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An introduction to the special issue on *interplay of crystallography, spectroscopy and theoretical methods for solving chemical problems*

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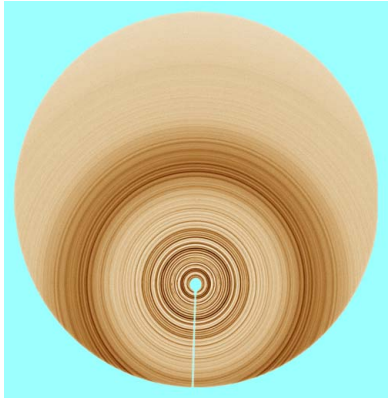

The crystal structures and molecular dimensions established by diffraction analysis have given an indisputably positive impulse to research efforts in many areas of chemistry, biochemistry, physics and materials science. In synthetic chemistry, the crystallographic result is often the most definitive means of establishing the nature of a new product. Indeed, the crystal structure is often taken as necessary proof that a compound exists; moreover, the importance of recognizing and characterizing polymorphic phases has made crystallographic analysis an indispensable tool in the pharmaceutical industry.

Meanwhile, the quality and quantity of diffraction analyses has increased over the years, with improved instrumentation and faster computers leading the charge in the massive production of new structural data. With these developments have come new practices for evaluating, communicating and storing structural results. It is fair to say that *Acta Crystallographica Section C* has been a leader in establishing 'best practice' procedures for the path from structure analysis through validation and on to publication and archival. With reliable diffraction instruments, readily available software for popular computers and automated procedures for checking and storing the results, the crystallographer has been liberated from the need which existed not that many years ago, to be at once an expert on crystallography and on electronics, computer programming, plumbing and the myriad other elements of the crystallographic endeavour. Crystallographic practice has improved to the point that non-experts can, in a large number of cases, produce verifiably reliable results.

At the same time, the appearance in print of dubious or materially incorrect crystallographic results, which can nonetheless have acceptable structure validation indicators (*R* factors, s.u. values *etc.*) belies the necessity of a critical examination of the science reported in a publication; and thus the role of the crystallographic practitioner as scientist is far from obsolete.

The results of structure determination alone – unit-cell dimensions, atomic coordinates and displacement parameters – cannot routinely be expected to reveal why the colour of a compound is what it is, why the compound undergoes the reactions that it does, or why it is produced in the first place. Such conclusions can only be drawn from the systematic analysis of structural parameters alongside concepts of bonding and reactivity, spectroscopic data, electronic structure calculations, or results from any other of a panoply of chemical and physical characterization techniques.

As this journal embarks on its science-facing mission as an outlet for research in structural chemistry in its broadest sense, we present this special issue on the '*Interplay of crystallography, spectroscopy and theoretical methods for solving chemical problems*.' The research articles and scientific comments presented here demonstrate that the vast utility of structure determination is manifest in other techniques in addition to single-crystal diffraction analysis, and that a description of structure can derive immense leverage from physical measurements and computational modelling.