Different Reasons for Packing with Z'=2: 4-nitroimidazole Derivatives

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The packing of the molecules in crystals is a result of the compromise between different intermolecular interactions, tendency towards close packing, symmetry requirements etc. All these factors, hierarchically organized and influencing one another, determine the unique three-dimensional structure, the molecular crystal.

The compromise between different requirements sometimes requires the presence of more than one molecule in the asymmetric unit. That means that there are molecules in the crystal which are not related by any symmetry operation while still being chemically identical. A study of the connections between this phenomenon and packing conflicts is essential for predicting organic crystal structures. A further goal could be to try to correlate the occurrence of multiple molecules in the asymmetric unit with the presence of certain functional groups in the molecules, space group symmetries etc.

The analysis of the frequency of different Z' values in the crystal structures shows that above-average percentage of the structures with Z'>1 is observed for imidazole derivatives.

The different reasons for packing with Z'=2 will be presented for 4-nitroimidazole derivatives. For example, in two closely-related 1-R-2-methyl-4-nitroimidazoles the creation of bilayers of molecules, the primary building blocks of the crystal structures, is possible because there are two symmetry-independent molecules that have either different conformations or take part in different intermolecular interactions.

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