

Fast Atom Bombardment Induced Decomposition Pattern of the Gold(III) Bis(carbene) Complex $[\{(p\text{-MeC}_6\text{H}_4\text{NH})(\text{EtO})\text{C}\}_2\text{AuI}_2]\text{ClO}_4$, a Retrosynthetic Process?

Anna Laura Bandini,^{1a} Guido Banditelli,^{*1a} Giovanni Minghetti,^{1b} Beatrice Pelli,^{1c} and Pietro Traldi^{1c}

Centro CNR, Dipartimento di Chimica Inorganica e Metallorganica, Università di Milano, 20133 Milano, Italy, Dipartimento di Chimica Università di Sassari, 07100 Sassari, Italy, and CNR Servizio di Spettrometria di Massa, Area di Ricerca di Padova, 35100 Padova, Italy

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The fast atom bombardment (FAB) induced decomposition pattern of the ionic bis(carbene)gold(III) complex $[\{(p\text{-MeC}_6\text{H}_4\text{NH})(\text{EtO})\text{C}\}_2\text{AuI}_2]\text{ClO}_4$ (1) is described and discussed in detail with the aid of metastable data. A lack of $[\text{M}]^+$ ions is observed when sulfolane is used as the matrix. Instead, the molecular species observed is the $[\text{M} - \text{H}]^{*+}$ ion. The fragmentation pattern can be considered as a retrosynthetic process of the compound itself, never previously observed for an organometallic under FAB conditions. The MS pattern suggests the synthesis of the new carbene-methanide derivative 2, $[\{(p\text{-MeC}_6\text{H}_4\text{NH})(\text{EtO})\text{C}\}(p\text{-MeC}_6\text{H}_4\text{N}=\text{C})(\text{EtO})\text{C}\text{Au}]$, observed under FAB-MS conditions as the most stable ion. An independent synthesis was successful.

Introduction

Since the discovery of the first Fischer carbene complex, the studies on metal carbene complexes have continuously grown so that they, as well as the isoelectronic alkylidene derivatives, appear now to be one of the most important topics in the metal-carbon chemistry. Their importance has led to a great variety of research concerning synthesis, structure, theory, and reactivity.² Thus, it is strange that their behavior in the vapor phase, as far as we know, has not been investigated, even though mass spectrometry has proved to be a valid tool in structural characterization of organic and organometallic compounds.³

The employment of ionization energy (IE) or appearance energy (AE) measurements, the development of collisional spectroscopy, and the extensive use of metastable ion data have allowed energetics and kinetics of decomposition pathways to be described and have consequently provided important information on the structure of gaseous ions.⁴ Furthermore, the very narrow time window of mass spectrometric experiments (10^{-12} – 10^{-7} in the ion source, 10^{-6} – 10^{-5} s in the flight tube)⁴ can lead, in principle, to the structural definition of short-lived ionic species. This last approach has been mainly utilized by organic chemists, who consider mass spectrometry not only as a molecular weight machine but also as a chemical reactor that can give fundamental data on both structure and reactivity of different compounds in the gas phase.

In this context, it is noteworthy that the retrosynthetic approach,⁵ recently reviewed by Selva^{5a} on organic com-

pounds, has as its basis the hypothesis that decomposition patterns are really retrosynthesis processes. In electron-impact MS, many efforts have been devoted to the identification of retrosynthetic pathways. This approach led, for example, to the description of the McLafferty rearrangement (analogous to the Norris type II photochemical process),^{5b} to retro Diels-Alder reactions^{5c} and 1,3-dipolar retrocycloadditions.^{5d} Kametani and Fukumoto employed this principle as a tool for the synthesis of natural products.^{5e}

The new ionization methods⁶ now available, which are alternatives to the well-established electron ionization (EI), have allowed entire classes of compounds, thermally or EI labile, to be analyzed by using mass spectrometry. Among these new methods, fast atom bombardment (FAB) mass spectrometry has shown a vigorous growth in the last years in the organometallic field, proving its utility on metal derivatives of most of the elements.⁷ Leaving aside the intimate mechanism of FAB ionization, which is still debated,⁸ we note that very often the fragmentation pathways observed under FAB conditions are not simple to understand and that the deposition of energy in the molecular species is usually lower than that deposited under EI conditions. Furthermore, the successful design of differently structured matrices may be in accord with the idea that FAB desorption is a solution-phase rather than a gas-phase process.⁸

The above considerations motivated us to study the MS behavior under FAB conditions of related classes of or-

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ganometallic derivatives, never studied before (i.e., carbene, methanide, and isocyanide derivatives of gold(I) and gold(III)), whose solid-state characterization was recently completed by using Mössbauer spectroscopy and X-ray structure determinations.⁹ We wish to report here the first results obtained with $[(p\text{-MeC}_6\text{H}_4\text{NH})(\text{EtO})\text{C}_2\text{AuI}_2]\text{ClO}_4$.

Experimental Section

Elemental analyses and molecular weight determinations were performed by the Microanalytical Laboratory of the University of Sassari and by Mikroanalytisches Labor Pascher (Remagen, FRG). The analytical samples were pumped to constant weight (ca. 0.1 Torr; 298 K). Evaporation was always carried out under reduced pressure (water aspirator).

All mass spectrometric experiments were performed on a double-focusing, reverse geometry VG ZAB-2F instrument.¹⁰ FAB experiments were carried out with different matrices (glycerol, thioglycerol, glycerol + acetic acid, thioglycerol + acetic acid, sulfolane). Molecular species were present only when the sample was dissolved in sulfolane. The bombarding Xe atom beam had a translational energy of 8 KeV.

Metastable transitions were detected in both the first and the second field-free regions by means of B/E = constant linked scans¹¹ and mass analyzed ion kinetic energy (MIKE) spectrometry,¹² respectively.

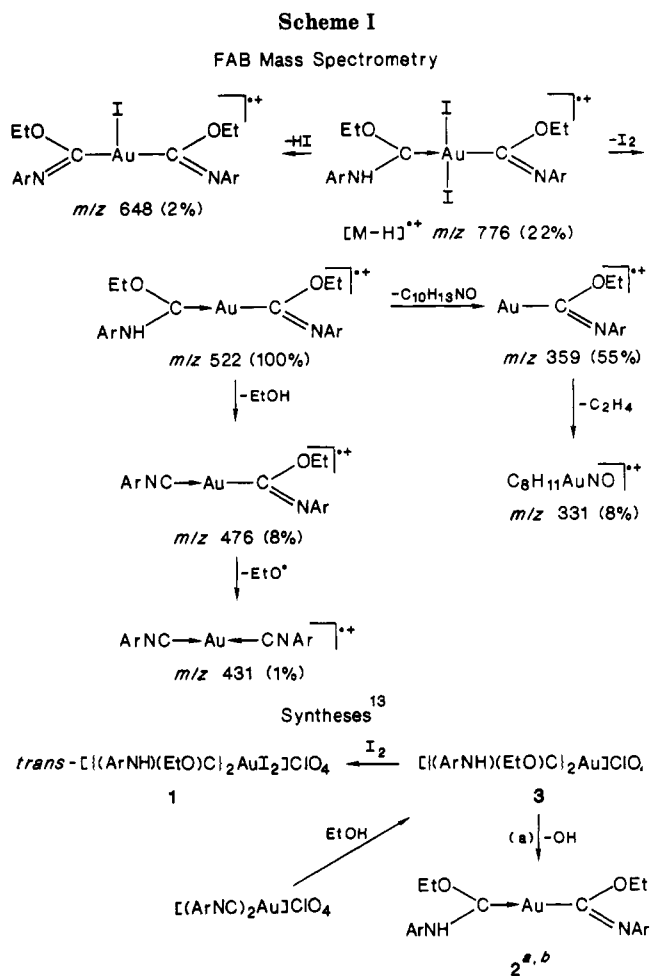
$[(p\text{-MeC}_6\text{H}_4\text{NH})(\text{EtO})\text{C}_2\text{AuI}_2]\text{ClO}_4$ (1) and $[(p\text{-MeC}_6\text{H}_4\text{NH})(\text{EtO})\text{C}_2\text{Au}]\text{ClO}_4$ (3). Complexes 1 and 3 were obtained and purified according to the literature.¹³ Their purity was checked through melting points, elemental analyses (C, H, N, and Au), and infrared and proton NMR spectra. According to these data, compound 1 contains ca. 0.25 molecule of diethyl ether and compound 3 is a mixture of different isomers, as already observed.⁹

$[(p\text{-MeC}_6\text{H}_4\text{NH})(\text{EtO})\text{C}]\{(p\text{-MeC}_6\text{H}_4\text{N}=\text{C})(\text{EtO})\text{C}\text{Au}\}$ (2). To a solution of $[(p\text{-MeC}_6\text{H}_4\text{NH})(\text{EtO})\text{C}_2\text{Au}]\text{ClO}_4$ (191 mg, 0.31 mmol) (3) in ethanol (60 mL) was added potassium hydroxide in the same solvent (2.17 mL, 7.93 g/L, 0.31 mmol) under stirring. After 10 min, a small amount of a colorless solid was filtered off and identified as KClO_4 . The clear solution was evaporated to dryness and the waxy residue taken up with a mixture of diethyl ether (10 mL) and *n*-hexane (20 mL). By scratching, a white solid (131 mg) was obtained and collected by filtration. The crude solid was next suspended in dichloromethane (2 mL). By addition of diethyl ether (30 mL), a solid precipitated and was filtered off (27 mg). The white microcrystalline compound was identified as unreacted starting complex 3 (C, H, N analyses; mp, and IR spectrum).

The colorless filtrate was then evaporated in the presence of diethyl ether (4 × 10 mL). Next, *n*-hexane (30 mL) was added to the concentrated colorless solution (5 mL) to give the analytical sample (54 mg). Compound 2: mp 100 °C with decomposition; molecular weight calcd 522, found 552 in chloroform solution (0.51%); IR (Nujol) $\delta_{\text{NH}} + \nu_{\text{C}=\text{N}}$ ca. 1600 cm^{-1} (s); the ν_{NH} stretch is observed as weak and broad absorptions (ca. 3250–2200 cm^{-1} ; ca. 1900 cm^{-1}). Anal. Calcd for $\text{AuC}_{20}\text{H}_{25}\text{N}_2\text{O}_2$ (2): C, 45.98; H, 4.79; N, 5.36; O, 6.13; Au, 37.74. Found: C, 45.10; H, 4.61; N, 5.37; O, 6.42; Au, 37.9.

Results and Discussion

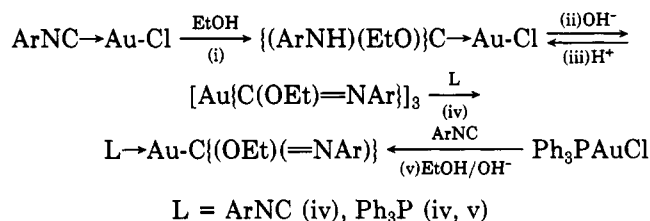
In the upper part of Scheme I, the FAB-induced decomposition pattern of compound 1 is reported. The lack of $[\text{M}]^+$ ions, usually observed in FAB ionization of ionic



^aThis work.

^bNot previously observed.¹⁴

Scheme II



compounds (M^+X^-), is to be emphasized. The presence of $[\text{M}-\text{H}]^+$ odd-electron ions at m/z 776 can be reasonably attributed to a chemical interaction with the matrix. A good solubility of 1 was obtained by using, as the matrix, sulfolane (see Experimental Section). As already published by Lloyd and Cotter,¹⁵ this unusual odd-electron ion could originate by extraction of H^+ by reaction with $[\text{sulfolane-H}]^-$ and/or with $[\text{SO}_2]^-$.

The one-step, metastably supported, I_2 loss leads to a gold(I) ionic species (m/z 522, base peak) from which, through sequential losses of $\text{C}_2\text{H}_5\text{OH}$ and $\text{C}_2\text{H}_5\text{O}^+$, the bis(isocyanide)gold(I) derivative of m/z 431 is obtained. Hence, by positive ion FAB mass spectrometry of compound 1, the starting material for synthesis of 1 has been obtained, as described in the lower part of Scheme I. FAB mass spectrometry has caused a reverse synthesis to occur.

Although the ions at m/z 431 have exactly the mass of the starting material for the synthesis, the ions of m/z 522

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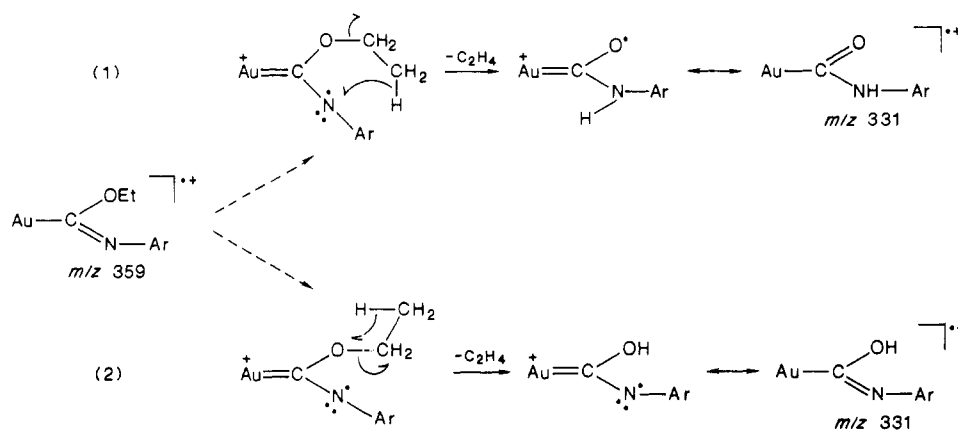
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Scheme III



may be the dehydrogenated ($-\text{H}^*$) forms of the well-known bis(carbene)gold(I) derivative (i.e., the starting compound for 1 by oxidative addition of I_2). The former could be reasonably regarded as a monocarbene-monomethanide derivative, $\text{L} \rightarrow \text{AuC}(\text{OR})=\text{NAr}$, comparable to gold(I) methanide complexes that were isolated and characterized in the condensed phase when L is, e.g., PPh_3 (see Scheme II, iv).¹⁶ In addition, we recall that the conversion of a carbene to a methanide ligand is known to occur reversibly: thus in alkaline solution, deprotonation of a coordinated carbene gives a methanide (Scheme II, ii); the reverse occurs in acidic media (Scheme II, iii).^{17a} In this respect, the ionic species at m/z 476 can be considered a gold(I) derivative, $\text{ArNC} \rightarrow \text{Au}-\text{C}(\text{OR})=\text{NAr}$, not observed in the synthesis of the carbene complexes although isolated from the trimeric derivatives $[\text{Au}-\text{C}(\text{OEt})=\text{NAr}]_3$ by reaction with ArNC (Scheme II, iv).^{16b} The loss addition of I_2 parallels the above findings, even though the molecular species differs by a H^* only.

The $\text{C}_{10}\text{H}_{13}\text{NO}$ loss from the carbene-methanide species of m/z 522, leading to gold(I) methanide radical ions at m/z 359 is noteworthy. Because the fragmentation occurs as observed, the methanide-gold bond must be stronger than the carbene-gold bond. In addition, the high stability of the product ion is proved either by its relative abundance (55%) or by the further loss of C_2H_4 , which does not imply, quite surprisingly, the Au-C bond. This behavior can be explained by considering the ion at m/z 359 to have an alkylidene-type structure.

Such a species explain both the gold-carbon bond strength and the easy ethylene loss. For this fragmentation pathway two different mechanisms can be proposed (see Scheme III), i.e., a H^* rearrangement on the nitrogen or on the oxygen atom (pathways 1 and 2, respectively). Gold(I) methanides have already been studied by some of us and shown to be stable in trimeric form in the solid state, in solution and in the gas phase.¹⁷ In particular, the ions at m/z 359, never found under EI conditions,^{17b} could represent, in principle, the monomeric unit of such molecules. However, other possible structures for the ions at m/z 359 cannot be excluded; a difficulty with the proposed structure in Scheme I lies in the coordination number of gold, formally monocoordinated, whereas gold(I) complexes

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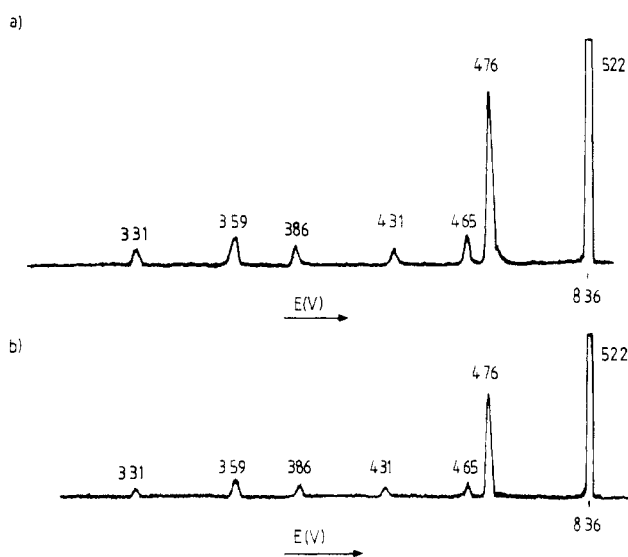


Figure 1. MIKE spectra of (a) ions at m/z 522 originated from FAB of compound 1 and (b) molecular ions of compound 2.

are usually linear bicoordinated species. Hence possible structures, e.g., $\text{EtO}Au \leftarrow \text{C} \equiv \text{NAr}$ arising from rearrangements subsequent and/or concerted with the carbene loss could be present. Nevertheless, it is worth noting that the Au-O bonds are uncommon in the condensed phase, which is consistent with the different hard and soft character of an oxygen donor and a gold(I) acceptor, respectively.

Finally, all the odd-electron ionic species from the simple H^* loss are species that are not observable in solution chemistry. All of them are described as containing the methanide group. Alternatively, they could be described as allylic-like, i.e., involving a η^3 -coordination rather than a σ gold-carbon bond. The structures of an allylic-type involve a difference of two electrons in the overall electron bookkeeping: as a consequence the stability of the ions at m/z 359 could be justified, in principle, by the achievement of a 14-electron system, i.e. the same which in condensed phase results from the oligomerization process (Scheme II, ii).

These FAB-MS results prompted us to isolate, even in condensed phase, the carbene-methanide species observed in gas phase. Using as selective criterium the relative stability of the different observed ions, we made a first attempt to obtain the $\{[(p\text{-MeC}_6\text{H}_4\text{NH})(\text{EtO})\text{C}]\{p\text{-MeC}_6\text{H}_4\text{N}=\}(\text{EtO})\text{C}\}\text{Au}$ complex. Indeed the expected carbene-methanide derivative $\{[(p\text{-MeC}_6\text{H}_4\text{NH})(\text{EtO})\text{C}]\{p\text{-MeC}_6\text{H}_4\text{N}=\}(\text{EtO})\text{C}\}\text{Au}$ (2) was obtained by reaction of $\{[(p\text{-MeC}_6\text{H}_4\text{NH})(\text{EtO})\text{C}]_2\text{Au}\}\text{ClO}_4$ (3) with a stoichiometric

metric amount of alkali. The identity of compound **2** was confirmed by using the MIKE spectrum, which is, as required, exactly like those of the m/z 522 ions (see Figure 1). Identical abundances and kinetic energy release¹² values ($T_{1/2}$) in the MIKE spectra of two isobaric ionic species implicate their structural identity.¹⁸

In conclusion, the data herein reported constitute a strict analogy between the FAB-induced decomposition pathways and solution synthesis. To our knowledge, this is the first example of a retrosynthetic pathway in organometallic chemistry observed under FAB conditions. Furthermore,

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the identification of highly stable product ions has suggested the possibility of synthesizing these stable species in the condensed phase, which has been successfully performed. Hence FAB mass spectrometry not only has analytical interest but also gives useful information on the stability of different species to be used in the synthesis of new compounds.

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Organometallic Donor-Acceptor Complexes with Nonplanar Donors: The Zigzag Linear Chain Complex $[(C_6Me_6)_2M^{2+}][iso-C_4(CN)_6^{2-}]$ (M = Fe, Ru)

Michael D. Ward* and J. C. Calabrese

Central Research and Development Department, † E. I. du Pont de Nemours and Co., Inc., Experimental Station E328, Wilmington, Delaware 19898

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Donor-acceptor solids $[(C_6Me_6)_2Me^{2+}][iso-C_4(CN)_6^{2-}] \cdot MeNO_2$ (M = Fe, **1a**; M = Ru, **2a**) and $[(C_6Me_3H_3)_2M^{2+}][iso-C_4(CN)_6^{2-}]$ (M = Fe, **1b**; M = Ru, **2b**) prepared from $(arene)_2M^{2+}$ and $iso-C_4(CN)_6^{2-}$ are described. Single-crystal X-ray studies show that **1a** crystallizes in the space group $P2_1/c$ with $a = 19.875$ (6) Å, $b = 10.512$ (2) Å, $c = 15.981$ (4) Å, $\beta = 96.65$ (3)°, $V = 3316$ (3) Å³, $\rho = 1.36$ g cm⁻³, $Z = 4$, $R_u = 0.061$, and $R_w = 0.080$. The ruthenium analogue **2a** also crystallizes in the space group $P2_1/c$ with $a = 19.973$ (2) Å, $b = 10.553$ (2) Å, $c = 16.144$ (1) Å, $\beta = 96.80$ (7)°, $V = 3378$ (3) Å³, $\rho = 1.36$ g cm⁻³, $Z = 4$, $R_u = 0.070$, and $R_w = 0.068$. Both complexes exhibit "zigzag" linear chains of closely spaced alternating cations and anions. Donor-acceptor interactions arise from close intermolecular contacts between the C_6Me_6 ligands of the dications and nitrogen atoms of the nonplanar dianion with dianions "bridging" the dications via three of its cyano groups. The complexes exhibit strong charge-transfer bands and are best described as donor-acceptor (DA) complexes with nominally doubly charged ($D^{2+}A^{2+}$) ground states and (D^+A^+) excited states. The difference between the charge-transfer absorption energies of **1** and **2** is equivalent to the difference in the solution reduction potentials of the isostructural $(arene)_2M^{2+}$ cations. The structure of the 19e $(C_6Me_6)_2Fe^+$ monocation, reported here for the first time, is essentially identical with that of the 18e dication, suggesting that the charge-transfer transitions of these DA complexes can occur without the formation of energetically unfavorable molecular conformations.

Introduction

Donor-acceptor (DA) interactions in molecular solids are to a large extent the foundation of the extensive interest in these materials.¹ We have been particularly interested in DA solids with organometallic constituents, since the diverse variety of this class of reagents suggests the possibility for systematic investigation of these phenomena as well as the discovery of new materials. Our goal has been to better understand structure-function relationships in these materials, which may result in new concepts for rational modification of structural and electronic properties that are relevant to possible electronic applications.²

The structural motif observed for many organic DA complexes³ and organometallic complexes such $[(C_5H_5)_2Fe^+][TCNE]^-$ ⁴ and $[(C_5Me_5)_2Fe^+][TCNQ]^-$ ⁵ consists of mixed stacks of planar π -donors and π -acceptors in a face-to-face arrangement. Similarly, we recently re-

ported $[(C_6Me_3H_3)_2M^{2+}][C_3[C(CN)_2]_3^{2-}]$ (M = Fe, Ru)^{6a} complexes which possessed this conventional mixed-stack motif with $(C_6Me_3H_3)_2M^{2+}$ acceptors and $C_3[C(CN)_2]_3^{2-}$ donors, in which the close approach of the π -systems of these species resulted in DA interactions associated with a rather unusual doubly charged "superionic" ground state.⁷⁻⁹ In contrast, we have recently demonstrated that

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