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The Hazards of Using Space Groups of Too High Symmetry. Frank R. Fronczek, Dept. of Chemistry, Louisiana State Univ., Baton Rouge, LA, 70803.

Marsh and others have heightened the awareness of the crystallographic community about the hazards of describing structures in space groups of unnecessarily low symmetry. Nowadays, excellent software is widely available to check for such problems, and the probability of committing such an error is low, as long as one is moderately attentive. A hazard which is less easily detectable is that of using popular space groups when the true symmetry is actually lower, and the structure is pseudosymmetric. Examples will be described in which the structure masquerades as P-1, but is really P1, as C2/c, but is really Cc, etc. Although a somewhat acceptable refinement is usually possible in the higher-symmetry space group, making this inverse-Marsh error can also lead to incorrect chemical conclusions. A clue to the presence of this problem is disorder in the higher-symmetry model, when it would not be expected from the Wilson-plot B and from the appearance of the diffraction pattern.

Examples of unexpectedly racemic natural products will be discussed, as will the related phenomenon of kryptoracemic structures, in which the space group is chiral, but the asymmetric unit consists of racemic pairs.

Time permitting, some Dick Marsh stories from the early 1970s will be told, some of which may even be true.