s14.m39.o1 **Neutron Diffraction Studies on Optically-Active Deuterated Molecules.** Robert Bau, *Chemistry Department, University of Southern California, Los Angeles, CA 90089, U.S.A. E-mail: bau@usc.edu*

Keywords: Neutron Diffraction, Chiral Molecules, H/D Substitution, Absolute Configuration

The ability of the neutron diffraction process to differentiate between hydrogen and deuterium atoms is well known. This unique property makes it possible to determine the absolute configuration of stereospecifically-labelled organic molecules, that are chiral by virtue of an H/D difference, using singlecrystal neutron diffraction. Earlier work that we had carried out in collaboration with the group of T.F. Koetzle, on molecules containing a chiral methylene group (i.e., molecules of the type CHDRR*) will be reviewed together with related results from other groups. We will also discuss, in this presentation, ongoing research on an aromatic hydrocarbon that is optically active by virtue of selective deuteration in two specific positions, dideuterotetrabenzocyclooctateraene ($C_{24}H_{14}D_2$). The results of the single-crystal neutron diffraction analysis[1] of this compound will shed some light on the inversion barrier of non-planar tetraphenylene rings.

This type of research is an example of a broad range of applications of neutron diffraction in chemistry, that is being advanced by newly upgraded small-molecule facilities, like the SXD instrument at ISIS (Didcot, U.K.), the SCD diffractometer at IPNS (Argonne, U.S.A.), and the Vivaldi diffractometer at ILL (Grenoble, France). Further revolutionary advances are anticipated with the advent of the new single-crystal diffractometer that will be constructed at the new Spallation Neutron Source that is being built in Oak Ridge, Tennessee.

[1] R. Bau, M. Gutmann, H. N. C. Wong *et al.*, unpublished work (2004)

s14.m39.o2 **Neutron Diffraction and Magnetic Structures**. F. Bouree, *Laboratoire Léon Brillouin [CEA-CNRS], CEA/Saclay, F-91190 GIF-SUR-YVETTE, France. E-mail: bouree@llb.saclay.cea.fr*

Keywords: 75-25; 75-30; 75-50

Magnetic neutron powder diffraction is, and will remain in the future, the most straightforward technique to get magnetic structures, as a function of temperature, pressure… The successive steps of a magnetic structure determination (description of the microscopic arrangement of magnetic moments in a crystal) will be described in this presentation, from the experiment (2-axis diffractometer and sample environment) to the results: commensurate and/or incommensurate long-range/short-range magnetic order, via data analysis (selection rules, Bertaut's representation analysis, Rietveld FULLPROF refinement…). Some examples are selected, among terbium fluorides [1] and in the $R_4Mo_4O_{11}$ system (R = Lanthanide) [2].

[1] M. Josse, PhD, December 2003, Université de Clermont-Ferrand, France
[2] P. Gougeon, P. Gall and RE McCarley *Acta Cryst*. C**47** (1991) 1585-1588