \hat{b}^2)/a_1 \cdot c_1$
43	$\overline{1}10/\overline{1}\overline{1}2/100$	$a_1 = [\hat{a}^2 + \hat{b}^2 - 2\|\hat{\mathbf{a}} \cdot \hat{\mathbf{b}}\|]^{1/2}$ $b_1 = [4\hat{c}^2 - \hat{a}^2 - \hat{b}^2 + 2\|\hat{\mathbf{a}} \cdot \hat{\mathbf{b}}\|]^{1/2}$ $c_1 = \hat{a}$ $\cos \beta_1 = (\|\hat{\mathbf{a}} \cdot \hat{\mathbf{b}}\| - \hat{a}^2)/a_1 \cdot c_1$

Table 2. *The conditions under which a reduced matrix of a given form describes a C, A, or I lattice*

Number	$\hat{\mathbf{a}} \cdot \hat{\mathbf{a}}$ $\hat{\mathbf{b}} \cdot \hat{\mathbf{c}}$	$\hat{\mathbf{b}} \cdot \hat{\mathbf{b}}$ $\hat{\mathbf{a}} \cdot \hat{\mathbf{c}}$	$\hat{\mathbf{c}} \cdot \hat{\mathbf{c}}$ $\hat{\mathbf{a}} \cdot \hat{\mathbf{b}}$	C lattice	Conditions for A lattice	I lattice
10	A D	A D	C F	$2A + 2F \le C$	$2A + 2F \ge C \ge 4D$	$C \le 4D$
14	A $-D$	A $-D$	C $-F$	$2A - 2F \le C$	$2A - 2F \ge C \ge 4D$	$C \le 4D$
20	A D	B E	B E		$A \ge 4E$	$A \le 4E$
25	A $-D$	B $-E$	B $-E$		$A \ge 4E$	$A \le 4E$
37	A $-D$	B $-\frac{1}{2}A$	C 0		$B \ge 4D$	$B \le 4D$
39	A $-D$	B 0	C $-\frac{1}{2}A$	$4B - A \le C$	$4B - A \ge C \ge 4D$	$C \le 4D$
41	A $-\frac{1}{2}B$	B $-E$	C 0		$A \ge 4E$	$A \le 4E$

Table 4. *The shape of the C-centred conventional cell for the different types of reduced cell*

Relations between cell dimensions					Number
$b_1 < a_1$	$b_1 < d_1$	$c_1 < b_1$			41
		$b_1 \le c_1$	$c_1 < d_1$		37
			$d_1 \le c_1$	$c_1 < l_1$	39
				$l_1 \le c_1$	27
	$d_1 \le b_1$	$l_1 < c_1$			17
		$c_1 \le l_1$	$c_1 < d_1$		
			$d_1 = c_1$	$a_1^2 - b_1^2 < -2\mathbf{a}_1 . \mathbf{c}_1$	20
				$-2\mathbf{a}_1 . \mathbf{c}_1 < a_1^2 - b_1^2$	
			$d_1 < c_1$		10
$a_1 \le b_1$	$d_1 < a_1$	$d_1 < m_1$	$c_1 < d_1$		
			$c_1 < d_1$	$b_1^2 - a_1^2 < -2\mathbf{a}_1 . \mathbf{c}_1$	25
			$d_1 = c_1$	$-2\mathbf{a}_1 . \mathbf{c}_1 < b_1^2 - a_1^2$	
			$d_1 < c_1$		14
		$m_1 \le d_1$			43
	$a_1 \le d_1$	$c_1 < a_1$			30
		$a_1 \le c_1$	$c_1 < d_1$		28
			$d_1 \le c_1$		29

From equation (1) we obtain for I lattices

$$\mathbf{a}_1 . \mathbf{b}_1 = \mathbf{b}_1 . \mathbf{c}_1 = 0,$$
$$-\mathbf{a}_1 . \mathbf{c}_1 < c_1^2 \le -2\mathbf{a}_1 . \mathbf{c}_1 \le a_1^2 . \tag{3}$$

Combining equations (1–3) and putting $\mathbf{a}_1 = \mathbf{a}$, $\mathbf{b}_1 = \mathbf{b}$, $\mathbf{c}_1 = \mathbf{c}$ for C lattices, we see that all three kinds of centred monoclinic lattice can be obtained by C centring a cell $\mathbf{a}_1$, $\mathbf{b}_1$ $\mathbf{c}_1$ satisfying

$$\mathbf{a}_1 . \mathbf{b}_1 = \mathbf{b}_1 . \mathbf{c}_1 = 0,$$
$$0 < -2\mathbf{a}_1 . \mathbf{c}_1 \le a_1^2, \quad -\mathbf{a}_1 . \mathbf{c}_1 < c_1^2 . \tag{4}$$

We shall call this cell the C-centred conventional cell. Given a centred monoclinic lattice, this new conventional cell can be characterized as follows: $\mathbf{b}_1$ has the direction of the twofold symmetry axis, $\mathbf{a}_1$ is the shortest vector perpendicular to $\mathbf{b}_1$ such that the rectangular net in the $\mathbf{a}_1\mathbf{b}_1$ plane is centred, and $\mathbf{c}_1$ is the shortest vector perpendicular to $\mathbf{b}_1$ that makes an obtuse angle β_1 with $\mathbf{a}_1$.

Table 3 gives the connexion between the reduced cell and our C-centred cell for the cases in which MSD use an I-centred conventional cell.

Donnay, Donnay, Cox, Kennard & King (1963) use a conventional cell defined by vectors $\bar{\mathbf{a}}$, $\bar{\mathbf{b}}$, $\bar{\mathbf{c}}$ satisfying $\bar{c} \le \bar{a}$. This choice is related to ours by

$$\bar{\mathbf{a}} = \mathbf{c}_1, \quad \bar{\mathbf{b}} = -\mathbf{b}_1, \quad \bar{\mathbf{c}} = \mathbf{a}_1 \quad \text{for } C \text{ lattices}$$
$$\bar{\mathbf{a}} = \mathbf{a}_1, \quad \bar{\mathbf{b}} = \mathbf{b}_1, \quad \bar{\mathbf{c}} = \mathbf{c}_1 \quad \text{for } A \text{ lattices}$$
$$\bar{\mathbf{a}} = \mathbf{a}_1 + \mathbf{c}_1, \quad \bar{\mathbf{b}} = -\mathbf{b}_1, \quad \bar{\mathbf{c}} = -\mathbf{c}_1 \quad \text{for } I \text{ lattices.}$$

In Table 4, we describe in a systematic manner how the type of the reduced cell can be deduced from the shape of the C centred conventional cell. Notice that

$$d_1 = \tfrac{1}{2}(a_1^2 + b_1^2)^{1/2} < a_1 \quad \text{or} \quad < b_1$$
$$l_1 = (d_1^2 + \mathbf{a}_1 . \mathbf{c}_1 + c_1^2)^{1/2} > d_1$$
$$m_1 = (a_1^2 + 2\mathbf{a}_1 . \mathbf{c}_1 + c_1^2)^{1/2} > c_1 .$$

Centred orthorhombic lattices

MSD use a conventional cell satisfying $a_1 < b_1 < c_1$ for face- and body-centred orthorhombic lattices; they choose the side-centred orthorhombic lattice to be C-

centred with $a_1 < b_1$. The relations between the dimensions of these conventional cells for the various forms of reduced bases are given in Table 5.

Table 5. *Relations between the dimensions of the conventional cell for centred orthorhombic lattices*

Bravais class	Relations between cell dimensions			Number
Orthorhombic F	$b_1 < \sqrt{3}a_1$			16
	$b_1 \ge \sqrt{3}a_1$			26
Orthorhombic I	$a_1 > e$			8
$e = \tfrac{1}{2}(a_1^2 + b_1^2 + c_1^2)^{1/2}$	$a_1 \le e \le b_1$			19
	$e > b_1$			42
Orthorhombic C	$b_1 < \sqrt{3}a_1$	$c_1 \ge d$		13
		$c_1 < d$		23
$d = \tfrac{1}{2}(a_1^2 + b_1^2)^{1/2}$	$b_1 > \sqrt{3}a_1$	$c_1 \ge d$		38
		$c_1 < d$	$a_1 \le c_1$	36
			$a_1 > c_1$	40

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