NMR Crystallography. Information on Structure, Symmetry, and Dynamics from Solid-State Multinuclear Magnetic Resonance Spectroscopy

David L. Bryce

Department of Chemistry and Biomolecular Sciences, University of Ottawa

The term 'NMR crystallography' has been employed in the literature to cover a wide array of approaches to structure determination, refinement, or selection.[1,2] Following the establishment of a *Commission on NMR Crystallography and Related Methods* in Montreal in 2014, this field has taken on increased prominence in the International Union of Crystallography as evidenced by the well-attended NMR Crystallography symposium of the 24th Congress & General Assembly of the IUCr, held in Hyderabad last year.

In this presentation, I will describe recent advances from my research group in using NMR data, often in concert with diffraction and density functional theory data, to provide structural, crystallographic, and dynamic insights into a range of organic and inorganic materials. For example, I will describe a series of halogen-bonded architectures and their characterization via NMR spectroscopy. These samples may be prepared by traditional slow-evaporation methods or by mechanochemical ball milling; solid-state NMR is an essential tool in many cases for characterizing powdered samples, particularly when amorphous fractions may be present. I also show how solid-state deuterium NMR is key to characterizing dynamic processes catalyzed by halogen bonds. Other examples include the *in-situ* monitoring of halogen-bonded cocrystals formation in real time by solid-state ^{31}P NMR spectroscopy.[3]

Solid-state NMR spectra of other quadrupolar (spin > ½) nuclei are exquisitely sensitive to structure, symmetry, and dynamics. I will describe various applications of ^{11}B, ^{61}Ni, $^{69/71}$Ga, and $^{79/81}$Br solid-state nuclear magnetic resonance and nuclear quadrupole resonance experiments to provide relevant insights into a range of compounds and supramolecular architectures.

References

1. Bryce, D. L. *IUCrJ* **2017**, *4*, 350-359.
2. Bryce, D. L.; Taulelle, F. *Acta Cryst.* **2017**, *C73*, 126–127.
3. Xu, Y.; Champion, L.; Gabidullin, B.; Bryce, D. L. *Chem. Commun*. **2017**, *53*, 9930-9933.