

N3—C5	1.497 (6)	1.493 (6)
N3—C6	1.500 (6)	1.487 (6)
N4—C7	1.489 (6)	1.503 (6)
N4—C8	1.474 (7)	1.501 (6)
C1—C2	1.476 (8)	1.484 (8)
C3—C31	1.519 (7)	1.543 (7)
C3—C4	1.514 (7)	1.513 (7)
C4—C5	1.525 (8)	1.502 (7)
C5—C51	1.524 (7)	1.529 (7)
C6—C7	1.474 (8)	1.475 (8)
C8—C81	1.520 (8)	1.523 (8)
C8—C9	1.518 (8)	1.512 (8)
C9—C10	1.513 (8)	1.519 (8)
C10—C101	1.526 (8)	1.493 (8)
N1—Ni—N2	86.6 (2)	86.4 (2)
N1—Ni—N3	177.4 (2)	176.9 (2)
N1—Ni—N4	94.9 (2)	94.2 (2)
N2—Ni—N3	91.9 (2)	92.7 (2)
N2—Ni—N4	175.6 (1)	177.4 (2)
N3—Ni—N4	86.8 (2)	86.9 (2)
C10—N1—C1—C2	-171.4 (6)	-179.6 (5)
C3—N2—C2—C1	161.2 (5)	169.9 (5)
C6—N3—C5—C4	-173.6 (5)	-174.4 (5)
C8—N4—C7—C6	177.9 (6)	174.5 (5)
N1—C1—C2—N2	-52.3 (3)	-54.1 (3)
C3—C4—C5—N3	-63.9 (4)	-64.5 (4)
N4—C8—C9—C10	-72.3 (4)	-61.8 (4)
C1—N1—C10—C9	-163.3 (6)	173.1 (5)
C2—N2—C3—C4	173.3 (5)	175.4 (5)
C5—N3—C6—C7	-166.4 (5)	-165.5 (5)
C7—N4—C8—C9	-174.9 (6)	166.9 (5)
N2—C3—C4—C5	63.9 (4)	65.0 (4)
N3—C6—C7—N4	53.2 (3)	52.0 (3)
C8—C9—C10—N1	59.9 (4)	73.2 (4)

The structure was solved by direct and Fourier methods. Refinement was by full-matrix least-squares methods. H atoms were located by difference Fourier methods. *NRCVAX* (Gabe, Le Page, White & Lee, 1987) was used for all crystallographic computations.

The authors thank the National Science Council for support under grants NSC84-2112-M007-019 and NSC84-2113-M007-021. They are also indebted to Ms Shu-Fang Tung for collecting the X-ray diffraction data.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and least-squares-planes data have been deposited with the IUCr (Reference: AB1193). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1995). **C51**, 2020–2023

Tetrakis(μ -benzoato-*O:O'*)bis(*N,N*-diethylnicotinamide-*N'*)dicopper(II)

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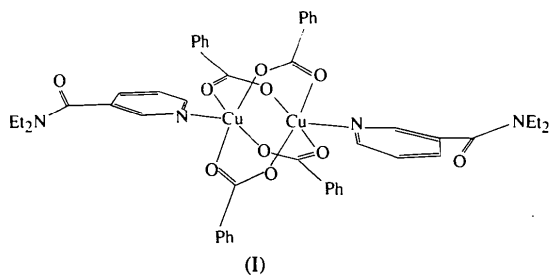
(Received 23 August 1994; accepted 13 January 1995)

Abstract

The title molecule, [Cu₂(C₆H₅COO)₄(C₁₀H₁₄N₂O)₂], is a crystallographically centrosymmetric binuclear complex, with Cu atoms [Cu...Cu' = 2.613 (1) Å] bridged by four benzoate ligands. The four nearest O atoms around each Cu atom form a square-planar arrangement with the square-pyramidal coordination completed by the pyridine N atom of the *N,N*-diethylnicotinamide ligand at a distance of 2.162 (6) Å. Each Cu atom is displaced by 0.190 (1) Å from the plane of the four O atoms, with an average Cu—O distance of 1.974 (6) Å.

Comment

N,N-Diethylnicotinamide (DENA) is known as an important respiration stimulant. The structures of some complexes obtained from the reactions of transition metal(II) ions with DENA have been determined previously: Cd(DENA)(SCN)₂ (Bigoli, Braibanti, Pellinghelli & Tiripicchio, 1972), Mn(DENA)₂(NCS)₂ (Bigoli, Braibanti, Pellinghelli & Tiripicchio, 1973*a*), Zn(DENA)₂(NCS)₂(H₂O)₂ (Bigoli, Braibanti, Pellinghelli, 1973*b*). In Mn(DENA)₂(NCS)₂, DENA is a bidentate ligand, bonded to the metal atom through the pyridine N and amide O atoms. Alternatively, in Cd(DENA)(SCN)₂ and Zn(DENA)₂(NCS)₂(H₂O)₂, DENA is a monodentate ligand coordinated through only the pyridine N atom, which is more basic than the O atom. The title compound, (I), is a binuclear com-



plex, consisting of two DENA and four benzoate ligands. The structures of similar complexes of the Cu^{2+} ion, $[\text{Cu}(\text{C}_6\text{H}_5\text{COO})_2(\text{C}_5\text{H}_5\text{N})]_2$ (Usabaliev *et al.*, 1980) and $[\text{Cu}(\text{C}_6\text{H}_5\text{CO}_2)_2(\text{py})]_2$ (Speier & Fulop, 1989), have also been determined. In these structures, the benzoate ion acts as a bidentate ligand. The structure determination of the title compound (a copper complex of DENA and benzoate ligands) was undertaken in order to define the ligand properties of DENA and the benzoate ligand, and to compare the results obtained here with those reported earlier. A view of the molecule and the atomic numbering scheme is shown in Fig. 1.

The dimeric complex, $[\text{Cu}_2(\text{C}_6\text{H}_5\text{COO})_4(\text{DENA})_2]_2$, has a centre of symmetry and two Cu^{II} atoms surrounded by four benzoate groups and two DENA ligands. The DENA ligands are coordinated to Cu atoms through the pyridine N atoms only. The benzoate groups act as bridging ligands. The $\text{Cu}\cdots\text{Cu}'$ distance [2.613 (1) Å] is shorter than in $[\text{Cu}_2(\text{C}_6\text{H}_5\text{COO})_4(\text{py})_2]$ [2.681 (1) Å; Usabaliev *et al.*, 1980], $[\text{Cu}(\text{C}_6\text{H}_5\text{CO}_2)_2(\text{py})]_2$ [2.658 (1) Å; Speier & Fulop, 1989] and $[\text{Cu}_2(\text{CH}_3\text{COO})_4(\text{H}_2\text{O})_2]$ (2.64 Å; van Niekerk & Schoening, 1953). In metallic copper, the $\text{Cu}\text{—}\text{Cu}$ bond length is 2.55 Å (Lee, 1986). The title compound has the smallest $\text{Cu}\cdots\text{Cu}$ distance

after metallic copper. Therefore, a weak orbital interaction may exist between the two Cu atoms. The average $\text{Cu}\text{—}\text{O}$ distance is 1.974 (6) Å, and four O atoms of the bridging benzoate ligands around each Cu atom form a square plane. The Cu atom lies 0.190 (1) Å below the least-squares plane. The average $\text{O}\text{—}\text{Cu}\text{—}\text{O}$ bond angle is 89.5 (2)°. A square-pyramidal arrangement around each Cu atom is completed by the pyridine N atom of a DENA ligand at 2.162 (6) Å from the Cu atom. The $\text{N1}\text{—}\text{Cu}\cdots\text{Cu}'$ angle is 173.8 (1)° and the dihedral angle between plane through Cu, O1, C1, O2', Cu', O1', C1' and O2 and the plane through Cu, O3, C8, O4', Cu', O3' and C8' is 89.9 (1)°. Bond lengths and angles are in good agreement with the values reported for other copper complexes: $[\text{Cu}(\text{CH}_3\text{CO}_2)_2(\text{py})]_2$ (Barclay & Kennard, 1961; Hanic, Stempelova & Hanicova, 1964), $[\text{Cu}(\text{CH}_2\text{ClCO}_2)_2\text{—}(2\text{Me-py})]_2$ (Davey & Stephens, 1970), $[\text{Cu}_2(\text{CH}_3\text{CO}_2)_4\text{—}(\text{pyrazine})]$ (Morosin, Hughes & Soos, 1975) and $[\text{Cu}(\text{C}_6\text{H}_5\text{CO}_2)_2(\text{py})]_2$ (Speier & Fulop, 1989).

Experimental

The title compound was prepared from the reaction of 0.01 mol of $\text{Cu}(\text{C}_6\text{H}_5\text{COO})_2 \cdot 3\text{H}_2\text{O}$ and 0.017 mol of DENA in 120 ml of ethanol. The blue mixture was filtered and set aside for crystallization at ambient temperature for a few weeks. Suitable green crystals were obtained by slow evaporation from ethanol.

Crystal data

$[\text{Cu}_2(\text{C}_7\text{H}_5\text{O}_2)_4\text{—}(\text{C}_{10}\text{H}_{14}\text{N}_2\text{O})_2]_2$
 $M_r = 968.2$
 Orthorhombic
Pcab
 $a = 10.881 (2) \text{ \AA}$
 $b = 19.772 (3) \text{ \AA}$
 $c = 21.563 (3) \text{ \AA}$
 $V = 4639 (1) \text{ \AA}^3$
 $Z = 8$
 $D_x = 2.772 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation
 $\lambda = 0.71069 \text{ \AA}$
 Cell parameters from 25 reflections
 $\theta = 7\text{—}10^\circ$
 $\mu = 1.954 \text{ mm}^{-1}$
 $T = 298 \text{ K}$
 Block like
 $0.22 \times 0.22 \times 0.22 \text{ mm}$
 Green

Data collection

Enraf–Nonius CAD-4 diffractometer
 $\omega/2\theta$ scans
 Absorption correction: none
 5121 measured reflections
 3676 independent reflections
 2770 observed reflections
 $[I > 2\sigma(I)]$
 $R_{\text{int}} = 0.0141$

$\theta_{\text{max}} = 24^\circ$
 $h = -1 \rightarrow 12$
 $k = -1 \rightarrow 22$
 $l = -1 \rightarrow 24$
 3 standard reflections monitored every 250 reflections
 frequency: 120 min
 intensity decay: 1%

Refinement

Refinement on F
 $R = 0.0453$
 $wR = 0.0486$

$(\Delta/\sigma)_{\text{max}} = 0.01$
 $\Delta\rho_{\text{max}} = 0.01 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.01 \text{ e \AA}^{-3}$

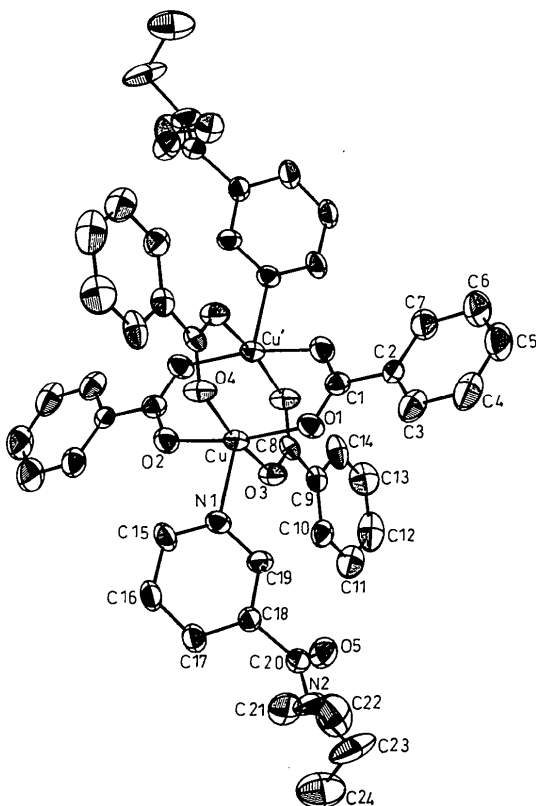


Fig. 1. An ORTEP (Johnson, 1976) drawing of the title molecule with the atom-numbering scheme. The displacement ellipsoids are drawn at the 40% probability level.

S = 0.36

2770 reflections

289 parameters

Modified unit weights

[F < 28.39, w = 1.0;

F ≥ 28.39, w = (28.39/F);

F² ≤ 2σ(F²), w = 0]

Extinction correction: none

Atomic scattering factors

from *International Tables*for *X-ray Crystallography*

(1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)

$$B_{\text{eq}} = (8\pi^2/3) \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j.$$

	x	y	z	B _{eq}
Cu	0.05949 (9)	0.05366 (4)	0.01854 (4)	2.94 (2)
O1	-0.0931 (5)	0.1048 (3)	0.0009 (3)	4.1 (1)
O2	0.1936 (5)	-0.0125 (3)	0.0305 (3)	4.1 (1)
O3	-0.0094 (5)	0.0276 (3)	0.0996 (2)	4.0 (1)
O4	0.1109 (5)	0.0643 (3)	-0.0684 (2)	4.1 (1)
O5	0.0409 (6)	0.2244 (3)	0.2181 (3)	5.4 (2)
N1	0.1656 (6)	0.1358 (3)	0.0575 (3)	3.1 (1)
N2	0.1305 (7)	0.3260 (4)	0.1930 (3)	5.0 (2)
C1	-0.1854 (7)	0.0756 (4)	-0.0219 (4)	3.2 (2)
C2	-0.2942 (8)	0.1176 (4)	-0.0391 (3)	3.3 (2)
C3	-0.2856 (9)	0.1882 (5)	-0.0347 (4)	4.7 (2)
C4	-0.388 (1)	0.2269 (5)	-0.0548 (5)	6.2 (3)
C5	-0.492 (1)	0.1956 (6)	-0.0799 (5)	6.7 (3)
C6	-0.498 (1)	0.1237 (6)	-0.0832 (5)	7.0 (3)
C7	-0.3986 (8)	0.0850 (5)	-0.0626 (4)	4.6 (2)
C8	-0.0795 (7)	-0.0228 (4)	0.1094 (3)	3.1 (2)
C9	-0.1287 (7)	-0.0321 (4)	0.1732 (4)	3.6 (2)
C10	-0.0931 (8)	0.0143 (5)	0.2199 (4)	4.3 (2)
C11	-0.148 (1)	0.0066 (5)	0.2800 (4)	5.6 (2)
C12	-0.2337 (9)	-0.0445 (6)	0.2903 (4)	6.2 (3)
C13	-0.265 (1)	-0.0908 (6)	0.2435 (4)	6.2 (3)
C14	-0.2130 (8)	-0.0847 (5)	0.1841 (4)	4.3 (2)
C15	0.2874 (8)	0.1409 (4)	0.0466 (4)	3.9 (2)
C16	0.3578 (7)	0.1863 (4)	0.0808 (4)	3.9 (2)
C17	0.3051 (7)	0.2273 (4)	0.1262 (4)	3.8 (2)
C18	0.1782 (7)	0.2215 (4)	0.1343 (4)	3.2 (2)
C19	0.1113 (7)	0.1749 (4)	0.1005 (3)	2.9 (2)
C20	0.1104 (8)	0.2582 (4)	0.1848 (4)	4.2 (2)
C21	0.1952 (9)	0.3704 (5)	0.1479 (5)	5.5 (2)
C22	0.117 (1)	0.4307 (5)	0.1277 (5)	6.3 (3)
C23	0.077 (1)	0.3555 (5)	0.2511 (4)	7.5 (3)
C24	0.155 (1)	0.3380 (6)	0.3063 (5)	8.2 (4)

O2—Cu—N1	93.0 (2)	C8—C9—C10	118.6 (7)
O3—Cu—O4	168.9 (2)	C8—C9—C14	118.8 (7)
O3—Cu—N1	93.2 (2)	C10—C9—C14	122.5 (7)
O4—Cu—N1	97.9 (2)	C9—C10—C11	117.4 (8)
Cu—O1—C1	120.6 (5)	C10—C11—C12	120.0 (8)
Cu—O3—C8	125.5 (5)	C11—C12—C13	121.4 (8)
Cu—N1—C15	120.8 (5)	C12—C13—C14	120.0 (9)
Cu—N1—C19	117.7 (5)	C9—C14—C13	118.7 (8)
C15—N1—C19	120.6 (7)	N1—C15—C16	119.7 (7)
C20—N2—C21	124.7 (7)	C15—C16—C17	121.4 (7)
C20—N2—C23	115.2 (7)	C16—C17—C18	116.6 (7)
C21—N2—C23	120.1 (7)	C17—C18—C19	120.6 (7)
O1—C1—C2	118.3 (7)	C17—C18—C20	122.5 (7)
C1—C2—C3	118.9 (7)	C19—C18—C20	116.4 (7)
C1—C2—C7	118.5 (7)	N1—C19—C18	120.1 (7)
C3—C2—C7	122.5 (8)	O5—C20—N2	123.4 (8)
O5—C20—C18	117.4 (8)	N2—C21—C22	112.5 (8)
N2—C20—C18	119.1 (7)	N2—C23—C24	111 (1)
O1—Cu—O3—C8	85.7 (6)	O2—Cu—O3—C8	-83.4 (6)
O3—Cu—O1—C1	-85.4 (6)	O4—Cu—O1—C1	83.5 (6)
O1—Cu—N1—C15	-143.2 (6)	O1—Cu—N1—C19	47.4 (6)
O2—Cu—N1—C15	37.5 (6)	O2—Cu—N1—C19	-131.9 (5)
O3—Cu—N1—C15	127.3 (6)	O3—Cu—N1—C19	-42.2 (5)
O4—Cu—N1—C15	-52.0 (6)	O4—Cu—N1—C19	138.5 (5)
Cu—O1—C1—C2	-175.0 (5)	Cu—O3—C8—C9	-176.4 (5)
C21—N2—C20—O5	-168.7 (9)	C23—N2—C20—C18	-169.4 (8)
C20—N2—C21—C22	123.6 (9)	C20—N2—C23—C24	77.5 (12)

H atoms were geometrically positioned 0.95 Å from the corresponding atoms and a riding model was used in the refinement process. Initially, a unit weighting scheme was used, but in the final stages of refinement modified unit weights were assigned using the method described in *MolEN* (Fair, 1990). This may explain the small S value. The asymmetric unit comprises only half a molecule.

Data collection, cell refinement and data reduction: *MolEN* (Fair, 1990). Structure solution: *SHELXS86* (Sheldrick, 1990). Structure refinement *MolEN*. Molecular graphics: *ORTEPII* (Johnson, 1976). Preparation of material for publication: *MolEN*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and bond angles involving H atoms have been deposited with the IUCr (Reference: AB1221). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

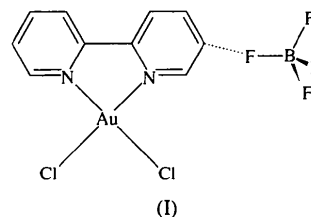
Table 2. Selected geometric parameters (Å, °)

Cu—O1	1.981 (6)	C4—C5	1.40 (2)
Cu—O2	1.976 (6)	C5—C6	1.42 (2)
Cu—O3	1.970 (5)	C6—C7	1.40 (1)
Cu—O4	1.969 (5)	C8—C9	1.49 (1)
Cu—N1	2.162 (6)	C9—C10	1.42 (1)
O1—C1	1.259 (9)	C9—C14	1.41 (1)
O3—C8	1.273 (9)	C10—C11	1.43 (1)
O5—C20	1.24 (1)	C11—C12	1.39 (2)
N1—C15	1.35 (1)	C12—C13	1.40 (1)
N1—C19	1.343 (9)	C13—C14	1.41 (1)
N2—C20	1.37 (1)	C15—C16	1.39 (1)
N2—C21	1.49 (1)	C16—C17	1.39 (1)
N2—C23	1.50 (1)	C17—C18	1.40 (1)
C1—C2	1.49 (1)	C18—C19	1.38 (1)
C2—C3	1.40 (1)	C18—C20	1.50 (1)
C2—C7	1.40 (1)	C21—C22	1.53 (1)
C3—C4	1.42 (1)	C23—C24	1.50 (2)
O1—Cu—O2	169.0 (2)	C2—C3—C4	117.6 (8)
O1—Cu—O3	89.1 (2)	C3—C4—C5	120.9 (9)
O1—Cu—O4	90.1 (2)	C4—C5—C6	120 (1)
O1—Cu—N1	98.0 (2)	C5—C6—C7	119 (1)
O2—Cu—O3	89.6 (2)	C2—C7—C6	119.4 (9)
O2—Cu—O4	89.1 (2)	O3—C8—C9	117.9 (7)

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recrystallized from methanol. A view of the cation in a direction perpendicular to its approximate molecular plane is given in Fig. 1.

Acta Cryst. (1995). C51, 2023–2025

2,2'-Bipyridinedichlorogold(III) Tetrafluoroborate

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(Received 10 February 1995; accepted 11 April 1995)

Abstract

The crystallographically determined structure of the title compound, $[\text{AuCl}_2(\text{C}_{10}\text{H}_8\text{N}_2)]\text{BF}_4$, is reported. The cation is approximately planar and of C_{2v} local symmetry. Both Au—Cl distances are 2.252 (4) Å and the average Au—N distance is 2.037 (13) Å. One pyridine ring of the bipyridyl ligand is hydrogen bonded to the adjacent BF_4^- anion. There is no significant cation–cation stacking in the solid state.

Comment

The compound (bipy)PtCl₂ (bipy = 2,2'-bipyridine) undergoes a facile 1e reduction to afford the anion [(bipy)PtCl₂][−] in which the platinum oxidation state is formally +1. However, recent work (Macgregor, McInnes, Sorbie & Yellowlees, 1993) has conclusively demonstrated that the lowest unoccupied molecular orbital of the neutral species is bipy-based, and that consequently the anion is correctly formulated as [(bipy[−])Pt^{II}Cl₂]. As a prelude to similar electrochemical studies of the isoelectronic species [(bipy)AuCl₂]⁺, we considered it of importance to establish unequivocally the structure of the cation, particularly in view of the recently suggested possibility of solid-state stacking interactions in the perchlorate salt (Yam, Choi, Lai & Lee, 1993).

The title compound, (I), was synthesized in near quantitative yield by an established procedure and

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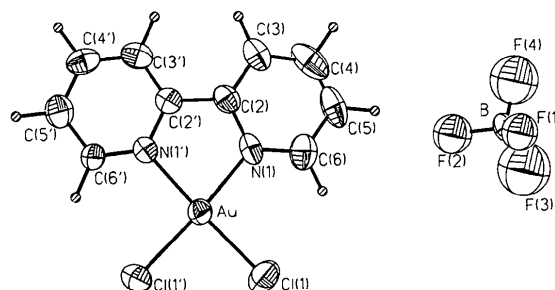


Fig. 1. View of the 2,2'-bipyridinedichlorogold(III) cation and associated tetrafluoroborate anion. 50% probability ellipsoids are shown except for H atoms which are represented by spheres of arbitrary size.

The $[\text{AuN}_2\text{Cl}_2]$ fragment of the cation is approximately planar (maximum atomic deviation from the least-squares plane < 0.05 Å) and the cation as a whole has near C_{2v} local symmetry. While the ring of N(1') is essentially located in this plane [maximum deviation 0.24 Å by C(5')], all the atoms in the N(1) ring lie to one side of the metal coordination plane, with C(3) and C(4) exhibiting the maximum elevation (0.38 Å). It may be of relevance that H(5) is involved in hydrogen bonding to F(2), characterized by C—H···F 2.18 Å, C—H···F 167 and H···F—B 141°.

As far as we are aware, the title compound represents only the second bipyridyl gold(III) species to be crystallographically characterized. The lengths of Au—N(1) and Au—N(1') are not significantly different from each other [average 2.037 (13) Å], but do vary significantly from the average value in [(bipy)Au(mes)₂]⁺ (mes = C₆H₂Me₃-2,4,6) [2.125 (6) Å; Yam, Choi, Lai & Lee, 1993]. This presumably arises from the differing *trans* influences of Cl and mes. The Au—Cl distances in [(bipy)AuCl₂]⁺ are identical [2.252 (4) Å] and the C(2)—C(2') bridge distance is 1.457 (15) Å.

In the crystal, the shortest intermolecular distance between Au atoms is 6.850 Å, *i.e.* the unit-cell repeat in the *a* direction. Clearly this distance does not represent a significant interaction [*cf.* 3.45 and 4.43 Å in the red and yellow forms, respectively, of (bipy)PtCl₂ (Osborn & Rogers, 1974; Herber, Croft, Coyer, Bilash & Sahiner, 1994)]. It is highly probable that [(bipy)AuCl₂]⁺ClO₄[−] and