

## MS29-P01 | KOALA - ROUTINE H-ATOM DETERMINATIONS BY LAUE NEUTRON DIFFRACTION

Edwards, Alison (Australian Centre for Neutron Scattering, Lucas Heights, AUS); Piltz, Ross (Australian Centre for Neutron Diffraction, Lucas Heights, AUS)

KOALA entered the ANSTO neutron beam user program in 2009 following the example of VIVALDI at the ILL which proposed relatively rapid neutron diffraction studies of molecular crystals ( $0.1\text{mm}^3$  minimum crystal volume) for which a broad range of determination constitutes “accuracy”. In some instances, the presence or absence of a hydrogen nucleus constitutes an accurate result and this can, where necessary, be achieved via a relatively low resolution determination from specimens of limited crystallinity. In other cases, exact hydrogen atom positions are sought for comparison with methods seeking to extend the utility of X-ray diffraction in cases such as quantum crystallographic refinement or purely theoretical methods. Two major enhancements to our operation of KOALA have been the implementation of a COBRA cryostream to facilitate the handling of samples which are air and moisture sensitive and to speed sample change; and the creation of a user friendly data reduction procedure which facilitates timely presentation of the neutron structure determination with the full chemical study. The achievements with KOALA demonstrate that the promise of VIVALDI was achievable and there is no reason why VIVALDI or a similar Laue instrument could not be successfully made available at a reactor source, capitalising on the development initiated at the ILL.