Keynote Lecture

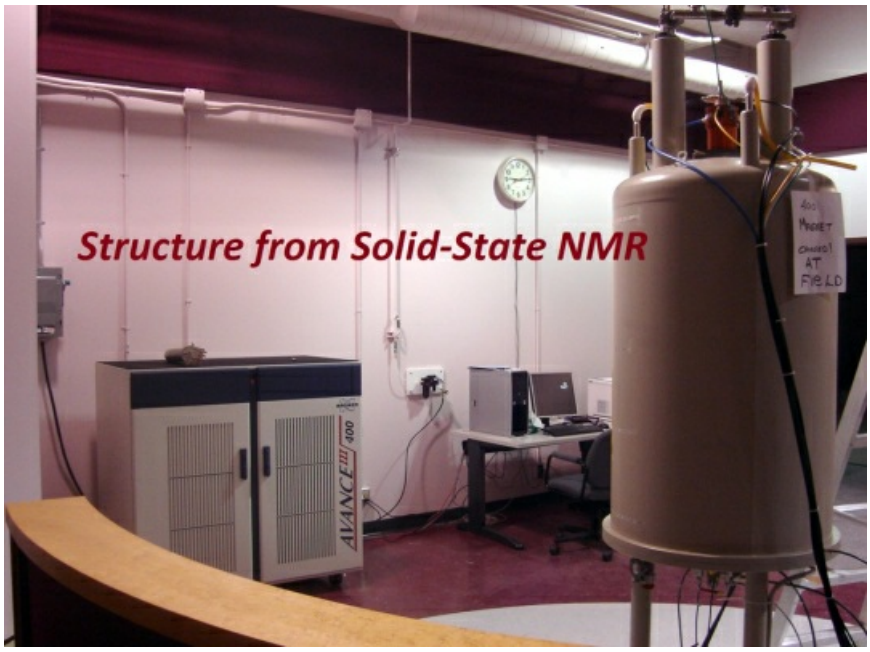
KN-05

Structure and properties of materials by solid-state nuclear magnetic resonance

David Lawson Bryce[1]
[1]*Department Of Chemistry And Biomolecular Sciences, University Of Ottawa, Ottawa, Canada*
E-mail: dbryce@uottawa.ca

Since the early days of nuclear magnetic resonance (NMR) spectroscopy, experiments on crystalline materials have provided structural and crystallographic information. The scope of this information may range from a single internuclear distance to a complete structural model. In this lecture, I will provide an overview of the field of NMR Crystallography, a topic on which the IUCr established a Commission in 2014, as well as NMR applications to crystal engineering [1]. NMR crystallographic methods are frequently used in combination with diffraction methods, and offer particular advantages for studying disorder, dynamics, and heterogeneous systems, for example. I will then present a survey of applications of solid-state NMR spectroscopy to the study of various organic and inorganic materials, with an emphasis on work from my own laboratory. For example, we have developed and applied a multinuclear magnetic resonance crystallographic structure refinement and cross-validation protocol using experimental and computed electric field gradients [2]. A second aspect of our work is the characterization of halogen-bonded cocrystals and frameworks, often prepared via mechanochemical approaches. Solid-state NMR spectroscopy is used in this context to provide insights into the formation and structure of cocrystals, as well as the nature of the halogen bond [3]. As a third example, I will describe various intriguing applications of two-dimensional double-quantum filtered NMR experiments. In favourable cases, such experiments may be employed to provide direct information on crystallographic symmetry and on dynamic disorder in solids.

[1] Xu, Y.; Southern, S. A.; Szell, P. M. J.; Bryce, D. L. (2016) CrystEngComm, 18, 5236-5252.
[2] Perras, F. A.; Bryce, D. L. (2012) J. Phys. Chem. C, 116, 19472-19482.
[3] Szell, P. M. J.; Bryce, D. L. (2016) Modern Magn. Reson. pp 1-18. DOI 10.1007/978-3-319-28275-6_92-1.



Keywords: nuclear magnetic resonance, solid-state NMR, NMR crystallography