perchlorate ions and the amine groups. The deposited material (Table $S5$) shows four O···N contacts in the range 2·9–3·1 Å for the second perchlorate ion, which are shorter than any of the O···C contacts. The shortest interionic hydrogen bond, N(1) to F(1) at x, $0\cdot5-y$, $z-0\cdot5$, has a length of 2·768 (9) Å, involves H(13) [F···H = 1·90 (8) Å, angle F···H—N = 163 (7)°], and is between c-glide-plane-related cations. The hydrogen bonds of this kind therefore run continuously through the crystal structure.

References

CLAMP, S., CONNELLY, N. G., TAYLOR, G. E. & LOUTTIT, T. S. (1980). *J. Chem. Soc. Dalton Trans.* pp. 2162–2169.

COREY, E. J. & BAILAR, J. C. JR (1959). *J. Am. Chem. Soc.* **81**, 2620–2629.
CROMER, D. T. & WABER, J. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV, pp. 99 and 149. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)
EVANS, R. C. (1966). *An Introduction to Crystal Chemistry*, 2nd ed., pp. 70–74. Cambridge Univ. Press.
HOUSE, D. A. (1977). *Coord. Chem. Rev.* **23**, 223–322.
JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3794, revised. Oak Ridge National Laboratory, Tennessee.
KIRK, A. D. (1981). *Coord. Chem. Rev.* **39**, 225–263.
KIRK, A. D. & KELLY, T. L. (1974). *Inorg. Chem.* **13**, 1613–1616.
PURCELL, K. F. & KOTZ, J. C. (1977). *Inorganic Chemistry*, p. 637. Philadelphia: W. B. Saunders.
SHELDRICK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.
SLATER, J. C. (1964). *J. Chem. Phys.* **41**, 3199–3204.
VANQUICKENBORNE, L. G. & CEULEMANS, A. (1983). *Coord. Chem. Rev.* **48**, 157–202.
VAUGHN, J. W. (1981). *Inorg. Chem.* **20**, 2397–2402.
WONG, C. F. C. & KIRK, A. D. (1975). *Can. J. Chem.* **53**, 3388–3393.

Structure of Bis(pyridine)(5,10,15,20-tetraphenylporphyrinato)iron(II)–Pyridine Solvate, [Fe(C₄₄H₂₈N₄)(C₅H₅N)₂].2C₅H₅N

BY NAIYIN LI, VACLAV PETŘÍČEK* AND PHILIP COPPENS†

Department of Chemistry, State University of New York at Buffalo, Buffalo, NY 14214, USA

AND JOHN LANDRUM

Department of Chemistry, Florida International University, Miami, FL 33199, USA

Abstract. $M_r = 985\cdot0$, triclinic, $P\bar{1}$, $a = 9\cdot472$ (5), $b = 10\cdot325$ (2), $c = 13\cdot545$ (8) Å, $\alpha = 80\cdot25$ (3), $\beta = 77\cdot79$ (4), $\gamma = 77\cdot79$ (3)°, $V = 1254\cdot5$ Å³, $Z = 1$, $D_x = 1\cdot304$ g cm⁻³, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 3\cdot65$ cm⁻¹, $F(000) = 514$, $T = 298$ K, $R = 0\cdot034$ for 3577 observed reflections. The structure consists of Fe(tetraphenylporphyrin)(py)₂ and two pyridine molecules of solvation. The average Fe—N(pyrrole) distance is 1·993 Å, while the axial Fe—N(pyridine) distance is 2·039 (1) Å. Because of the center of symmetry the Fe atom is located exactly in the plane of the porphinato ring, but is displaced by 0·064 Å from each of the pyridine planes.

---

* Permanent address: Department of Structures and Bonding, Institute of Physics, Czechoslovakian Academy of Sciences, Na Slovance 2, 180 40 Praha 8, Czechoslovakia.
† Author to whom correspondence should be addressed.

Introduction. The relevance of porphyrin stereochemistry in biology is well documented (see, for example, Lever & Gray, 1983). The study of the title compound was undertaken as part of a program to map the electron density in iron porphyrins as a function of oxidation state, coordination number and spin state (Lecomte, Chadwick, Coppens & Stevens, 1983; Coppens & Li, 1984).

Experimental. Feᴵᴵ tetraphenylporphyrin [Fe(tpp)] was prepared from Feᴵᴵᴵ tetraphenylporphyrin chloride by reduction with chromous acetylacetonate in a benzene–ethanol mixture (Collman, Hoard, Kim, Lang & Reed, 1975). The crystals were subsequently recrystallized from a benzene–heptane mixture. The bis(pyridine) complex was prepared by dissolving 100 mg of Fe(tpp) in boiling dry pyridine. The reaction mixture was rapidly filtered through a medium-porosity sintered

glass frit and set aside to crystallize. Suitable crystals were obtained after 24–48 h. All manipulations were performed under exclusion of oxygen in a Vacuum Atmospheres glove box.

The purple crystals of the title compound are not stable in air. All diffraction work was therefore carried out with a crystal mounted in a sealed capillary tube with a small amount of the parent solution. CAD-4 diffractometer, graphite-monochromatized Mo $K\alpha$ radiation. Crystal dimensions $0.32 \times 0.45 \times 0.53$ mm. Cell parameters by least-squares fit of 25 2θ values ($16 < 2\theta < 32°$). All hkl and $h\bar{k}l$ reflections with $2\theta < 50°$ measured. θ–2θ scan technique, variable scan rate 0.6 to 4.0° min^{-1}, background correction made with a local modification of the Lehmann–Larsen formalism (Blessing, Coppens & Becker, 1972). Three standard reflections measured at intervals of 30 reflections showed no systematic decrease ($< 1\%$) of scattering power during data collection. No absorption correction made ($\mu R_{max} = 0.17$). Equivalent reflections merged into a set of 3722 independent reflections, $h\ 0 \to 12$, $k\ \bar{13} \to 13$, $l\ \bar{17} \to 17$. Of these, 3577 with $F_o > 3\sigma(F_o)$ used in structure analysis. Positions of Fe, N and most of the C atoms deduced from a Patterson synthesis; remaining non-H atoms located in a subsequent Fourier synthesis. Difference Fourier synthesis clearly indicated positions of all H atoms of the tetraphenylporphyrin ring. Positions of pyridine H atoms calculated and then refined. Refinement by least squares, $\sum w(F_o - k|F_c|)^2$ minimized, $w = 1/\sigma^2(F) = 4F^2/\sigma^2(F^2)$; $\sigma^2(F^2) = (0.02\ F^2)^2 + \sigma^2_{counting}(F^2)$. Scattering factors for (neutral) Fe, N, C, H and dispersion correction for Fe, N, and C from *International Tables for X-ray Crystallography* (1974). All calculations performed with Enraf–Nonius *SDP* (Frenz, 1982). Non-H atoms refined with anisotropic thermal parameters. H atoms on non-ligated pyridine molecules not refined. Each ring atom of the solvent pyridine is considered as consisting of $\frac{1}{6}$ N and $\frac{5}{6}$ C; in addition, half the solvent molecules are rotated by 30° around the plane normal, thus giving 12 half C/N atoms for each ring. They were treated with isotropic temperature parameters. No extinction parameter refined. Final R and wR 0.034 and 0.041 respectively. Goodness of fit 1.92. Final max. Δ/σ for atomic parameters 0.35. Peaks on final $\Delta\rho$ map < 0.35 e Å^{-3}.

Discussion. The atomic coordinates and isotropic thermal parameters are listed in Table 1.* Bond lengths and angles are given in Table 2. A diagram of the

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, distances and angles in the solvent pyridine molecules, and the results of the mean-plane calculations have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42096 (39 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Non-H-atom positional parameters, isotropic thermal parameters and their e.s.d.'s*

	x	y	z	B_{eq}*/B(Å²)
Fe	0.0000	0.0000	0.0000	2.254 (7)
N(1)	−0.0267 (2)	0.0417 (1)	0.1416 (1)	2.55 (3)
N(2)	0.1109 (2)	−0.1814 (1)	0.0413 (1)	2.42 (3)
N(3)	0.1926 (2)	0.0703 (2)	−0.0355 (1)	2.82 (3)
C(7)	0.1501 (2)	−0.2325 (2)	0.1350 (1)	2.55 (4)
C(8)	0.1710 (2)	−0.2813 (2)	−0.0199 (1)	2.72 (4)
C(9)	0.0222 (2)	−0.0400 (2)	0.2239 (1)	2.83 (4)
C(10)	−0.1004 (2)	0.1596 (2)	0.1793 (1)	2.90 (4)
C(5)	0.1094 (2)	−0.1672 (2)	0.2212 (1)	2.72 (4)
C(6)	−0.1634 (2)	0.2735 (2)	0.1221 (1)	2.80 (4)
C(3)	−0.0282 (3)	0.0256 (2)	0.3141 (2)	3.72 (5)
C(4)	−0.1022 (3)	0.1473 (2)	0.2865 (2)	3.75 (5)
C(1)	0.2391 (2)	−0.3636 (2)	0.1303 (2)	3.23 (4)
C(2)	0.2499 (2)	−0.3940 (2)	0.0364 (2)	3.43 (5)
C(11)	0.1667 (2)	−0.2341 (2)	0.3157 (1)	3.10 (4)
C(12)	0.2557 (3)	−0.1744 (2)	0.3560 (2)	3.96 (5)
C(13)	0.3099 (3)	−0.2341 (3)	0.4434 (2)	5.18 (6)
C(14)	0.2767 (3)	−0.3545 (3)	0.4913 (2)	5.64 (7)
C(15)	0.1898 (3)	−0.4160 (3)	0.4530 (2)	5.32 (7)
C(16)	0.1340 (3)	−0.3560 (2)	0.3658 (2)	4.13 (5)
C(17)	−0.2224 (2)	0.3974 (2)	0.1736 (1)	2.88 (4)
C(18)	−0.1304 (3)	0.4845 (2)	0.1743 (2)	4.21 (5)
C(19)	−0.1824 (3)	0.5974 (2)	0.2243 (2)	5.23 (6)
C(20)	−0.3238 (3)	0.6227 (2)	0.2734 (2)	4.88 (6)
C(21)	−0.4166 (3)	0.5385 (3)	0.2721 (2)	4.81 (6)
C(22)	−0.3661 (3)	0.4260 (2)	0.2219 (2)	4.00 (5)
C(23)	0.2130 (2)	0.1722 (2)	0.0068 (2)	3.79 (5)
C(24)	0.3430 (3)	0.2185 (2)	−0.0129 (2)	4.95 (6)
C(25)	0.4599 (3)	0.1611 (3)	−0.0796 (2)	5.03 (6)
C(26)	0.4414 (3)	0.0580 (3)	−0.1239 (2)	4.90 (6)
C(27)	0.3089 (2)	0.0154 (2)	−0.1001 (2)	3.78 (5)
X(1)†	0.3502 (8)	0.2259 (7)	0.2831 (6)	8.8 (2)‡
X(2)	0.4327 (8)	0.1553 (7)	0.3344 (6)	8.7 (2)‡
X(3)	0.4050 (9)	0.1193 (8)	0.4355 (6)	9.6 (2)‡
X(4)	0.2730 (9)	0.1517 (8)	0.4802 (6)	9.4 (2)‡
X(5)	0.1622 (6)	0.2192 (6)	0.4290 (4)	5.9 (1)‡
X(6)	0.2125 (9)	0.2464 (8)	0.3275 (6)	9.6 (2)‡
X(7)	0.1560 (7)	0.2725 (6)	0.3775 (5)	7.1 (1)‡
X(8)	0.2100 (7)	0.2091 (7)	0.4741 (5)	7.5 (2)‡
X(9)	0.3584 (9)	0.1532 (8)	0.4675 (6)	9.5 (2)‡
X(10)	0.4412 (8)	0.1377 (8)	0.3717 (6)	9.1 (2)‡
X(11)	0.3853 (6)	0.1880 (6)	0.2809 (5)	6.4 (1)‡
X(12)	0.2482 (8)	0.2634 (7)	0.2843 (5)	8.0 (2)‡

* Equivalent isotropic thermal parameter defined as: $\frac{4}{3} \sum_i \sum_j \beta_{ij} \mathbf{a}_i . \mathbf{a}_j$.
† $X(n)$: solvent atom.
‡ Isotropically refined atom.

molecule indicating the atomic-numbering scheme and a packing diagram are shown in Figs. 1 and 2.

N—C and C—C distances and angles in the ring are in excellent agreement with the values in the similar compound Fe(tpp) bis(piperidine) (Radonovich, Bloom & Hoard, 1976). The equatorial Fe—N bond lengths are also identical in the two complexes, the values being 1.993 (4) Å in the present study, and 2.004 (4) Å in the bis(piperidine) complex. But the axial Fe—N distances are very different, with values of 2.039 (1) and 2.127 (3) Å in the two complexes respectively. Radonovich *et al.* (1976) have explained the unusually long axial distance found in their study as being mainly due to steric interactions between the piperidine H atoms and the N atoms. At comparable values of the axial bond length such interactions are much weaker in the pyridine compound, which does not have an H atom attached to N or α-H atoms close to the pyrrole N atoms. In addition, conjugation between the pyridine π-electrons and the Fe d-orbitals will contribute to the shorter axial distance found here and in the Fe^{II}

Table 2. *Bond lengths (Å) and angles (°) in*
Fe(tpp)(py)₂

Numbers in parentheses are e.s.d.'s in the least-significant digits.

Fe—N(1)	1·989 (1)	C(3)—C(4)	1·338 (2)
Fe—N(2)	1·997 (1)	C(1)—C(2)	1·339 (2)
Fe—N(3)	2·039 (1)	C(11)—C(12)	1·384 (2)
N(1)—C(9)	1·379 (2)	C(11)—C(16)	1·388 (2)
N(1)—C(10)	1·390 (2)	C(12)—C(13)	1·386 (2)
N(2)—C(7)	1·384 (2)	C(13)—C(14)	1·368 (3)
N(2)—C(8)	1·385 (2)	C(14)—C(15)	1·365 (3)
N(3)—C(23)	1·345 (2)	C(15)—C(16)	1·391 (2)
N(3)—C(27)	1·341 (2)	C(17)—C(18)	1·382 (2)
C(7)—C(5)	1·391 (2)	C(17)—C(22)	1·373 (2)
C(7)—C(1)	1·439 (2)	C(18)—C(19)	1·393 (2)
C(8)—C(2)	1·438 (2)	C(19)—C(20)	1·356 (3)
C(9)—C(5)	1·397 (2)	C(20)—C(21)	1·365 (3)
C(9)—C(3)	1·441 (2)	C(21)—C(22)	1·391 (2)
C(10')—C(6)	1·389 (2)	C(23)—C(24)	1·372 (2)
C(10)—C(4)	1·432 (2)	C(24)—C(25)	1·369 (3)
C(5)—C(11)	1·499 (2)	C(25)—C(26)	1·366 (3)
C(6)—C(17)	1·507 (2)	C(26)—C(27)	1·374 (2)
N(1)—Fe—N(2)	89·63 (4)	C(9)—C(3)—C(4)	107·3 (1)
N(1)—Fe—N(3)	89·67 (5)	C(10)—C(4)—C(3)	107·5 (1)
N(2)—Fe—N(3)	89·22 (4)	C(7)—C(1)—C(2)	107·3 (1)
Fe—N(1)—C(9)	127·77 (9)	C(8)—C(2)—C(1)	107·5 (1)
Fe—N(1)—C(10)	127·27 (9)	C(5)—C(11)—C(12)	120·0 (1)
C(9)—N(1)—C(10)	105·0 (1)	C(5)—C(11)—C(16)	122·3 (1)
Fe—N(2)—C(7)	127·87 (9)	C(12)—C(11)—C(16)	117·6 (2)
Fe—N(2)—C(8)	126·90 (9)	C(11)—C(12)—C(13)	121·2 (2)
C(7)—N(2)—C(8)	105·2 (1)	C(12)—C(13)—C(14)	120·2 (2)
Fe—N(3)—C(23)	122·2 (1)	C(13)—C(14)—C(15)	120·0 (2)
Fe—N(3)—C(27)	122·2 (1)	C(14)—C(15)—C(16)	120·1 (2)
C(23)—N(3)—C(27)	115·5 (1)	C(11)—C(16)—C(15)	120·9 (2)
N(2)—C(7)—C(5)	125·2 (1)	C(6)—C(17)—C(18)	119·8 (1)
N(2)—C(7)—C(1)	110·0 (1)	C(6)—C(17)—C(22)	121·8 (1)
C(5)—C(7)—C(1)	124·8 (1)	C(18)—C(17)—C(22)	118·3 (2)
N(2)—C(8)—C(2)	110·0 (1)	C(17)—C(18)—C(19)	120·5 (2)
N(1)—C(9)—C(5)	125·6 (1)	C(18)—C(19)—C(20)	120·5 (2)
N(1)—C(9)—C(3)	110·1 (1)	C(19)—C(20)—C(21)	119·7 (2)
C(5)—C(9)—C(3)	124·3 (1)	C(20)—C(21)—C(22)	120·3 (2)
N(1)—C(10)—C(6')	125·4 (1)	C(17)—C(22)—C(21)	120·7 (2)
N(1)—C(10)—C(4)	110·1 (1)	N(3)—C(23)—C(24)	123·5 (2)
C(6)—C(10)—C(4)	124·5 (1)	C(23)—C(24)—C(25)	119·9 (2)
C(7)—C(5)—C(9)	123·7 (1)	C(24)—C(25)—C(26)	117·7 (2)
C(7)—C(5)—C(11)	118·5 (1)	C(25)—C(26)—C(27)	119·6 (2)
C(9)—C(5)—C(11)	117·8 (1)	N(3)—C(27)—C(26)	123·8 (2)
C(10')—C(6)—C(17)	117·7 (1)		

The pyridine ligand is planar within experimental error but the Fe atom is displaced by 0·064 Å from each of the pyridine planes.

The dihedral angles between the plane of the porphyrinato core and the planes of the two independent phenyl groups are 58·8 and 87·2° respectively.

From the packing diagram, Fig. 2, it is clear that voids exist between Fe(tpp)(py)₂ molecules in which two additional pyridine molecules fit. Since the pyridine molecules of solvation are distorted no charge-density analysis of these crystals is planned. However, non-solvated crystals of the title compound have been obtained and are presently being studied.
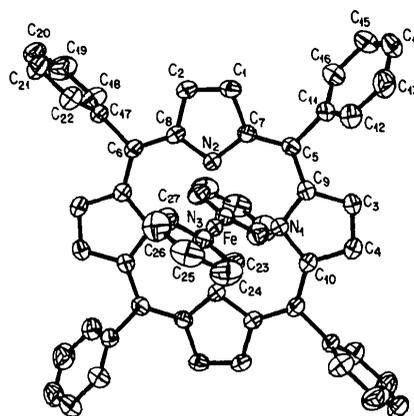
Fig. 1. *ORTEP* (Johnson, 1971) drawing of the molecule. Ellipsoids are 50% probability surfaces.

bis(1-methylimidazole) complex [2·014 (5) Å (Scheidt & Gouterman, 1983)].

The φ angle defined as the angle between the plane of the axial ligand and the closest Fe—N(pyrrole) bond is 34·4°, compared with 45° in Fe(tpp)(py)(CO) (Peng & Ibers, 1976). In the latter compound the axial bond length is 2·10 (1) Å, suggesting weaker π-bonding because of competition from the *trans* CO ligand. This also explains the larger value of the φ angle in the latter complex, notwithstanding the reduction of steric hindrance due to the increased axial bond length to the pyridine N atom.

The largest deviation from planarity of the porphyrinato ring is 0·097 (2) Å for C(6). Other large displacements are found for C(1) = 0·081 (2), C(3) = −0·079 (3), C(4) = −0·053 (3), C(5) = 0·045 (2), and C(8) = −0·067 (2) Å. The displacements are irregular and not obviously related to the molecular symmetry. Because of the center of symmetry the Fe atom is located exactly in the plane of the porphyrinato ring.
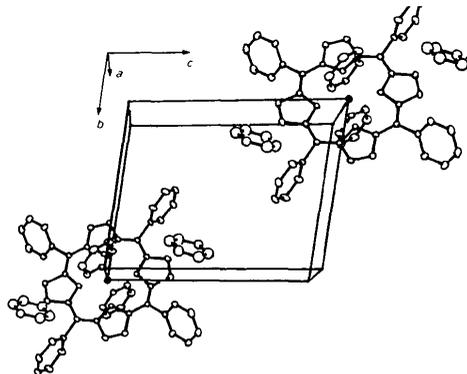

Fig. 2. Packing diagram. Note that additional molecules are located at the other six corners of the unit cell.

References

BLESSING, R. H., COPPENS, P. & BECKER, P. (1972). *J. Appl. Cryst.* 7, 488–492.

COLLMAN, J. P., HOARD, J. L., KIM, N., LANG, G. & REED, C. A. (1975). *J. Am. Chem. Soc.* 97, 2676–2681.

COPPENS, P. & LI, L. (1984). *J. Chem. Phys.* 81, 1983–1993.

FRENZ, B. A. (1982). *Structure Determination Package.* Enraf-Nonius, Delft.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

JOHNSON, C. K. (1971). *ORTEPII.* Report ORNL-3794. Oak Ridge National Laboratory, Tennessee.

LECOMTE, C., CHADWICK, D. L., COPPENS, P. & STEVENS, E. D. (1983). *Inorg. Chem.* 22, 2982–2992.

LEVER, A. B. P. & GRAY, H. B. (1983). Editors, *Iron Porphyrins,* Vols. I and II. Reading, MA: Addison–Wesley Publishing Co.

PENG, S. M. & IBERS, J. A. (1976). *J. Am. Chem. Soc.* 98, 8032–8036.

RADONOVICH, L. J., BLOOM, A. & HOARD, J. L. (1976). *J. Am. Chem. Soc.* 94, 2073–2078.

SCHEIDT, W. R. & GOUTERMAN, M. (1983). In *Iron Porphyrins,* edited by A. B. P. LEVER & H. B. GRAY, Vol. II. Reading, MA: Addison–Wesley Publishing Co.

Benzoato(triphenylphosphine)gold(I) Benzene Solvate,* [Au(C₇H₅O₂){P(C₆H₅)₃}].C₆H₆

BY PETER G. JONES

Institut für Anorganische Chemie der Universität Göttingen, Tammannstrasse 4, D-3400 Göttingen, Federal Republic of Germany

Abstract. $M_r = 658.49$, monoclinic, $P2_1/n$, $a = 10.825$ (2), $b = 13.896$ (3), $c = 17.411$ (4) Å, $\beta = 94.43$ (2)°, $V = 2611$ (2) Å³, $Z = 4$, $D_x = 1.675$ (2) g cm⁻³, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 57$ cm⁻¹, $F(000) = 1288$, $T = 293$ K, $R = 0.042$ for 3433 observed reflections. The linear coordination at gold is slightly distorted [P—Au—O 173.7 (2)°]. The pattern of bond lengths, compared with the analogous acetate, can be explained by postulating better π-acceptor properties for benzoate. The benzene of solvation is well ordered and occupies holes in the lattice without participation in stacking interactions.

Introduction. As part of our study of gold carboxylate complexes, the title compound was synthesized [from Ph₃PAuCl and silver(I) benzoate] and recrystallized from benzene as colourless prisms. Elemental analysis suggested the presence of benzene of crystallization. The crystals slowly disintegrate when exposed to air, presumably by loss of benzene, and so were sealed in glass capillaries for structure determination.

Experimental. Crystal $0.5 \times 0.25 \times 0.05$ mm, elongated along **b**, 5833 profile-fitted intensities (Clegg, 1981) measured on a Stoe–Siemens four-circle diffractometer; monochromated Mo $K\alpha$ radiation, $2\theta_{max}$ 50°, quadrant $-h + k \pm l$ ($|h| \le 12$, $|k| \le 16$, $|l| \le 20$) and some $+h$ equivalents; three check reflections, no intensity change; empirical absorption correction (ψ scans, transmissions 0.60–0.97); averaging equivalents gave 4587 unique reflections (R_{int} 0.021), 3433 with $F > 4\sigma(F)$ used for all calculations; cell constants refined from 2θ values of 36 reflections in range 20–23°; structure solution by heavy-atom method; refinement on $|F|$ to R 0.042, wR 0.037 [non-H atoms anisotropic, H atoms included using riding model with C—H 0.96 Å, $U(\text{H}) = 1.2U_{eq}(\text{C})$; 317 parameters, $w^{-1} = \sigma^2(F) + 0.00015F^2$, $S = 1.23$, slope of normal probability plot = 1.1], max. $\Delta/\sigma < 0.01$, max. and min. heights in final $\Delta\rho$ map +0.6, −0.8 e Å⁻³. Calculations with program system *SHELXTL* (Sheldrick, 1978). Atomic scattering factors those of Sheldrick (1981).

Discussion. Final atomic coordinates and derived parameters are given in Tables 1 and 2.† The gold atom shows the expected linear coordination (Fig. 1), albeit slightly distorted, with P—Au—O(1) 173.7 (2)°; the Au···O(2) contact of 3.037 (8) Å is too long to be regarded as an appreciable bonding interaction. Compared with the corresponding acetate (Jones, 1984), the following marginally significant changes are noted in the bond lengths of the PAuOCO group: Au—O(1) is shorter [2.033 (6) Å in the benzoate, 2.063 (6) Å in the

---

* Carboxylate and Related Complexes of Gold. 3. Part 2: Jones (1984).

† Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and bond angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42122 (31 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.