Modification of the program FOX for using intermolecular distances from ssNMR

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The direct-space approach used for crystal structure determination from powder diffraction data is a powerful tool that has enabled many crystal structures to be solved. However, this approach is still severely limited by the complexity of the model. In terms of degrees of freedom, the current limit is around 40 [1,2]. The main reasons for such a limit are the time consumption and the impossibility of distinguishing between correct and wrong solutions according to the measured powder diffraction pattern. The direct-space methods find the structural model by changing the position and shape of the molecular fragments in the unit cell. They allow defining additional restrictions for the optimized model, handled as additional observations. Thus, the model can be restricted, for example, by torsion angles or rigid groups, as it is already implemented in existing software [3,4]. All these additional observations aim to make it possible to find a solution or at least significantly reduce the calculation time.

The probability of finding the correct solution can be increased using information about non-bonding intermolecular interactions. This kind of information can be obtained by performing a specific ssNMR measurement which usually offers a list of short-range interactions between atoms. Alternatively, the distances of expected hydrogen bonds of a usual dimer of the studied compound can also be used. We have implemented the ability to add intermolecular distance constraints to the existing FOX software and have tested it on several compounds. Based on the ssNMR experiment, we defined intermolecular distances between several selected atoms with various precisions, and we used them as additional restrictions for the structure solution from X-ray powder diffraction data.


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