Powder Struture resolution of 1,7-Dioxaspiro[4.4]nonane

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Different attempts to crystallise compound 1,7-dioxaspiro[4.4]nonane, led to very small and irregular crystals which were not good enough to be analysed by the single-crystal X-ray diffraction technique. Moreover, the data collected with powder diffraction technique, was very poor to work with conventional direct methods for the structure solution.

The powder pattern was indexed using the program suite Crysfire. We have modeled different configurations in agreement with the other experimental analyses in order to test them with the powder diffraction data. We have located the different modeled solutions into the refined unit cell with the F.O.X. program. The Rietveld method was used for the refinement of the positions of non H atoms using the Bruker AXS Topas program.

Based on the results of the above mentioned method, it is possible to conclude that the technique of structural resolution by powder diffraction data is sensitive to changes of the atomic positions, or on the nature of atoms of the modeled molecule, and that this technique has allowed the confirmation of the structure of mentioned compound as it was suggested by means of spectroscopic techniques.

Keywords: powder structure resolution, organic structure determination, 1,7-dioxaspiro[4.4]nonanes