Relationships between Independent Molecules in *Z*′=2 Structures

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Approximately 11% of organic structures in the Cambridge Structural Database (CSD) [1] have more than one molecule in the asymmetric unit ($Z'>1$) and of these almost 90% have $Z'=2$. Disorder in these structures is more common than in structures with $Z'=1$ and the distribution of disorder between the crystallographically-independent molecules has been investigated.

A sizeable proportion of $Z'=2$ structures are thought to exhibit pseudosymmetry. A method for assessing the extent of pseudo-symmetry in $Z'=2$ structures which do not exhibit disorder has been developed and suitable structures from the CSD have been evaluated using *CRYSTALS* [2].

Using this method, an analysis of the different relationships between molecules has been carried out. In particular, the nature of the rotation-translation operator relating the molecules in pseudosymmetric structures has been examined. The frequencies of different types of operator were considered for some common space groups, with emphasis on pseudo-translations and pseudo-inversions in non-centrosymmetric space groups which can pose particular problems in refinement [3]. This analysis is compared with previous work on the prevalence of certain symmetry elements [4].

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Keywords: pseudosymmetry, space-group symmetry, disorder