LETTERS TO THE EDITOR

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Space-group frequencies

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In a recent note, Srinivasan (1991) criticized Donohue's (1985) revision of the space-group frequency distribution table given by Mighell, Himes & Rodgers (1983). Donohue had proposed that the observed frequency of chiral space groups should be doubled or, for the eleven enantiomorphic pairs of space groups, added together. His argument was that the determination of a given compound in a chiral space group automatically determines that the enantiomeric compound will crystallize in the same or, for the eleven pairs, in the enantiomeric space group. Srinivasan argues that Donohue's revision is unwarranted since only experimentally observed structures should enter the statistics; in his view the assumption of equal probability of occurrence of enantiomeric structures is unjustifiable.

Since enantiomorphic structures are isometric it follows that they are equienergetic, and hence they do have the same probability of occurrence, at least in a thermodynamic sense (we ignore the practical problems of synthesizing the enantiomer of a complex natural product). However, since these structures are isometric we agree that there is no point in counting them twice. Only non-isometric structures should be included in a list of space-group frequencies.

However, if this line of argument is accepted, it follows that the original tabulation of Mighell, Himes & Rodgers (1983) does still require revision. From this table one could get the impression that there is an intrinsic preference for right-handed screw axes over left-handed ones: for example, $P4_1$ (47) against $P4_3$ (7), or $P4_12_12$ (101) against $P4_32_12$ (44). Only for $P6_1$ (14) and $P6_5$ (16) is this swing reversed. We have not checked, but it is likely that the absolute sense of chirality of many of these structures was not established. Even where it is known, the space-group chirality depends on the molecular chirality (for resolved non-interconverting enantiomers) or on chance (for crystals built from intrinsically achiral molecules or from solutions containing both enantiomers). One may suspect that the apparent preference for right-handed screw axes arises because the corresponding space group usually precedes the enantiomorphic one in tabulations. In view of this arbitrariness and the isometric relation between enantiomorphs, the eleven pairs of enantiomorphic space groups should be combined for this purpose and their frequencies added together. For the unlikely event that both enantiomeric structures have actually been determined in enantiomorphic space groups, then, of course, the pair should only be counted once.

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