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LETTER

A revision on gold(I)–carbon stretching frequencies

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To our knowledge only a few studies have been published concerning the identification, in IR and/or Raman spectra, of bands attributable to gold–carbon stretching modes, ν(Au–C), for gold(I) compounds. The compounds already examined in the literature (Table 1) exhibit Au–C stretching frequencies ranging from 540 to 330 cm^{-1} [1–5].

In order to extend the available data, we deemed it of interest to study the gold(I)–carbon vibrational frequencies of a number of other compounds (see Table 2).

Experimental

All compounds were prepared according to the literature [5–8]. Analytical per cent data were in agreement with the theoretical values. Carbon, nitrogen and hydrogen were determined with a Perkin-Elmer 2400 elemental analyzer. Gold was determined with a Varian AA-5 atomic absorption spectrophotometer. IR spectra were obtained at room temperature on polythene pellets of the samples in the range 500–80 cm^{-1}, using a Digilab FTS-40 FT-IR spectrometer. FT-Raman spectra were recorded at room temperature on powdered samples, using a Bruker IFS 66 spectrometer equipped with a Bruker FRA 106 accessory.

TABLE 1. IR gold(I)–carbon stretching frequencies (cm^{-1}) reported in the literature

Compound	ν(Au–C)	Reference
CH_3AuPPh_3	539m	1,2
Au(CO)Cl	443w	3
$K[Au(CN)_2]$	427	4
$[Au(CH_3NC)_2]BF_4$	330ms	5

m = medium, w = weak, ms = medium strong.

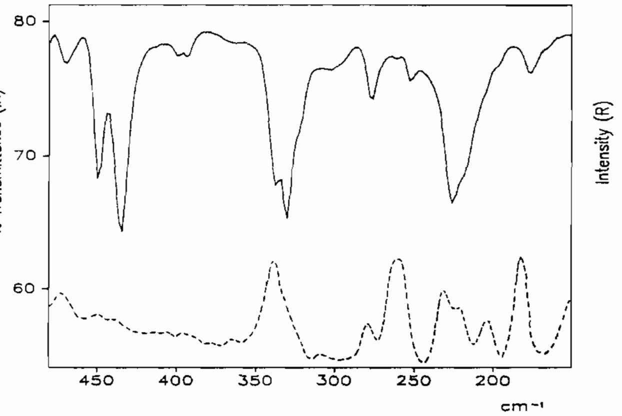

Fig. 1. Far-IR (polythene pellet) (——) and Raman (powder) (– – –) spectra of (acac)$AuPPh_3$.

Results and discussion

We examined the IR and Raman spectra of some two-coordinate gold(I) complexes $[L_2Au]X$ ($X = ClO_4$, BF_4), where L can be an isonitrile or a carbene, together with the spectra of the complex of Au(I) with acetylacetonate (acac), coordinated through a carbon atom [8], and triphenylphosphine. Our results are reported in Table 2.

It should be noted that we observed Au–C stretching frequencies lying between 350 and 330 cm^{-1}, i.e. at lower values than those reported in Table 1. A possible explanation is that the ligands L of our complexes have a mass which is greater than that of methyl or cyanide groups or of carbon oxide.

In the IR and Raman spectra of compounds **2** and **5** (Table 2), a shoulder appears beside the band of stronger intensity assigned to Au–C stretching (see for example Fig. 1). Yet we could predict a single IR active band and a single Raman active band due to the Au–C stretching vibrations for the linear centrosymmetric cation of compound **2**. At the same time, as the molecule of compound **5** contains only one gold–carbon bond, it is obvious that just a single vibrational mode of this bond should be observed. However we can explain these anomalies on the basis of site symmetry or factor group effects.

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TABLE 2. Selected IR and Raman frequencies (cm^{-1})

No.	Compound	ν(Au–C) IR	ν(Au–C) Raman	δ(Au–C) IR
1	$[(CH_3NC)_2Au]ClO_4$	330m	334s	102m
2	$[(C_6H_5NC)_2Au]ClO_4$	350s, 342sh	351m	102m
3	$[(p\text{-}CH_3C_6H_4NC)_2Au]BF_4$	348s	350m	99m
4	$\{[(p\text{-}CH_3C_6H_4NH)_2C]_2Au\}BF_4$	330m	336m	96m
5	$(acac)Au(PPh_3)$	336sh, 330m	338m, 330sh	105w

s = strong, m = medium, w = weak, sh = shoulder.

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