Aggregation of Au(I)-complexes on Amorphous Substrates Governed by Aurophilicity

Petra Gründlinger,[a] Michael Györök,[a] Sebastian Wolfmayr,[a] Tobias Breuer,[b] Daniel Primetzhofer,[c] Barbara Bruckner,[c] Uwe Monkowius[d] and Thorsten Wagner[a]**

** Corresponding authors*

Supplementary Information

a Johannes Kepler University Linz
Institute of Experimental Physics, Surface Science Division
Altenberger Str. 69
4040 Linz, Austria

b Philipps University Marburg
Physics Department, Molecular Solids Group
Renthof 7
35032 Marburg, Germany

c Uppsala University
Department of Physics and Astronomy
Box 516
S-75120 Uppsala, Sweden

d Johannes Kepler University Linz
School of Education, STEM Didactics
Altenberger Str. 69
4040 Linz, Austria

The three complexes (NapNC)AuCl, (NapNC)AuBr, and (NapNC)AuI were characterized complementary by IR spectroscopy. Fig. S1 shows the corresponding IR spectra for the three compounds supporting the proposed chemical connectivity. The –N≡C bond gives rise to a characteristic stretching band at 2221 cm^{-1}.[1] For the chlorido complex the corresponding band is found at 2206 cm^{-1} (Fig. S1 (a)), for the bromido one at 2209 cm^{-1} (Fig. S1 (b)), and for the iodido one at 2207 cm^{-1} (Fig. S1 (c)).

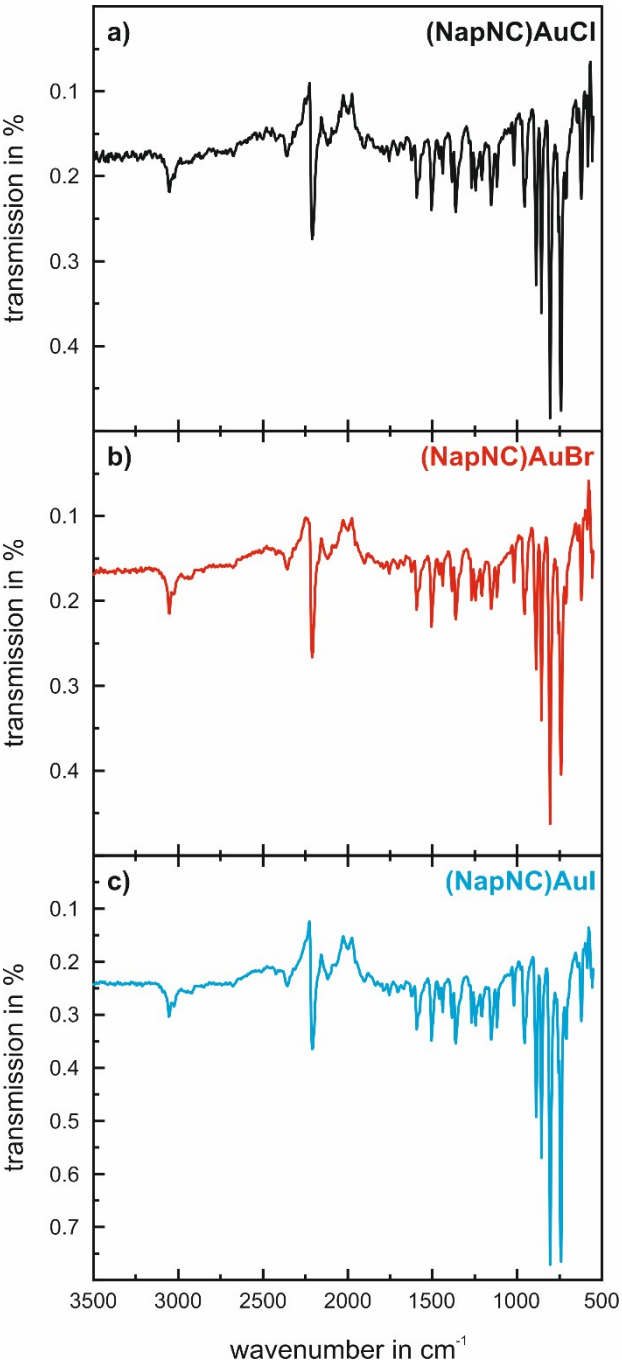

Figure S1. IR spectra of the three synthesized complexes.

As a complement to RBS for characterization of gold and halogen species the overall chemical composition of the (NapNC)AuCl and (NapNC)AuBr films deposited on glass substrate was also checked by means of Time-of-Flight Elastic Recoil Detection Analysis (ERDA). As for RBS, experiments were performed at the 5 MV tandem accelerator at Uppsala University. Details of the employed set-up as well as the analysis are described elsewhere.[2,3] Fig. S2 shows the mass-energy plots as obtained from ERDA. The films with nominal thickness around 25 nm had been grown on standard microscopy slides. The large information depth of ERDA gives in this particular case rise to a huge signal of the substrate (low energy channels) and only a very tiny signal from the films (higher energy channels). As typical for a soda-lime glass, we clearly see contributions from quartz and typical additives like NaO and CaO. Whereas the signal from Au and C was clear, the signal from Cl was minor. While the signal from Br was more pronounced, it was still considered of insufficient quality to assess the integrity of the chlorido complex. Comparing the counts for 197 u (Au) and 12 u (C) at least the correct order of magnitude for the Au:C ratio is found, thus suggesting intact molecules.

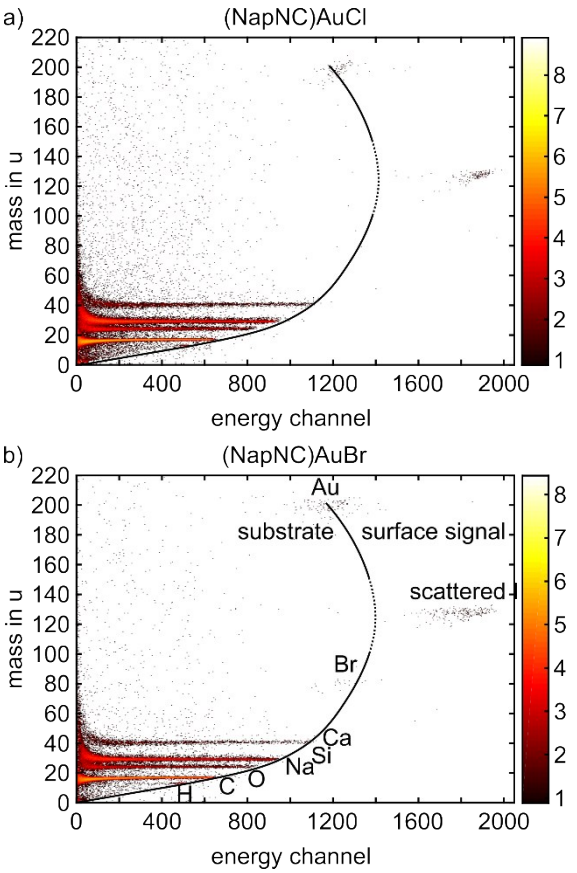

Figure S2. ERDA plots of the (NapNC)AuCl and (NapNC)AuBr film grown on soda lime glass.

Fig. S3 shows additional in-plane X-ray diffraction data for the (NapNC)AuCl film grown on glass. While the out-of-plane XRD measurements provided in the main paper quantified the vertical lattice plane distances within the thin films, we furthermore performed in-plane X-ray diffraction measurements for an (NapNC)AuCl film grown on glass. In these, we observe several reflections, all of which can be assigned to the diffraction signals, which are predicted by the bulk crystal structure. This furthermore proves that the crystal structure adopted in the thin films is equal to the bulk structure (see Table I of the main paper).

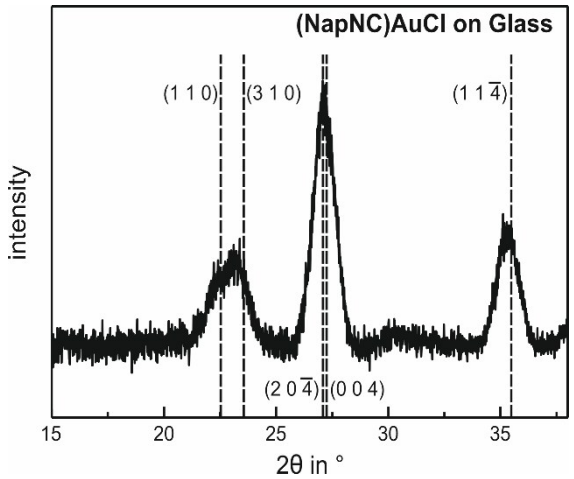

Figure S3. Grazing incidence X-ray diffraction (GIXD) measurement for the 25 nm thick film of (NapNC)AuCl on glass.

While trying to sublime (NapNC)AuI in a high vacuum chamber, the quartz crucible was heated up stepwise to a maximum temperature of 440 K. The quartz microbalance did not indicate any significant rate and the inspection of the glass substrate by eye did not confirm any deposited material, while the crucible used in the experiment was gilded afterwards (cf. Fig. S4). These observations indicate that (NapNC)AuI decomposes before sublimation.

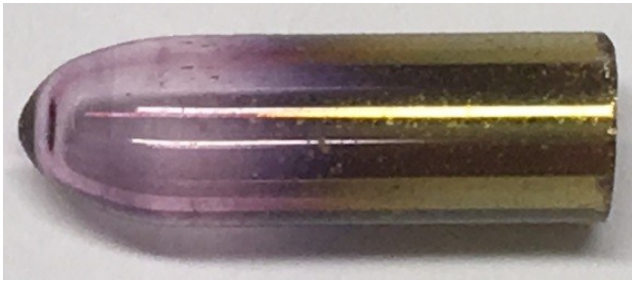

Figure S4. Gilded crucible originally filled with (NapNC)AuI and then heated to 440 K in high vacuum.

[1] I. Ugi, U. Fetzer, U. Eholzer, H. Knupfer, K. Offermann, Isonitrile Syntheses. *Angew. Chem. Int. Ed. Engl.* **1965**, *4*, 472-484.

[2] H.J. Whitlow, G. Possnert, C.S. Petersson, Quantitative mass and energy dispersive elastic recoil spectrometry: Resolution and efficiency considerations. *Nucl. Instr. And Meth. B* **1987**, *27*, 448.

[3] H.-Y. Qu, D. Primetzhofer, M. A. Arvizu, Z. Qiu, U. Cindemir, C. G. Granqvist, and G. A. Niklasson, Electrochemical Rejuvenation of Anodically Coloring Electrochromic Nickel Oxide Thin Films. *ACS Appl. Mater. Interfaces* **2017**, *9*, 42420-42424.