CMCC Mechanochemistry Discussions

Online Seminar Series

Crushing It: Probing Mechanochemistry with Solid-State NMR

Livestreaming at 10:00 AM (CT) **THURS., August 21, 2025**

on the CMCC YouTube Channel:

https://www.youtube.com/channel/UC7e CYPKbGTKpgO7W2bNABxg



Mechanochemical reactions are typically carried out on solid components. Reactants, intermediates and products are often characterized using diffraction experiments, or perhaps infrared and Raman spectroscopy. Solid-state nuclear magnetic resonance (SSNMR) holds great potential for in-situ and ex-situ characterization. NMR provides local, nuclear site-specific information on structure and chemical bonding as well as longer-range information on crystallinity, amorphism, and polymorphism. In this talk, I will describe our recent efforts to use various mechanochemical approaches (e.g., grinding, ball milling, resonant acoustic mixing (RAM)), as well as cosublimation, to generate known and novel cocrystals held together by various classes of non-covalent interactions including halogen bonding and chalcogen bonding. Multinuclear SSNMR spectra provide exquisitely detailed information on these crystal forms as well as realtime data for monitoring the conversions of such forms. Real-time in-situ solid-state 'aging' conversions in the NMR rotor can provide kinetic information on the formation of non-covalent bonds.



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