LETTERS TO THE EDITOR

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Non-conventional settings of crystal structures

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Abstract. The presentation of crystal structures in non-conventional settings not listed in *International Tables for Crystallography* is in some cases reasonable and justified. The arguments in favor of using space-group symbols such as $I\bar{1}$, $C1$ and similar, are put forward and discussed.

Crystal structures published in *Acta Crystallographica* are supposed to be presented in standard settings listed in *International Tables for Crystallography* (1983, Vol. A) unless objective reasons to the contrary are stated (*Notes for Authors*, 1991). In the following cases, however, the non-conventional setting appears to be the only reasonable choice. A small deformation of the conventional lattice cell may result in a lattice which, when using the standard setting, would have to be described in a quite different cell of lower symmetry. If in a series of isomorphic (or nearly isomorphic) compounds some crystal structures happen to be slightly deformed, their description in different settings would render any comparison very inconvenient. It seems reasonable in such cases to preserve the setting independent of symmetry lowering; see, for example, Pietraszko, Łukaszewicz & Augustyniak (1992).

Small deformations of the lattice can be easily overlooked in routine crystal structure determinations, and for many purposes such a simplified structure may be satisfactory, although knowledge of the true symmetry may help in understanding anomalies observed by other methods, *e.g.* ESR (Augustyniak, 1992). Structure analysis of slightly deformed crystal structures requires special attention and precise experiments. It is very probable, therefore, that the redetermination of some crystal structures may reveal small deformations. There are hints in the literature indicating possible deformations of this kind (Davis & Johnson, 1984).

Preservation of the setting of a deformed crystal lattice is also advisable in the publication of the closely related crystal structures of consecutive phases of the same compound. For instance, the ferroelectric $RbHSeO_4$, triclinic at ambient temperature, undergoes a phase transition at 370.5 K to the monoclinic (nearly orthorhombic) paraelectric phase. The crystal structure of triclinic $RbHSeO_4$ has been presented in the non-conventional $I1$ setting (Waśkowska, Olejnik, Łukaszewicz & Głowiak, 1978) in order to emphasize pseudosymmetry and to allow an easy comparison of the paraelectric $RbHSeO_4$ phase with $(NH_4)HSO_4$. A good reason for the application of the non-standard setting may also be the lowering of symmetry owing to ordering of atoms, *e.g.* Al/Si in silicides.

Naturally, in the case of publication of a crystal structure in a non-conventional setting (not listed in *International Tables for Crystallography*), the paper should contain the list of equivalent positions and the transformation matrix which transforms the given data to a new data set corresponding to a description of the structure based on the standard space-group setting.

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