FA4-MS37-P23

Comparative Charge Density Study: Gemini vs SuperNova. Hazel Sparkes^a, <u>Alexandra Griffin</u>^b, ^aDepartment of Chemistry, University of Durham, UK ^bAgilent Technologies (formerly Oxford Diffraction) E-mail: alex.griffin@oxford-diffraction.com

Accurate, high resolution X-ray charge density experiments provide information on the electron distribution within the system under study, allowing both the nature of the bonding and the atomic interactions to be determined [1]. Agilent Technologies (formerly Oxford Diffraction) have two diffractometers capable of collecting high quality data; the **Gemini**, which has a standard ceramic molybdenum source, and the **SuperNova**, with microfocus technology.

Data was collected on both diffractometers using a single crystal of a small rhodium complex. The results of multipole refinements carried out in *XD2006* [2] are presented for the complex, with comparisons drawn between the two data collections. The nature of the bonding and intermolecular interactions in the complex is discussed, with particular focus on the topological properties associated with the rhodium metal centre.

[1] D. Zobel, P. Luger, W. Dreissig & T. Koritsanszky (1992) Acta Cryst., B48, 837-848. [2] A. Volkov, P. Macchi, L. J. Farrugia, C. Gatti, P. R. Mallinson, T. Richter & T. Koritsanszky XD2006, a computer program package for multipole refinement and topological analysis of charge densities from diffraction data.

Keywords: charge density, supernova, gemini