LETTERS TO THE EDITOR

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Non-conventional unit cells

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As a long- time reader of *Acta Crystallographica*, I have become used to many of the non-conventional unit cells that some authors foist on me. I have learned to tolerate space groups $P2_1/a$ and $A2/a$, even though a simple interchange of axes would turn them into the standard $P2_1/c$ and $C2/c$; I have figured out $I2_1/a$, even though the *International Tables* do not recognize a body-centered monoclinic unit cell, and $C\bar{1}$, despite knowing that a triclinic cell must be primitive; I have deduced that *Pnca* is space group No. 60, customarily referred to as *Pbcn*, and that *Pbnm* is really *Pnma*. With somewhat less good will I have put up with unit cells which, for no good reason, have angles less than 60° or greater than 120°, resigning myself to carrying out a cell reduction if I wish to compare with another compound or with another investigation of the the same compound. But I feel that I must stand up and complain when I encounter a triclinic structure described in such a way that *not one* of the three shortest lattice vectors is used as a cell edge.

I refer to an article in the November 1987 issue of *Acta Crystallographica* Section C – '1,6-dioxacyclodeca-3,8-diene', on page 2245. This structure is described as triclinic (space group $P\bar{1}$), with $a = 7.263(15)$, $b = 7.683(15)$, $c = 7.225(12)$ Å, $\alpha = 72.62(5)$, $\beta = 137.37(8)$, $\gamma = 130.36(7)°$. (Just look at those last two angles!) It turns out that the three shortest lattice vectors are [110], [101] and $[\bar{1}\,\bar{1}\,\bar{1}]$; they define a cell with $a' = 6.285$, $b' = 5.266$, $c' = 6.903$ Å, $\alpha' = 103.00$, $\beta' = 113.76$, $\gamma' = 99.41°$. Couldn't at least *one* of these axes have been used by the authors?

Is there a purpose in using such an unusual cell? I see none. But neither, in most instances, do I see a purpose in $P2_1/a$, or $C\bar{1}$, or *Pbnm*. All I see is a *reason*; and the reason I see is laziness. The usual procedure, I believe, is to permit a computer to pick out the unit cell and let it go at that. Rather than going through, once and for all, the very simple (in most software packages that I am aware of) process of interchanging axes so as to produce a convenient unit cell, many investigators leave it to the reader to work things out for himself.

But there may be another reason. Some contributors to *Acta Crystallographica* may believe that the small amount of time they save by not converting to a convenient unit cell is more valuable than the combined time of all readers who might be enough interested in the results so as to carry out the conversions for themselves.

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