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Conventional cells: monoclinic *I*- and *C*-centered cells

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In the selection of a centered cell in the monoclinic system, it is recommended that the experimentalist select an *I*-centered cell for those cases in which it is the conventional cell — cases in which *a* and *c* are coincident with the shortest two translations in the net perpendicular to *b* (*b*-axis unique). The common practice of selecting a non-conventional *C*-centered cell in such cases should be discontinued.

1. Introduction

International Tables for X-ray Crystallography (1969) contains a section covering reduced cells, reduced forms and conventional cells (Mighell *et al.*, 1969). This section includes a key table that gives a metric classification of the 44 reduced forms. Recently, this table with appropriate revisions was republished in the *Journal of Research of the National Institute of Standards and Technology* (Mighell, 2001). An especially valuable feature of the table is that it defines and allows the user to determine standard conventional cells. For triclinic and monoclinic systems, the table permits one to select a *unique* conventional cell from a variety of possibilities. For the conventional cell in the triclinic system, one selects the reduced cell. For the conventional cell in the monoclinic system, *b* is taken as the unique axis, and *a* and *c* are chosen coincident with the shortest two translations in the net perpendicular to *b*. The angle β is taken as non-acute. This choice allows primitive, side-centered and body-centered lattices.

2. Current status

Since 1969 there has been an evolution towards acceptance and widespread use of such conventional cells. An inspection of the recent articles in *Acta Crystallographica Section C* reveals that most cells either follow these conventions exactly or follow them with minor variations such as re-labeling of cell edges. For example, in the most populous space group, No. 14, experimentalists routinely select the setting (*i.e.* $P2_1/a$, $P2_1/c$ or $P2_1/n$) which is consistent with a cell based on the shortest vectors in the *ac* plane (*b* axis unique).

One major exception remains: a subset of the centered monoclinic lattices. The table with the metric classification of the 44 reduced forms (Mighell, 2001) shows that the conventional monoclinic cell can be either *C*- or *I*-centered depending on the nature of the metric relations in the reduced form. In experimental practice, however, most centered monoclinic lattices are reported on the basis of a *C*-centered cell. When the conventional cell is *C*-centered, it is routinely selected. However, authors generally avoid using a conventional cell that is *I*-centered. Instead, they select a non-conventional *C*-centered cell. Typical examples of this practice are shown in Table 1. In each case, the non-conventional *C*-centered cell reported in *Acta Crystallographica Section C* can be transformed to an *I*-centered conventional cell in which the β angle is much closer to 90°. A detailed analysis of the nature of the problem and the reduced forms corresponding to monoclinic centered lattices are given in the *Journal of Research of the National Institute of Standards and Technology* (Mighell, 2002).

3. Discussion

Statistics using *NIST Crystal Data* (NIST, 1995) reveal that the ratio of monoclinic *side*-centered to *I*-centered conventional cells is approximately 2/1. However, as noted above, experimentalists generally avoid selecting conventional *I*-centered monoclinic cells. For example, in the July 2002 issue of *Acta Crys-*

Table 1
Crystallographic parameters reported for five centered monoclinic cells selected from the recent issues of *Acta Crystallographica Section C*.

The table shows that each literature *C*-centered cell can be transformed to a conventional *I*-centered cell – based on the shortest vectors in the *ac* plane – in which the β angle is closer to 90°. Numbers in parentheses represent standard deviations.

	Lattice I	Lattice II	Lattice III	Lattice IV	Lattice V
Literature cells: monoclinic *C*-centered					
Cell	LC1	LC2	LC3	LC4	LC5
a (Å)	26.454 (3)	24.388 (5)	27.742 (2)	42.785 (12)	18.8609 (3)
b (Å)	14.499 (3)	12.470 (2)	7.8344 (16)	10.320 (14)	15.4691 (4)
c (Å)	14.517 (3)	18.425 (4)	16.2658 (18)	32.238 (11)	11.6010 (2)
β (°)	120.276 (10)	127.74 (3)	125.679 (5)	130.785 (12)	123.145 (9)
V (Å^3)	4808.8 (16)	4431 (2)	2871.7 (7)	10778 (15)	2833.99 (10)
Space group	*C*2/*c*	*C*2/*c*	*C*2/*c*	*C*2/*c*	*C*2/*c*
Ref.	Suzuki *et al.* (2002)	Vojnović *et al.* (2002)	Bakir (2002)	Paavola *et al.* (2002)	Espinosa *et al.* (2002)
Standard conventional cells: monoclinic *I*-centered					
Cell	CC1	CC2	CC3	CC4	CC5
a (Å)	14.517	18.425	16.266	32.238	11.601
b (Å)	14.499	12.470	7.834	10.320	15.469
c (Å)	22.876	19.601	22.535	32.678	15.845
β (°)	92.96	100.28	90.22	97.54	94.66
V (Å^3)	4809	4431	2872	10778	2834
Space group	*I*2/*a*	*I*2/*a*	*I*2/*a*	*I*2/*a*	*I*2/*a*
Normalized reduced forms					
Form	RF1	RF2	RF3	RF4	RF5
a·**a**	1.00	1.00	1.00	1.00	1.00
b·**b**	1.00	1.21	3.38	4.55	1.11
c·**c**	1.08	1.62	3.41	5.85	1.11
b·**c**	−0.46	0.32	1.24	0.32	0.22
a·**c**	−0.50	0.50	0.50	0.50	0.44
a·**b**	0.00	0.50	0.50	0.50	0.44
Form No.	37	27	27	27	20

tallographica Section C, non-conventional *C*-centered cells are used in all five cases where the conventional cell is *I*-centered. Likewise, the same preference has been observed in recent issues of other journals that publish crystallographic data.

In spite of current practice, there are a number of essential advantages to using the conventional *I*-centered cell in such cases. First, the routine use of conventional cells helps prevent errors. In the course of evaluating thousands of unit cells over the years for crystallographic databases, it has been observed that it is not uncommon for the non-conventional skewed *C*-centered monoclinic cells to be associated with errors in space-group and crystal-system assignment. For example, in a recent publication (Sciarone *et al.*, 2002), the reported *C*-centered cell for $C_{54}H_{48}N_2FeBF_{15}$ with a β angle of 113.28° can be transformed to the conventional *I*-centered cell with a β of 90.10°. Clearly the use of the conventional cell immediately alerts one to check for potential orthorhombic symmetry. Second, the use of conventional cells facilitates – especially for the non-crystallographer – the use of structural data as it minimizes the necessity to transform parameters to make comparisons. For example, one can readily determine if two crystalline compounds, with the same composition, are identical or in a polymorphic relationship. Third, the use of the conventional *I*-cell represents the last step required to bring overall consistency and harmony with respect to cell choice in the monoclinic system, *i.e.* always select the shortest vectors in the *ac* plane (*b* unique) for all cells, whether centered or primitive.

Finally, the appropriate use of the *I*-centered cell is required to comply with *Acta Crystallographica*'s nomenclature conventions given in the 'Notes for Authors', which specify that 'the choice of axes should normally follow the recommendations of the Commission on Crystallographic Data [Kennard *et al.* (1967). *Acta Cryst.* **22**, 445–449]'. For the monoclinic system, these recommendations specifiy that one should 'select the shortest two translations in the net perpendicular to the symmetry direction *b*.....and use appropriate centering'. In contrast to earlier years, these recommendations can now readily be complied with as the latest version of Volume A of the *International Tables for Crystallography* (1996) explicitly gives the atomic positions for the various space group settings (*e.g.* *I*2/*a*).

4. Recommendations

For monoclinic centered lattices, it is recommended:

(i) that the crystallographic community routinely use the *I*-centered conventional cell when it is consistent with the shortest vectors in the *ac* plane (*b*-axis unique),

(ii) that instrument manufacturers enhance their software to smoothly guide the user to the *I*-centered cell when it is the conventional cell, and

(iii) that the *Acta Crystallographica* editors and reviewers actively support their own choice-of-axes policy in the editorial process.

The last point is especially important as *Acta Crystallographica* is the premier crystallographic journal whose rules and conventions others emulate. To facilitate the above, it would be especially helpful for *Acta Crystallographica* to add one sentence in the 'Notes for Authors' that explicitly gives the conventions for the choice of axes for monoclinic cells.

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