

Microsymposium

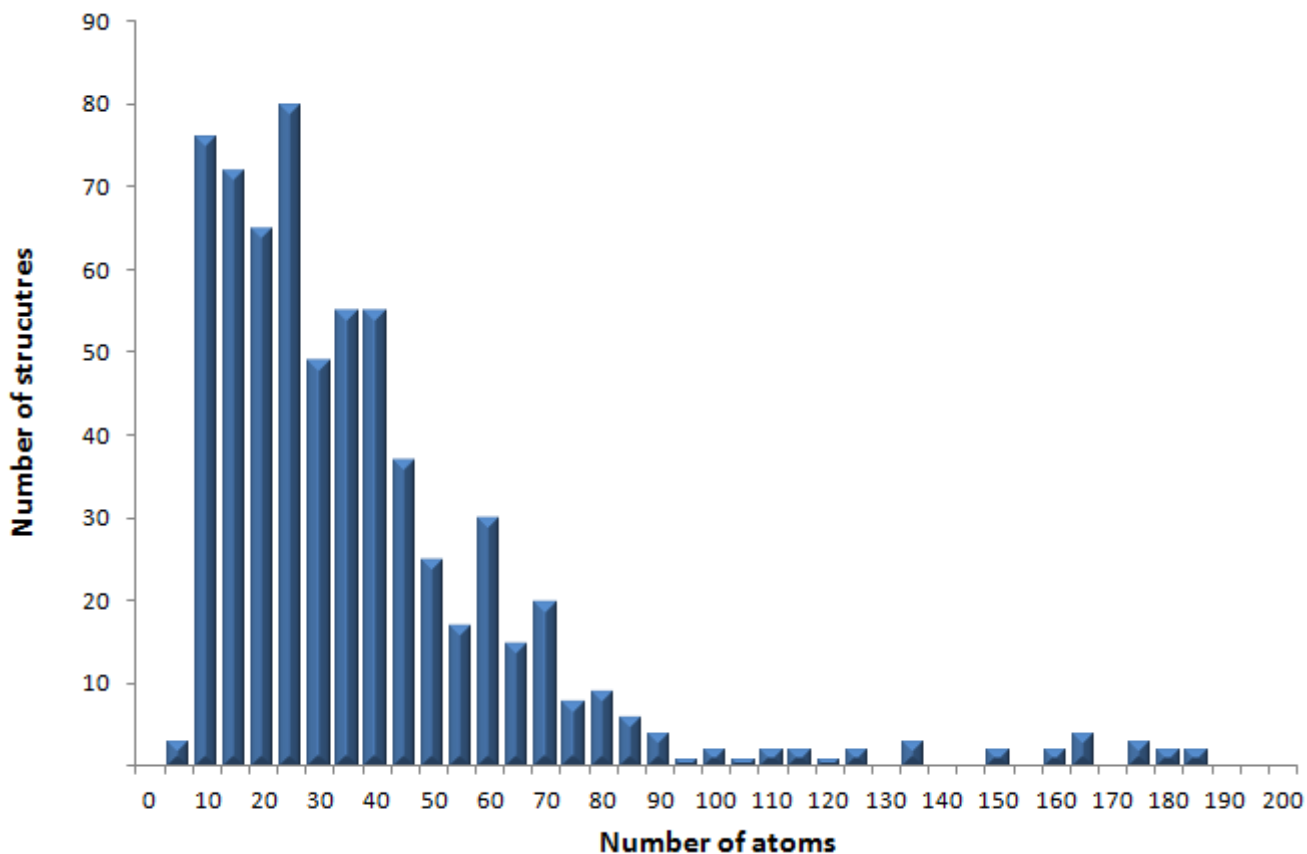
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Issues in solving complex molecular crystal structures from lab PXRD data

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Developments (both software and methodological) in crystal structure determination from powder X-ray diffraction data have resulted in increasingly complex molecular structures now being solved from relatively low-resolution diffraction data. This can lead to the publication of structures that clearly do not meet the rigorous chemical and crystallographic standards that one normally associates with published crystal structures. As such, considerable attention should be paid to the quality of the final refined crystal structure, with chemical sense playing as important a role as the fit of the structure to the data. This presentation will focus upon some issues that impact upon the final quality of the published structure as derived from lab PXRD data, and suggest strategies for maximising the chances of a successful structure solution and refinement. These include the preparation of structural models for use in global optimisation, the use of rigid-body-type refinements, the critical assessment of output crystal structures and the use of DFT-D to validate such crystal structures. The presentation will be illustrated with examples drawn mostly from the world of pharmaceutical research and will include an introduction that puts the role of structure determination from powder diffraction data into context in terms of accessible structural complexity.



Keywords: molecular crystal structures, solution and refinement, laboratory diffraction data