Microcrystal X-ray Diffraction and MAS NMR Studies of Zeolites

Russell E. Morris, *School of Chemistry, University of St Andrews, Purdie Building St Andrews KY16 9ST UK*. E-mail: rem1@st-and.ac.uk

Zeolites are notoriously difficult to prepare as large single crystals. Until the last decade we have had to rely on powder diffraction as our major tool for determining their structure. With the advent of single crystal X-ray diffraction as a standard tool at synchrotron sources this limitation has been somewhat reduced. In this presentation I will discuss some of our recent work on studying the structure and properties of zeolites using the single crystal X-ray diffraction station at the Synchrotron Radiation Source, Daresbury, UK.

Not only have new structures been solved using this facility, but we have also shown how the details of previous powder X-ray diffraction work have sometimes been incorrect. In addition, the facility has also allowed us to crystallographically study the thermal properties of zeolites, such as negative thermal expansion, in more detail than was previously possible.

I will also explain how solid state MAS NMR studies can be used to improve the accuracy of our crystallographic models, and I will discuss the possibilities for solving structures from NMR data.

Keywords: zeolites, microcrystal diffraction, NMR