

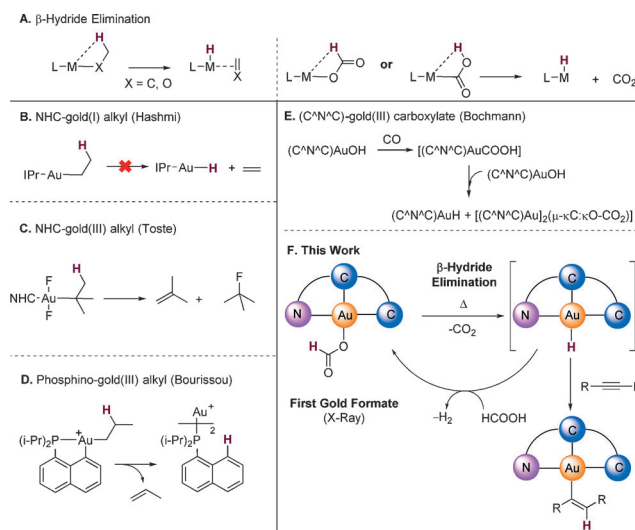
Gold Complexes

International Edition: DOI: 10.1002/anie.201705557
German Edition: DOI: 10.1002/ange.201705557The First Gold(III) Formate: Evidence for β -Hydride Elimination

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Abstract: The first stable gold(III) formate and experimental evidence for its β -hydride elimination are described. A catalytic dehydrogenation of formic acid together with mechanistic studies shed light on potential pathways operating in fundamental gold-catalyzed transformations.

The β -hydride elimination from a metal alkyl or alkoxy complex is an elementary reaction in catalysis that has been harnessed as a productive step in industrially relevant transformations such as olefin polymerization, Mizoroki–Heck couplings, or the Wacker process, among many others.^[1] Metal formates and carboxylates also undergo β -hydride elimination to produce CO₂ and metal hydrides (M–H; Scheme 1 A). This reactivity has been efficiently exploited in several transformations, including the water gas shift reaction (WGSR) as well as the dehydrogenation of formic acid (FA).^[2] Over the past years, in-depth mechanistic insight into β -hydride elimination processes has been gained for transition metals such as Pd, Ru, Ni, Pt, and Ir.^[1] In contrast, and despite prominent developments in gold catalysis,^[3] β -hydride elimination on gold was long deemed unfeasible,^[4] and reports on gold complexes undergoing β -hydride elimination are scarce.^[5] In pioneering work, Hashmi and co-workers demonstrated that the (IPr)gold(I) ethyl complex does not undergo β -hydride elimination even at high temperature (Scheme 1 B).^[6] In a seminal work towards C(sp³)–F bond-forming reductive elimination, Toste and Mankad showed that (NHC)gold(III) alkyl difluoride complexes form alkenes via β -hydride elimination along with the corresponding alkyl fluorides (Scheme 1 C).^[7] Recently, Bourissou and co-workers thoroughly investigated β -hydride elimination on low-coordinate (P[^]C)-type cyclometalated gold(III) alkyl complexes (Scheme 1 D).^[8] In 2015, Bochmann and co-workers reported the insertion of CO into a gold(III) hydroxo complex [κ^3 -(C[^]N[^]C)Au(OH)].^[9] Whereas the corresponding gold(III) carboxylate could not be isolated, its formation was supported by the observation of the corresponding Au^{III}–H species as a result of the β -hydride elimination (Scheme 1 E). The stability of this gold(III) hydride proved to be remarkable as it was stable in the presence of air, moisture, and even acetic



Scheme 1. A) General pathways for M–H formation by β -hydride elimination. B–D) Precedents of β -hydride elimination on gold. E) β -Hydride elimination on a (C[^]N[^]C)Au carboxylate. F) Evidence for β -hydride elimination on a novel gold(III) formate.

acid.^[10] Furthermore, these species were used for the hydroauration of alkynes in the presence of a radical initiator by homolytic cleavage of the Au–H bond to form the corresponding *trans*-vinylgold(III) complexes.^[11] Importantly, gold(III) carboxylates and formates have been proposed as intermediates prone to undergo β -hydride elimination in gold-catalyzed WGSRs^[12] and the dehydrogenation of formic acid,^[13] but the isolation and direct characterization of these species to substantiate these proposals has proven remarkably challenging. In this context, the resulting gold hydrides have also attracted significant attention^[14] although experimental validation for their participation in catalysis remains scarce.

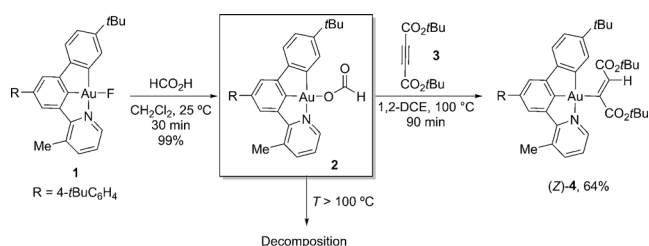
Our group has recently disclosed the synthesis of stable (N[^]C[^]C)gold(III) fluoride complexes that are nevertheless reactive towards nucleophiles (alkynes and boronic acids).^[15] We envisioned that the novel κ^3 -(N[^]C[^]C) pincer template could enable the synthesis of rather elusive gold(III) intermediates. Herein, we present the synthesis of a stable gold(III) formate together with a study of its reactivity towards β -hydride elimination and in the context of a catalytic dehydrogenation of formic acid (Scheme 1 F).

Cognizant of the basic nature of [(N[^]C[^]C)Au^{III}F] species,^[15] we envisioned their potential use as precursors of gold(III) formates. Indeed, after preliminary experiments, the reaction of gold(III) fluoride **1** in the presence of formic acid in CH₂Cl₂ at room temperature furnished the corresponding formate **2** in quantitative yield (Scheme 2).^[16] Gold(III) formate **2** is stable under ambient conditions as a solid but

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Supporting information for this article can be found under:
<https://doi.org/10.1002/anie.201705557>.



Scheme 2. Synthesis and reactivity of (N^{^C^C})gold(III) formate **2**.

decomposes in solution over prolonged periods of time (days). ¹H NMR analysis of **2** in CD₂Cl₂ showed a sharp singlet resonance at $\delta = 9.46$ ppm, characteristic of the formate moiety. Furthermore, a single crystal was grown by slow diffusion of MeOH into a concentrated solution of **2** in CH₂Cl₂, and the proposed structure was confirmed by X-ray diffraction analysis (Table 1).

Table 1: The solid-state molecular structures of **2**, **4**, and **6**.^[a]

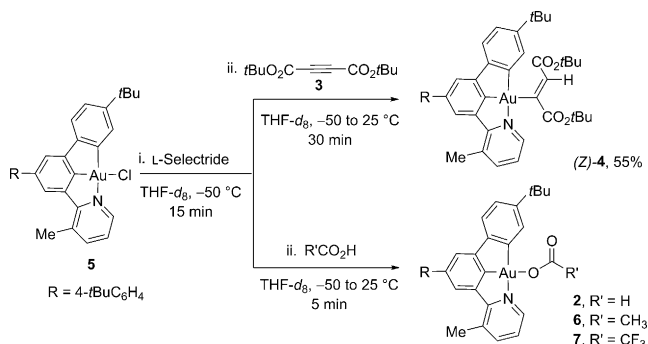
	2	4	6
Bond lengths [Å]	Au1–O1: 2.102(3) Au1–C8: 1.961(4)	Au1–C33: 2.083(9) Au1–C8: 2.004(8)	Au1–O1: 2.0873(17) Au1–C8: 1.952(2)
Bond angles [°]	O1–Au1–N1: 95.25(15) O1–Au1–C14: 103.51(17)	C33–Au1–N1: 104.5(3) C33–Au1–C13: 95.6(3)	O1–Au1–N1: 98.87(7) O1–Au1–C14: 99.46(8)

[a] Ellipsoids set at 50% probability. Hydrogen atoms have been omitted for clarity.

Interestingly, the Au–O bond [2.102(3) Å] is slightly longer than those previously reported for gold(III) oxo complexes,^[17] most probably owing to the strong *trans* influence of the central C(sp²) carbon atom of the (N^{^C^C}) ligand. As transition-metal formates are generally known to be precursors of hydrides,^[18] we next set out to confirm the ability of complex **2** to engage in a β -hydride elimination process. No conversion was observed by ¹H NMR spectroscopy after stirring **2** in aliphatic chlorinated solvents (CH₂Cl₂, 1,2-DCE) at temperatures up to 60 °C. However, heating **2** at 100 °C resulted in complete conversion and subsequent decomposition of the complex. This result suggested the possible formation of a highly reactive gold(III) hydride species. Interestingly, the reaction of formate **2** in the presence of di-*tert*-butyl acetylenedicarboxylate (**3**, 5 equiv) in 1,2-DCE at 100 °C afforded (*Z*)-gold(III) vinyl complex **4** in 64% isolated yield (Scheme 2). The reaction was monitored by ¹H NMR spectroscopy, revealing a first-order decay in **2** as well as first-order formation of **4** at comparable rates, which suggests a β -hydride elimination process (see the Supporting Information, Section S3.3). In solution, (*Z*)-**4** slowly isomerized to the *E* isomer,^[19] which could be characterized by X-ray diffraction analysis, revealing an elongated

Au1–C33 bond of 2.083(9) Å and a small C33–Au1–C13 angle of 95.6° (Table 1 and Ref. [16]).

To support the hypothesis of a putative gold(III) hydride intermediate^[20] that is able to insert into a triple bond, alternative methods for the synthesis of these species were sought (Scheme 3). Treatment of [(N^{^C^C})Au^{III}Cl] **5** with

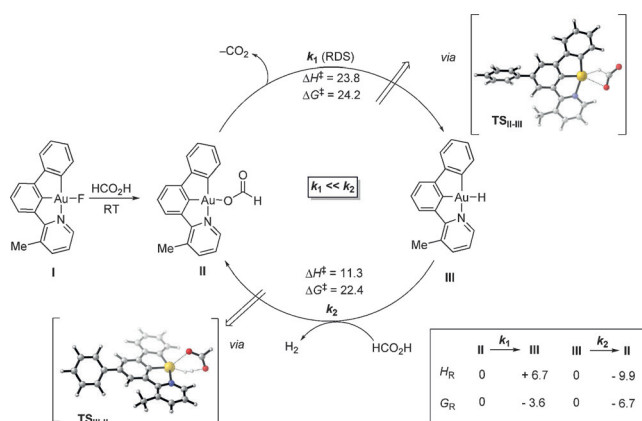


Scheme 3. Synthesis of vinyl gold(III) complex **4** and gold(III) esters **2**, **6**, and **7**.

L-selectride or LiHBEt₃ in dry THF-*d*₈ at –78 °C followed by addition of di-*tert*-butyl acetylenedicarboxylate furnished the corresponding *trans* addition product (*Z*)-**4** in 55% yield, in line with the results observed in Scheme 2. Interestingly, when the above-mentioned reaction mixture was exposed to formic, acetic, and trifluoroacetic acid, the corresponding gold(III) esters **2**, **6**, and **7** were cleanly obtained, all of which were unequivocally characterized by X-ray diffraction analysis (see Table 1 and the Supporting Information).^[21]

Having established the reactivity of gold(III) formate **2** towards β -hydride elimination, we envisioned the possibility of designing a homogeneous catalytic system for the dehydrogenation of formic acid. Gold-catalyzed dehydrogenations of FA in a heterogeneous fashion have been described, although typically basic additives or inorganic alkali metal salts are required for efficient performances.^[13,22] When complex **1** or **2** was heated at 100 °C in pure formic acid, a linear production of H₂ versus time and similar moderate catalytic activities (TOF = 3.1 ± 0.3 h⁻¹ for **1** and TOF = 3.5 ± 0.3 h⁻¹ for **2**) were obtained. Interestingly, neither decomposition nor a decrease in efficiency was noticed for a period of up to 44 h, which translated into a turnover number (TON) of > 137. The activation energy of the catalytic cycle, $E_a = 25.4 \pm 1.9$ kcal mol⁻¹, was calculated using an Arrhenius plot (see the Supporting Information).^[23] These results are also in line with the reactive nature of a putative gold(III) hydride intermediate whose reaction rate with formic acid should be fast at 100 °C compared to the β -hydride elimination of formate **2**. As a result, the mechanism of the dehydrogenation of formic acid can be pictured as a rate-determining β -hydride elimination of the gold(III) formate **2** upon heating to give a highly reactive hydride, which rapidly reacts with formic acid to release hydrogen and regenerate formate **2**, thereby closing the catalytic cycle (Scheme 4).

We turned to DFT studies to shed light on the overall reaction energy profile. We were interested in confirming the



Scheme 4. Proposed catalytic cycle for the dehydrogenation of formic acid. Structures and $\Delta H/\Delta G$ energies (kcal mol^{-1}) of the catalytic cycle computed at the M06/6-31G** (SDD) level of theory, including solvent effects (IEFPCM, solvent = formic acid).

feasibility of formate-to-hydride decarboxylation and dehydrogenation of FA from hydride to formate. Indeed, the first transition state $\text{TS}_{\text{II-III}}$ was located, which corresponds to the β -hydride-elimination-like decarboxylation step with a four-membered cyclic structure. The step is exergonic ($-3.6 \text{ kcal mol}^{-1}$) but needs a relatively high activation energy ($\Delta H^\ddagger = 23.8$, $\Delta G^\ddagger = 24.2 \text{ kcal mol}^{-1}$), justifying the high temperature required under the experimental conditions (Scheme 4). The high activation energy can be explained by the highly asynchronous and strained TS, showing an initial Au–O bond rupture (2.6 Å) that precedes the formation of the Au–H bond (2.0 Å). The reverse step $\text{TS}_{\text{III-II}}$ was also computed. The gold(III) hydride activates the formic acid molecule in a cyclic six-membered TS, which seems to be more synchronous than the previous one. Interestingly, the activation energies of $\text{TS}_{\text{III-II}}$ are significantly lower ($\Delta H^\ddagger = 11.3$, $\Delta G^\ddagger = 22.4 \text{ kcal mol}^{-1}$) than those of $\text{TS}_{\text{II-III}}$, and the formation of **II** from **III** is fairly exergonic ($-6.7 \text{ kcal mol}^{-1}$). Thus the relative k_1 and k_2 values calculated computationally and the high energy of $\text{TS}_{\text{II-III}}$ are in agreement with the experimental findings indicating that β -hydride elimination is the rate-determining step in this process. Alternative pathways, including those in which decoordination^[24] or protonation of the pyridine ligand precedes the decarboxylation step, were also studied. However, these calculations gave substantially higher activation energies compared to those reported in Scheme 4 (see Section S8).

In summary, we have described the synthesis and full characterization of the first gold(III) formate complex, which was obtained quantitatively from the reaction of an (N[^]C[^]C[^]) pincer gold(III) fluoride with formic acid. This complex undergoes β -hydride elimination upon heating, enabling a catalytic dehydrogenation of pure formic acid. While the efficiency of this catalytic system is far from representing a synthetically useful alternative to existing heterogeneous systems,^[13,22] we believe these results provide insightful guidance towards the development of more efficient systems in the near future.

Acknowledgements

We thank the European Research Council (ERC Starting Grant 307948) and the Forschungskredit of the University of Zürich for financial support. We acknowledge networking support by the COST Action CHAOS CA15106. The SGI/IZO-SGIker UPV/EHU is acknowledged for the allocation of computational resources. We also thank Dr. Olivier Blacque for the X-ray diffraction analysis of complex **4** and Benjamin Probst and Prof. Roger Alberto for technical support on the quantification of H_2 .

Conflict of interest

The authors declare no conflict of interest.

Keywords: β -hydride elimination · gold complexes · gold hydrides · reaction mechanisms · vinyl gold species

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Manuscript received: May 31, 2017

Version of record online: ■■■■■■, ■■■■■■

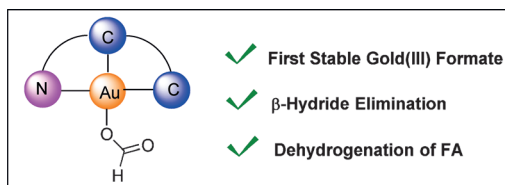
Communications



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The First Gold(III) Formate: Evidence for
 β -Hydride Elimination



An anionic ligand exchange reaction on $[(N^{\wedge}C^{\wedge}C)Au^{III}F]$ in the presence of formic acid delivered the first example of a stable gold(III) formate. Its ability to undergo β -

hydride elimination and its reactivity in the dehydrogenation of formic acid (FA) have been experimentally and computationally demonstrated.