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Space group *P*1: an update

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A new survey of the Cambridge Structural Database has uncovered 115 additional crystal structures that were described in the space group *P*1, but would be better described in groups of higher symmetries.

In 1999, a survey was carried out (Marsh, 1999) of all the crystal structures entered into the October 1998 release of the Cambridge Structural Database (Allen, 2002) and assigned to the space group *P*1; of approximately 1300 such entries, 279 were found to have inappropriate space-group designations. In 157 instances the reason for the incorrect designation was very simple: in the original paper, the 'overline' was missing from the space-group symbol '$P\bar{1}$', probably because of difficulties in producing the symbol on word processors. The remaining errors arose from either an incorrect assignment of lattice type or the failure to recognize a center of inversion, or occasionally both. This is a follow-up report. It is based primarily on a computer-controlled search, using the program *PLATON* (Spek, 2003), of the Cambridge Structural Database (CSD) release for the year 2003 plus a manual search of three update releases in 2004. As a result of this new survey, 115 additional structures that were improperly described in the space group *P*1 have been found. They are identified by their CSD refcodes in the supplementary material and coordinates for the revised structures have been submitted in CIF form to the CSD.[1]

What trend can we see in the frequency of incorrect structures? It seems to be an encouraging one. I found no additional examples of the 'missing overline' syndrome; the CSD has apparently searched out and corrected all past entries and is checking – and correcting, if necessary – current entries as they are submitted. However, there is, as yet, no clear evidence that errors of other sorts are on the decline. The three 2004 updates to the CSD contain, in all, 231 entries in space group *P*1; of these, 32 should be described in space groups of higher symmetry. This ratio is similar to that found in the Marsh (1999) survey. Some important journals, including *Acta Crystallographica*,[2] now carry out symmetry checks for all submitted structures, which should have led to a significant reduction in the number of errors; it is possible that this reduction is offset by an increasing tendency to rely, without careful inspection and consideration, on results produced by automated data-collection methods and structure-solving routines. However, we can hope that, in the near future, all crystal-structure reports will be routinely subject to inspection by one of the powerful symmetry-checking programs (such as *PLATON*; Spek, 2003) that are readily available.

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References

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