

Small Molecule Crystallography and Science--II

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Several years ago I talked at an ACA meeting on the relationship between science and small molecule crystallography. Since then I have become a co-editor of Acta Cryst., Section C. This has given me the unique opportunity to observe how others do crystallography both well and poorly. I have also noticed trends and problems that would not be noticed in their own research. This talk will deal with three areas gleaned from my experience. First, the problem of quantity of quality data will be examined. Second, refinement of hydrogen atoms will be discussed. Different criteria for basic refinement will be examined. Lastly, the change in the scope of Section C will be explained. This journal has changed from a totally crystallographic journal to one that is focused on structural science as it pertains to chemistry.