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Crystal structure of $(\mu_2\text{-}1,1'\text{-bis(diphenylphosphino)butane-}\kappa^2P,P')\text{-bis}[(Z)\text{-}N\text{-(3-fluorophenyl)-}O\text{-methylthiocarbamato-}\kappa S]\text{-di-gold(I)}$, $\text{C}_{44}\text{H}_{42}\text{Au}_2\text{F}_2\text{N}_2\text{O}_2\text{P}_2\text{S}_2$

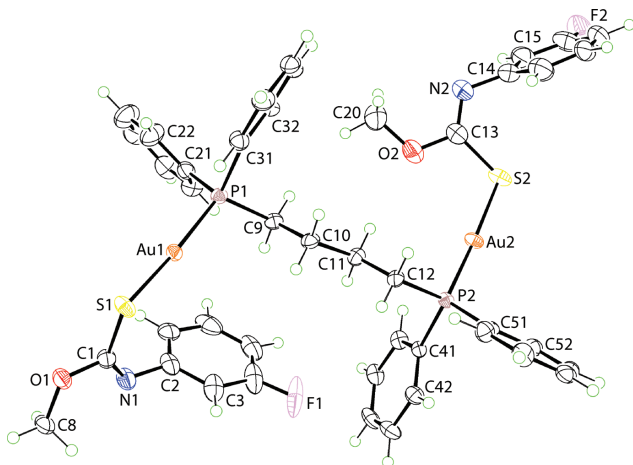


Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.23 × 0.19 × 0.18 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	7.19 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
θ_{\max} , completeness:	27.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	48879, 9642, 0.047
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 8323
$N(\text{param})_{\text{refined}}$:	527
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3], WinGX/ORTEP [4]

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Abstract

$\text{C}_{44}\text{H}_{42}\text{Au}_2\text{F}_2\text{N}_2\text{O}_2\text{P}_2\text{S}_2$, triclinic, $P\bar{1}$ (no. 2), $a = 8.8035(2)$ Å, $b = 11.4764(3)$ Å, $c = 21.2293(6)$ Å, $\alpha = 83.550(2)^\circ$, $\beta = 82.256(2)^\circ$, $\gamma = 83.793(2)^\circ$, $V = 2102.40(10)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0268$, $wR_{\text{ref}}(F^2) = 0.0577$, $T = 100(2)$ K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

NaOH (Merck; 0.020 g, 0.50 mmol) in water (5 mL) was added to a suspension of $(\text{Ph}_2\text{P}(\text{CH}_2)_4\text{PPh}_2)(\text{AuCl})_2$ (0.229 g, 0.25 mmol) in acetonitrile (20 mL), followed by the addition

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Au1	−0.39937(2)	0.87120(2)	0.26697(2)	0.02080(4)
Au2	0.28914(2)	0.25478(2)	0.27939(2)	0.02289(5)
S1	−0.57306(11)	0.96289(8)	0.34050(5)	0.0283(2)
S2	0.46758(12)	0.21256(9)	0.19285(6)	0.0334(2)
P1	−0.21561(11)	0.79847(8)	0.19320(5)	0.0209(2)
P2	0.12237(10)	0.31295(8)	0.36244(5)	0.01881(19)
O1	−0.8576(3)	0.9704(2)	0.37917(15)	0.0321(7)
O2	0.3025(4)	0.3984(3)	0.14240(17)	0.0478(8)
N1	−0.7699(4)	0.7857(3)	0.35487(19)	0.0346(9)
N2	0.5533(4)	0.3841(4)	0.0983(2)	0.0491(11)
C1 ^a	−0.7419(4)	0.8905(3)	0.3573(2)	0.0264(9)
C2 ^a	−0.6616(4)	0.6938(3)	0.3358(2)	0.0327(10)
C3 ^a	−0.5940(5)	0.6168(4)	0.3818(3)	0.0387(11)
H3 ^a	−0.607752	0.633393	0.425131	0.046*
C4 ^a	−0.5058(5)	0.5149(4)	0.3635(3)	0.0481(14)
F1 ^a	−0.4336(5)	0.4474(3)	0.4035(3)	0.068(2)
C5 ^a	−0.4823(5)	0.4867(4)	0.3022(3)	0.0460(13)
H5 ^a	−0.422520	0.416410	0.290909	0.055*
C6 ^a	−0.5494(5)	0.5652(4)	0.2565(3)	0.0487(13)
H6 ^a	−0.534109	0.548036	0.213178	0.058*
C7 ^a	−0.6375(5)	0.6670(4)	0.2724(2)	0.0363(10)
H7 ^a	−0.681742	0.718838	0.240205	0.044*
C2 ^b	−0.6616(4)	0.6938(3)	0.3358(2)	0.0327(10)
C3 ^b	−0.5940(5)	0.6168(4)	0.3818(3)	0.0387(11)
H3 ^b	−0.607752	0.633393	0.425131	0.046*
C4 ^b	−0.5058(5)	0.5149(4)	0.3635(3)	0.0481(14)
H4 ^b	−0.460216	0.462952	0.395261	0.058*
C5 ^b	−0.4823(5)	0.4867(4)	0.3022(3)	0.0460(13)

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Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H5 ^{rb}	−0.422520	0.416410	0.290909	0.055*
C6 ^{rb}	−0.5494(5)	0.5652(4)	0.2565(3)	0.0487(13)
F1 ^{rb}	−0.5165(10)	0.5453(7)	0.2012(4)	0.056(3)
C7 ^{rb}	−0.6375(5)	0.6670(4)	0.2724(2)	0.0363(10)
H7 ^{rb}	−0.681742	0.718838	0.240205	0.044*
C8	−1.0013(4)	0.9244(4)	0.4022(2)	0.0354(10)
H8A	−1.041706	0.893907	0.367171	0.053*
H8B	−1.074720	0.987159	0.419189	0.053*
H8C	−0.986166	0.860606	0.436224	0.053*
C9	−0.1512(4)	0.6440(3)	0.21371(18)	0.0229(8)
H9A	−0.240458	0.596795	0.218276	0.027*
H9B	−0.075813	0.615885	0.178440	0.027*
C10	−0.0776(4)	0.6246(3)	0.27535(19)	0.0241(8)
H10A	−0.155371	0.644906	0.311628	0.029*
H10B	0.006221	0.676657	0.272561	0.029*
C11	−0.0124(4)	0.4957(3)	0.28690(19)	0.0241(8)
H11A	−0.096182	0.444216	0.288067	0.029*
H11B	0.066476	0.476595	0.250748	0.029*
C12	0.0596(4)	0.4696(3)	0.34888(19)	0.0216(8)
H12A	−0.016647	0.493167	0.385003	0.026*
H12B	0.148873	0.516077	0.346698	0.026*
C13	0.4492(5)	0.3433(4)	0.1391(2)	0.0384(11)
C14 ^c	0.7054(5)	0.3287(4)	0.0980(2)	0.0431(12)
C15 ^c	0.7667(6)	0.2521(5)	0.0513(3)	0.0499(13)
H15 ^c	0.706326	0.237561	0.019632	0.060*
C16 ^c	0.9134(6)	0.1991(5)	0.0517(3)	0.0551(14)
F2 ^c	0.9678(5)	0.1232(5)	0.0121(2)	0.070(2)
C17 ^c	1.0078(6)	0.2237(5)	0.0948(3)	0.0596(16)
H17 ^c	1.110481	0.187958	0.093936	0.071*
C18 ^c	0.9474(6)	0.3032(5)	0.1401(3)	0.0470(13)
H18 ^c	1.010767	0.323052	0.169400	0.056*
C19 ^c	0.8004(6)	0.3512(5)	0.1420(3)	0.0538(14)
H19 ^c	0.760397	0.401583	0.174057	0.065*
C14 rd	0.7054(5)	0.3287(4)	0.0980(2)	0.0431(12)
C15 rd	0.7667(6)	0.2521(5)	0.0513(3)	0.0499(13)
H15 rd	0.706326	0.237561	0.019632	0.060*
C16 rd	0.9134(6)	0.1991(5)	0.0517(3)	0.0551(14)
H16 rd	0.951506	0.143997	0.021815	0.066*
C17 rd	1.0078(6)	0.2237(5)	0.0948(3)	0.0596(16)
H17 rd	1.110481	0.187958	0.093936	0.071*
C18 rd	0.9474(6)	0.3032(5)	0.1401(3)	0.0470(13)
F2 rd	1.0205(14)	0.2983(12)	0.1759(7)	0.100(5)
C19 rd	0.8004(6)	0.3512(5)	0.1420(3)	0.0538(14)
H19 rd	0.760397	0.401583	0.174057	0.065*
C20	0.2788(6)	0.5043(5)	0.0984(3)	0.0599(15)
H20A	0.330106	0.567881	0.111197	0.090*
H20B	0.168278	0.528198	0.099437	0.090*
H20C	0.322165	0.487682	0.054952	0.090*
C21	−0.2791(4)	0.8053(3)	0.11528(19)	0.0267(9)
C22	−0.2848(6)	0.9129(4)	0.0781(2)	0.0435(12)
H22	−0.253435	0.979908	0.093520	0.052*
C23	−0.3357(6)	0.9231(5)	0.0189(3)	0.0554(14)
H23	−0.338604	0.996806	−0.006366	0.067*
C24	−0.3832(5)	0.8247(5)	−0.0039(2)	0.0479(13)
H24	−0.416785	0.831225	−0.045001	0.057*
C25	−0.3810(5)	0.7199(4)	0.0331(2)	0.0413(11)

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H25	−0.415347	0.653486	0.018184	0.050*
C26	−0.3290(5)	0.7095(4)	0.0923(2)	0.0349(10)
H26	−0.327545	0.635734	0.117602	0.042*
C31	−0.0366(4)	0.8671(3)	0.18075(18)	0.0218(8)
C32	0.0816(4)	0.8290(3)	0.13536(19)	0.0264(8)
H32	0.064416	0.773093	0.107922	0.032*
C33	0.2250(5)	0.8722(3)	0.1298(2)	0.0296(9)
H33	0.305902	0.844600	0.099251	0.036*
C34	0.2500(5)	0.9552(3)	0.1688(2)	0.0310(9)
H34	0.347585	0.985276	0.164559	0.037*
C35	0.1338(5)	0.9941(4)	0.2134(2)	0.0332(10)
H35	0.151535	1.051018	0.240163	0.040*
C36	−0.0105(5)	0.9507(3)	0.2200(2)	0.0273(9)
H36	−0.090513	0.977963	0.251093	0.033*
C41	−0.0590(4)	0.2464(3)	0.37704(18)	0.0190(7)
C42	−0.1464(4)	0.2436(3)	0.4371(2)	0.0269(9)
H42	−0.107292	0.270327	0.471949	0.032*
C43	−0.2909(4)	0.2016(3)	0.4458(2)	0.0323(10)
H43	−0.349955	0.198022	0.486736	0.039*
C44	−0.3483(4)	0.1650(3)	0.3944(2)	0.0331(10)
H44	−0.447712	0.137573	0.400353	0.040*
C45	−0.2639(4)	0.1678(3)	0.3351(2)	0.0290(9)
H45	−0.305253	0.142948	0.300316	0.035*
C46	−0.1170(4)	0.2072(3)	0.3261(2)	0.0255(8)
H46	−0.056950	0.207156	0.285380	0.031*
C51	0.1976(4)	0.2931(3)	0.43882(18)	0.0193(7)
C52	0.2563(4)	0.1807(3)	0.46122(19)	0.0252(8)
H52	0.255685	0.116604	0.436564	0.030*
C53	0.3153(4)	0.1616(4)	0.5189(2)	0.0302(9)
H53	0.354455	0.084541	0.533967	0.036*
C54	0.3174(4)	0.2546(4)	0.5549(2)	0.0329(10)
H54	0.358256	0.241235	0.594549	0.039*
C55	0.2608(5)	0.3660(4)	0.5335(2)	0.0342(10)
H55	0.263130	0.429557	0.558258	0.041*
C56	0.2001(5)	0.3861(4)	0.4756(2)	0.0290(9)
H56	0.160341	0.463274	0.461132	0.035*

^aOccupancy: 0.639(8), ^bOccupancy: 0.361(8), ^cOccupancy: 0.665(9), ^dOccupancy: 0.335(9).

of MeOC(=S)N(H)C₆H₄F-3 (0.093 g, 0.50 mmol) [5] in acetonitrile (20 mL) and stirred for 3 h. The resulting mixture was left for slow evaporation at room temperature, yielding crystals after 3 weeks. Yield: 0.229 g (77%). **M. pt** (Biobase automatic melting point apparatus MP450): 410–411 K. Elemental Analysis for C₄₄H₄₂Au₂F₂N₂O₂P₂S₂ (Leco TruSpec Micro CHN Elemental Analyser): C, 44.45; H, 3.56; N, 2.36%. Found: C, 44.71; H, 3.72; N, 2.10%. **IR** (Bruker Vertex 70v FTIR Spectrophotometer; cm^{−1}): 1575 (s) ν(C=N), 1122 (s) ν(C–O), 1106 (s) ν(C–S). **¹H NMR** (Bruker Ascend 400 MHz NMR spectrometer with chemical shifts relative to tetramethylsilane in CDCl₃ solution at 298 K, ppm): δ 7.58–7.41 (m, br, 20H, Ph₂P), 6.95 (dt, 2H, aryl-H5, ⁴J_{HF} = 6.80 Hz, ³J_{HH} = 7.42 Hz),

6.60–6.56 (m, br, 4H, aryl-H2,6), 6.43–6.39 (m, br, 2H, aryl-H4), 3.88 (s, 6H, OCH_3), 2.30 (s, br, 4H, PCH_2), 1.67 (s, br, 4H, PCH_2CH_2). $^{13}C\{^1H\}$ NMR (as for 1H NMR): δ 165.5 (Cq), 163.1 (d, aryl-C3, $^1J_{CF} = 244.50$ Hz), 152.9 (d, aryl-C1, $^3J_{CF} = 9.80$ Hz), 133.2 (d, m- PC_6H_5 , $^3J_{CP} = 13.43$ Hz), 131.8 (p- PC_6H_5), 129.8 (d, aryl-C5, $^3J_{CF} = 9.54$ Hz), 130.1 (d, i- PC_6H_5 , $^1J_{CP} = 52.72$ Hz), 129.2 (d, o- PC_6H_5 , $^2J_{CP} = 11.09$ Hz), 117.9 (d, aryl-C6, $^4J_{CF} = 2.51$ Hz), 109.2 (d, aryl-C2, $^2J_{CF} = 21.95$ Hz), 109.0 (d, aryl-C4, $^2J_{CF} = 21.19$ Hz), 55.5 (OCH_3), 27.8 (d, PCH_2 , $^1J_{CP} = 34.01$ Hz), 26.9 (d, PCH_2CH_2 , $^2J_{CP} = 17.70$ Hz). $^{31}P\{^1H\}$ NMR (as for 1H NMR but with chemical shift referenced to 85% aqueous H_3PO_4 as the external reference): δ 32.9.

Experimental details

The C-bound H atoms were geometrically placed ($C-H = 0.95-0.99$ Å) and refined as riding with $U_{iso}(H) = 1.2-1.5U_{eq}(C)$. The maximum and minimum residual electron density peaks of 1.36 and $0.85 e\text{Å}^{-3}$, respectively, were located 0.78 and 0.67 Å, from the Au2 and S2 atoms, respectively. Each of the 3-fluorophenyl rings was disordered over two coplanar orientations so the C atoms were exactly coincident but, two positions were apparent for the F atoms; the latter were refined independently. At the conclusion of the refinement, the major component of the F1- and F2-rings had a site occupancy factor of 0.639(8) and 0.665(9), respectively.

Comment

Phosphane gold(I) thioamide molecules of the general formula $R_3PAu[SC(OR')=NAr]$ and their binuclear analogues are a well-studied class of compound [6, 7] owing, in part, to their biological activity against cancerous cells [8] and Gram-positive bacteria [9]. The compounds are relatively easy to prepare and furnish crystals readily. For example, the 3×3 matrix of crystals $(dppb)\{Au[SC(OR)=NC_6H_4Y-4]\}_2$ for $R = Me, Et$ or iPr and $Y = H, NO_2$ or Me has been studied [10]; $dppb$ is $Ph_2P(CH_2)_4PPh_2$. The specific motivation for the preparation of the title binuclear $dppb$ molecule, i.e. $(dppb)\{Au[SC(OMe)=N(C_6H_4F-3)]\}_2$ (I), with a fluorinated phenyl ring in the thiolate ligand arose from investigations into biological activity [5]. Herein, the crystal and molecular structures of (I) are described.

The molecular structure of the binuclear species in (I) is shown in the figure (50% displacement ellipsoids; the minor components of the disordered fluorophenyl rings are omitted for clarity). The Au1 atom is coordinated by thiolate-S1 [2.2933(10) Å] and phosphane-P1 [2.2552(10) Å] atoms which define a linear geometry with $P1-Au1-S1 = 173.96(3)^\circ$. The equivalent parameters for the Au2 atom are $Au2-S2 = 2.3097(11)$ Å, $Au2-P2 = 2.2505(10)$ Å and $P2-Au2-S2 = 174.67(3)^\circ$, indicating a close similarity. The mode

of coordination of the thiolate ligand and the gold atom coordination geometry in (I) is as found in all previous studies [5–7, 10]. The most notable feature of the molecular structure is the relative orientation of the thiolate ligands. For the Au1 atom, the aryl ring is disposed to be proximate to the gold atom with the $Au \cdots Cg(C2-C7)$ separation being 3.70 Å. A different disposition is noted for the second thiolate ligand arising from a rotation about the C–S bond which is now orientated to place the O2 atom in close proximity to the Au2 atom with the $Au2 \cdots O2$ separation being 3.172(4) Å. While both orientations have been observed previously [7], this is the first instance where both $Au \cdots \pi$ and $Au \cdots O$ interactions occur within the same molecule. However, there are conformational polymorphs for specific molecules, i.e. $Ph_3PAu[SC(OEt)=NPh]$, with intramolecular $Au \cdots O$ [11] and $Au \cdots \pi$ [12] interactions, and for $(4\text{-tolyl})_3PAu[SC(OEt)=NC_6H_4NO_2-4]$ with $Au \cdots O$ [13] and $Au \cdots \pi$ [14] contacts; the recently determined tetrahydrofuran (1/1) solvate of this compound features an intramolecular $Au \cdots O$ contact [15]. DFT calculations suggest the $Au \cdots \pi$ interaction is favoured over $Au \cdots O$ by about 6 kcal/mol [16].

A detailed analysis of the molecular packing for (I) is precluded owing to the disorder in the 3-fluorophenyl rings. Weak $Au \cdots S$ contacts [$Au2 \cdots S1^i = 3.5979(10)$ Å for symmetry operation (i) $1+x, -1+y, z$] connect molecules into a linear supramolecular chain along $[1 -2 0]$. The chains are connected into layers in the ab -plane by methylene- $C-H \cdots \pi$ (F-phenyl) [$C12-H12b \cdots Cg(C2-C7)^{ii} = 2.66$ Å with angle at $H12b = 163^\circ$ for (ii) $1+x, y, z$] and methyl- $C-H \cdots \pi$ (P-phenyl) [$C8-H8b \cdots Cg(C41-C46)^{iii} = 2.70$ Å with angle at $H8b = 142^\circ$ for (iii) $-1+x, 1+y, z$] interactions. The primary interactions between layers to consolidate the three-dimensional packing involve the disordered F atoms and are of the type $C-H \cdots F$ and $F \cdots \pi$.

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