

Theoretical XANES study of an organometallic cluster

C. T. Chantler¹, J. L. Glover¹, A. V. Soldatov², M. C. Feiters³

¹ School of Physics, University of Melbourne, Parkville, VIC, Australia

² Faculty of Physics, Rostov State university, Rostov-on-Don, 344090, Russian Federation

³ University of Nijmegen, Institute of Molecules and Materials, 1 Toemooiveld, 6525 ED Nijmegen, Netherlands

The study of catalytic systems can be of great practical benefit. XANES is one of the most powerful techniques for investigating active centres of such molecules. We have obtained XANES for the activated Ni (t-amylisocyanide) complex from a number of the latest and most advanced theoretical approaches. This system is a very large cluster for which it has been attempted to derive a converged solution, and has been linked to important chemical developments for catalysts for isocyanide polymerization. The predicted XANES for the nano-cluster are compared with experimental data, providing a critical test for different theoretical approaches. We found using novel finite element methods to be the most effective at predicting the structure seen in the near edge.