

## Poster Presentation

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### *Simultaneous infrared spectroscopy and X-ray PDF measurements*

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Combining insights from diffuse reflection infrared Fourier transform spectroscopy (DRIFTS) and X-ray pair distribution function (PDF) analysis has the potential to provide deeper insight into complex materials systems under reactive conditions, including heterogeneous catalysts and host-guest systems. We have developed instrumentation and non-ambient reaction cells that enable combined PDF-IR studies without compromise to either measurement. Through careful selection of the IR spectrometer and optics, the IR instrument and reaction cell were adapted to allow angular dispersive X-ray measurements without change to the active IR components, resulting in IR data that are entirely uncompromised. The associated PDF and diffraction data are shown to be of comparable quality and resolution to standard geometry PDF/diffraction measurements. We have demonstrated this approach through the study of desorption of coordinated and non-coordinated guests from the nanoporous Prussian blue analogue  $\text{MnII}_3[\text{CoIII}(\text{CN})_6]_2(\text{H}_2\text{O})_6 \cdot x\{\text{H}_2\text{O}\}$ . The combined data shows how the release of guests from different sites is coupled to structural relaxation of the framework. We will also discuss recent results where we have extended the approach to the study of zeolite catalysts.

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