Structural, Spectroscopic and Theoretical Studies of (t-Butyl-isocyanide)gold(I) Iodide

Ruei-Yang Liau a, Trevor Mathieson a, Annette Schier a, Raphael J. F. Berger a, Nino Runeberg b, and Hubert Schmidbaur a

a Anorganisch-chemisches Institut der Technischen Universität München, Lichtenbergstrasse 4, D-85747 Garching, Germany
b Department of Chemistry, University of Helsinki, POB 55 (A. I. Virtasen aukio 1), FI-N-00014 Helsinki, Finland

Reprint requests to Prof. Dr. Schmidbaur. E-mail: H.Schmidbaur@lrz.tum.de

Z. Naturforsch. 57 b, 881–889 (2002); received June 3, 2002

Isocyanide Complexes, Gold Complexes, Gold Iodide, Aurophilicity

The complexes (t-BuNC)AuCl and (t-BuNC)AuI 13 C-labeled at the isocyanide group were prepared and investigated by concentration- and temperature-dependent IR and NMR spectroscopy in dichloromethane solution. No indication for association of the molecules was obtained. The crystal structure of the iodide complex was determined by X-ray diffraction methods and shown to feature only monomers with extremely large intermolecular Au–Au contacts of 4.162 Å, well beyond the sum of the van der Waals radii. It therefore appears that (t-BuNC)AuI is a rare example of a sterically non-hindered L-Au-X complex which shows no aurophilic interactions whatsoever. In a quantum-chemical analysis (at the local MP2 level) of the dimerization of the model compounds (MeNC)AuCl and (MeNC)AuI in various dimer geometries it was demonstrated that the energy-balance of the dimerization is very delicate and not dominated solely by contributions from correlation / relativistic (aurophilic) effects.