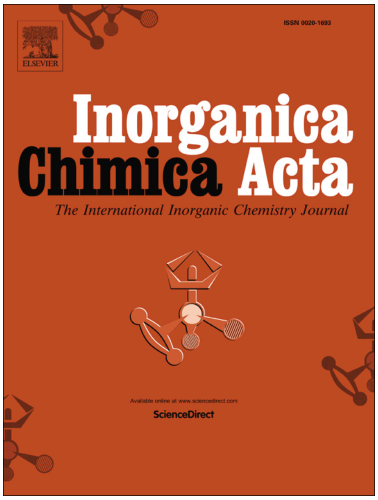

Research paper

What makes a crystal structure report valid?

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What makes a crystal structure report valid?

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Dedicated to Carlo Mealli on the occasion of his 70th birthday.

Abstract

Single crystal X-ray crystallography has developed into a unique, highly automated and accessible tool to obtain detailed information on molecular structures. Proper archival makes that referees, readers and users of the results of reported crystal structures no longer need to depend solely on the expertise of the analyst, often a non-professional crystallographer, who did the reported study. Deposited computer readable data should allow for an independent structure analysis, validation of the author’s interpretation of the experimental data and use of those data for follow-up research. This paper summarises what is needed for proper validation and archival. The difference between *valid* and *value* is discussed. As an example, the deposited data associated with the molecular structure determination of a guest molecule soaked into a MOF, based on the *Crystalline Sponge Method*, are analysed.

Keywords:
Validation
CheckCIF
PLATON
SQUEEZE
MOF
Crystalline Sponge Method

1. Introduction

The majority of papers published in chemical journals such as Inorganica Chemica Acta, Inorganic Chemistry and Organometallics include one or more crystal structure reports. In many cases those structures mainly serve as ‘solid proof’ of the identity of a compound in the context of the reported chemical research: *Seeing is Believing*. Many of those crystal structure determinations are nowadays, once suitable crystals are obtained, routine in the hands of experienced analysts. The reported structures do not necessarily offer significant new chemical or crystallographic insight on their own. For that reason, only limited details beyond a 3D representation and a footnote with selected data normally appear in print along with a deposition reference for more details. Often, the main added value of a structure determination lies in their subsequent inclusion in the Cambridge Structural Database (CSD) [1] that offers a rich source of data for all kinds of comparative, statistical and follow-up research. For the latter, quality, reliability and completeness of the deposited data is essential. It is important that all reported crystal structures are well documented and validated. Sufficient information should be made available to allow for an independent structure analysis with the archived data. Sometimes, those data are unique such as meta-stable polymorphs or difficult and costly to obtain again from scratch.