Gold and Hydrogen Bonding: Myth or Reality?

M. Rigoulet¹, E.D. Sosa Carrizo², K. Miqueu², A. Amgoune¹, D. Bourissou¹

(1) CNRS, Université Paul Sabatier, Laboratoire Hétérochimie Fondamentale et Appliquée (LHFA, UMR 5069), Toulouse, France
(2) Université de Pau et des Pays de l’Adour, Institut des Sciences Analytiques et de Physico-Chimie pour l’Environnement et les Matériaux (UMR 5254), Pau, Cedex 09, France

Hydrogen bonds involving transition metal centers as proton acceptors have attracted considerable attention over the last three decades. Besides their fundamental interest in terms of chemical bonding, they are also relevant to several organometallic transformations (such as the simple formation of metal hydrides by protonation). In contrast to the other transition metals,¹ there is so far no clear evidence for hydrogen bond to gold. A number of close Au···H contacts have been reported in crystal structures of aurides, gold(I) or gold(III) complexes, but no spectroscopic evidence for attractive Au···H interactions in solution have been reported and nothing substantiates unequivocally the presence of hydrogen bonds.² However, theoretical studies on model compounds suggest that hydrogen bonding to gold is indeed possible and actually favored energetically when an electron-rich gold(I) center bears a chelating ligand that positions a proton in close proximity to the metal.³ Starting from chelating ligands, we have prepared and thoroughly characterized cationic gold(I) complexes of type A. The presence of N–H···Au hydrogen bonds has been unambiguously demonstrated by experimental means (NMR, IR, D-labeling…) and theoretical calculations. These data will be presented and discussed.

Figure 1. Schematic representation of gold complex displaying N–H···Au gold-hydrogen bonding.

References

Corresponding author email: rigoulet@chimie.ups-tlse.fr