Combined X-ray and Neutron Charge Density Studies on C-H activation catalysts

Wolfgang Scherer[a], Bjørn Pedersen[b], G. Sean McGrady[c], [a]*Institute of Physics, University of Augsburg.* [b]*FRM-II, TU Munich, Germany.* [c]*Department of Chemistry, University of New Brunswick, Canada.* E-mail: wolfgang.scherer@physic.uni-augsburg.de

The new single crystal diffractometer RESI (*RE*ciprocal *S*pace *I*nvestigator) at the new high-flux neutron source FRM-II (www.frm2.tum.de) has been optimized for the demands of combined X-ray and neutron charge density studies (high resolution data at low backgrounds) by employing an X-ray and neutron sensitive imaging plate detector, a flexible κ-goniometer geometry and a focusing neutron guide for thermal neutrons. The new diffractometer concept will be outlined, and the advantage of combined X-ray and neutron charge density studies illustrated by first applications in the field of catalyzed C-H activation.We will demonstrate that so-called 'ligand-induced charge concentrations' in the valence shell of main group and transition metal complexes (*i*) can be identified by experimental charge density studies; and (*ii*) act as controlling parameters in C-H activation processes.[1,2] Systematic experimental studies of molecular charge distributions will thus lead to significant advances in the design and chemical control of catalysts for C-H activation and other processes, with central relevance to many reactions of academic and commercial importance.

[1] Scherer W., McGrady G.S., *Angew. Chem. Int. Ed*, 2004, **43**, 1782. [2] Scherer W., Sirsch P., Shorokhov D., Tafipolsky M., McGrady G.S., Gullo E., *Chem. Eur. J.,* 2003, **9**, 6057.

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