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*New refinement approach for crystal structure analysis of organic compounds*

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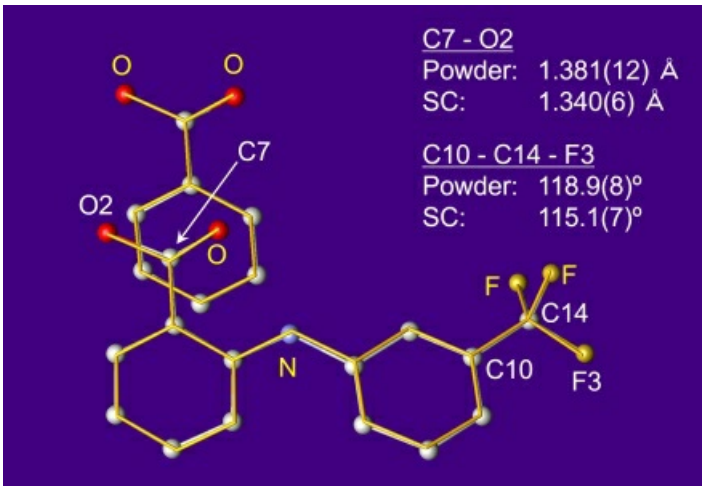
Crystal structure analysis from powder diffraction data has become, for a decade, an effective and powerful technique when the single crystalline state of a sample cannot be maintained due to hydration, dehydration, or phase transition as well as when single crystals are not obtained. One of the big reasons is that several one-stop software have widely been used, providing all the features required for the structure analysis. However, the last step of the analysis "refinement of crystal structures" is still challenging. In case of, in particular, powder samples of organic compounds and metal complexes, the crystal structures are usually refined by setting restraints to bond lengths and angles to keep the molecular structures from collapsing. However, good results will not sometimes be obtained without setting proper restraints: the molecular structure may collapse if the restraints are weak, or the observed pattern may not agree with the calculated pattern if the restraints are strong. The effect of restraint strength factor on crystal structures and calculated profiles varies with observed intensities, peak profiles, etc. Therefore, the restraint strength factor should be estimated for each analysis.
We will report several analysis examples from organic powder samples and validate the way of estimating restraint strength factors by comparing each result with the corresponding single crystal structure.

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