Single-Crystal Neutron Diffraction on Sigma Complexes: Recent Results from IPNS

<u>Thomas F. Koetzle</u>, Arthur J. Schultz, *IPNS Division, Argonne National Laboratory, Argonne, IL 60439 U.S.A.* E-mail: tkoetzle@anl.gov

For a number of years we have been employing single-crystal neutron diffraction to investigate structures of sigma complexes of transition metals. Sigma complexes are of special interest because they are ubiquitous intermediates in metal-catalyzed reactions including hydrogenations, activation and functionalization of hydrocarbons, and hydroborations. Here we will report on some recent results obtained using the SCD instrument at Argonne's Intense Pulsed Neutron Source, which has been upgraded with two new position-sensitive Anger detectors to achieve increased data collection efficiency. In the future, we hope to be able to dramatically extend these studies at the Spallation Neutron Source (SNS) using the single-crystal diffractometer (Topaz) that is currently under development there. *Acknowledgement*. This work was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, under Contract W-31-109-ENG-38.

Keywords: neutron crystallography, organometallic complexes, single-crystal diffraction