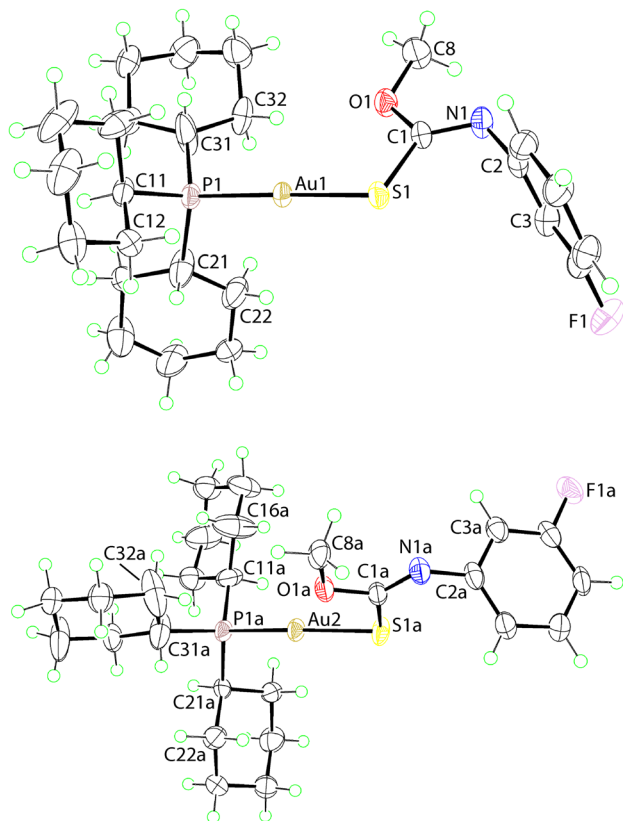


Chien Ing Yeo, Yee Seng Tan and Edward R. T. Tiekink\*

# Crystal structure of (tricyclohexylphosphane-κP)-[(Z)-N-(3-fluorophenyl)-O-methylthiocarbamato-κ<sub>1</sub>S]gold(I), C<sub>26</sub>H<sub>40</sub>AuFNOPS



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## Abstract

C<sub>26</sub>H<sub>40</sub>AuFNOPS, triclinic, *P*1 (no. 1), *a* = 9.62498(7) Å, *b* = 11.78239(10) Å, *c* = 12.74349(13) Å,  $\alpha$  = 78.7411(8)°,  $\beta$  = 73.5635(8)°,  $\gamma$  = 76.6096(1)°, *V* = 1335.34(2) Å<sup>3</sup>, *Z* = 2, *R*<sub>gt</sub>(*F*) = 0.0224, *wR*<sub>ref</sub>(*F*<sup>2</sup>) = 0.0557, *T* = 100 K.

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The molecular structures are shown in the Figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.14 × 0.08 × 0.06 mm
Wavelength:	Cu K $\alpha$ radiation (1.54184 Å)
$\mu$ :	11.8 mm <sup>-1</sup>
Diffractometer, scan mode:	XtaLAB Synergy, $\omega$
$\theta$ <sub>max</sub> , completeness:	75.3°, >99%
<i>N</i> ( <i>hkl</i> ) <sub>meas.</sub> , <i>N</i> ( <i>hkl</i> ) <sub>unique</sub> , <i>R</i> <sub>int</sub> :	66,451, 10,653, 0.030
Criterion for <i>I</i> <sub>obs</sub> , <i>N</i> ( <i>hkl</i> ) <sub>gt</sub> :	<i>I</i> <sub>obs</sub> > 2 $\sigma$ ( <i>I</i> <sub>obs</sub> ), 10,567
<i>N</i> ( <i>param</i> ) <sub>ref.</sub> :	638
Programs:	CrysAlis <sup>PRO</sup> [1], SHELX [2, 3], WinGX/ORTEP [4]

## Source of material

NaOH (Merck; 0.020 g, 0.50 mmol) in water (5 mL) was added to a suspension of (cyclohexyl)<sub>3</sub>PAuCl (0.256 g, 0.50 mmol) in acetonitrile (20 mL), followed by the addition of MeOC(=S)N(H)C<sub>6</sub>H<sub>4</sub>F-3 [5] (0.093 g, 0.50 mmol) in acetonitrile (20 mL) and stirred for 3 h. The resulting mixture was left for slow evaporation at room temperature, yielding crystals after 2 weeks. Yield: 0.261 g (79%). **M. pt.:** (Biobase automatic melting point apparatus MP450): 425–426 K. **Elemental Analysis** for C<sub>26</sub>H<sub>40</sub>AuFNOPS (Leco TruSpec Micro CHN Elemental Analyser): C, 47.20; H, 6.09; N, 2.12%. Found: C, 47.04; H, 6.19; N, 1.82%. **IR** (Bruker Vertex 70v FTIR Spectrophotometer; cm<sup>-1</sup>): 1575 (s)  $\nu$ (C=N), 1155 (s)  $\nu$ (C–O), 1124 (s)  $\nu$ (C–S). **<sup>1</sup>H NMR** (Bruker Ascend 400 MHz NMR spectrometer with chemical shifts relative to Me<sub>4</sub>Si in CDCl<sub>3</sub> solution at 298 K, ppm):  $\delta$  7.20 (dt, 1H, aryl-H5, <sup>4</sup>*J*<sub>HF</sub> = 6.92 Hz, <sup>3</sup>*J*<sub>HH</sub> = 7.33 Hz), 6.71–6.64 (m, br, 3H, aryl-H2,4,6), 3.84 (s, 3H, OCH<sub>3</sub>), 1.96–1.22 (m, br, 33H, Cy<sub>3</sub>P). **<sup>13</sup>C {<sup>1</sup>H} NMR** (as for <sup>1</sup>H NMR):  $\delta$  165.9 (C<sub>q</sub>), 163.2 (d, aryl-C3, <sup>1</sup>*J*<sub>CF</sub> = 243.79 Hz), 152.7 (d, aryl-C1, <sup>3</sup>*J*<sub>CF</sub> = 9.77 Hz), 129.5 (d, aryl-C5, <sup>3</sup>*J*<sub>CF</sub> = 9.56 Hz), 118.0 (d, aryl-C6, <sup>4</sup>*J*<sub>CF</sub> = 2.36 Hz), 109.4 (d, aryl-C2, <sup>2</sup>*J*<sub>CF</sub> = 22.06 Hz), 109.0 (d, aryl-C4, <sup>2</sup>*J*<sub>CF</sub> = 21.19 Hz), 55.1 (OCH<sub>3</sub>), 33.3 (d, i-PC<sub>6</sub>H<sub>11</sub>,

$J_{CP} = 28.01$  Hz), 30.7 (o-PC<sub>6</sub>H<sub>11</sub>), 27.1 (d, m-PC<sub>6</sub>H<sub>11</sub>,  $J_{CP} = 11.89$  Hz), 25.9 (p-PC<sub>6</sub>H<sub>11</sub>).  $^{31}\text{P}\{^1\text{H}\}$  NMR (as for  $^1\text{H}$  NMR but with chemical shift referenced to 85% aqueous H<sub>3</sub>PO<sub>4</sub> as the external reference):  $\delta$  57.7.

## Experimental details

The C-bound H atoms were geometrically placed (C–H = 0.95–1.00 Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2$ – $1.5U_{\text{eq}}(\text{C})$ . Disorder was modelled in four regions of the structure. Each 3-fluorophenyl ring was disordered over two co-planar 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 C2- and C2a-rings had site occupancy factors of 0.763(14) and 0.741(14), respectively. The cyclohexyl-C31 ring exhibited two, partially overlapping chair conformations. Thus, while the C31, C33 and C36 atoms were coincident, the remaining atoms were statistically disordered (from refinement) and refined independently. The cyclohexyl-C31a ring exhibited two conformations, i.e. chair and boat, depending on the relative orientation of the C34a atom. From independent refinement, the chair conformation was most pronounced with a site occupancy factor of 0.77(3). For the different orientations of the two disordered cyclohexyl rings, soft distance constraints were introduced with 1,1-C–C and 1,2-C···C separations being  $1.53 \pm 0.01$  and  $2.52 \pm 0.01$  Å, respectively. Finally, the crystal was refined as an inversion twin with the minor component contributing 0.109(8) to the measured crystal.

## Comment

The specific interest leading to the synthesis and characterization of the title compound, Cy<sub>3</sub>Au[SC(OMe)=NC<sub>6</sub>H<sub>4</sub>F-3], (I), revolves around the noted biological activity of related species, such as anti-cancer [6] and anti-bacterial [7] potential; Cy = cyclo-C<sub>6</sub>H<sub>11</sub>. The inclusion of a fluoride atom in the molecular structure was motivated by suggestions in the literature that such chemical substitution enhances biological activity [8]. Herein, the synthesis, spectroscopic characterization and X-ray crystal structure determination of (I) are described.

The crystallographic asymmetric unit of (I) comprises two formula units and their molecular structures are shown in the figure (50% displacement ellipsoids; minor disorder components are omitted). Each of the gold(I) atoms in (I) is

**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Au1	0.66877 (2)	0.94917 (2)	0.86592 (2)	0.02693 (7)
S1	0.50132 (16)	0.88755 (13)	1.02309 (13)	0.0296 (3)
P1	0.83683 (16)	1.00086 (14)	0.70931 (13)	0.0283 (3)
O1	0.3991 (5)	1.1114 (4)	0.9725 (4)	0.0328 (9)
N1	0.2734 (6)	1.0304 (5)	1.1402 (5)	0.0337 (11)
C1	0.3771 (6)	1.0189 (5)	1.0521 (5)	0.0267 (11)
C2 <sup>a</sup>	0.2638 (7)	0.9264 (5)	1.2191 (5)	0.0309 (13)
C3 <sup>a</sup>	0.3376 (8)	0.9039 (6)	1.3020 (6)	0.0366 (14)
H3 <sup>a</sup>	0.390074	0.959564	1.309723	0.044*
C4 <sup>a</sup>	0.3340 (7)	0.8001 (6)	1.3726 (6)	0.0355 (13)
F1 <sup>a</sup>	0.4082 (7)	0.7793 (5)	1.4510 (5)	0.0464 (18)
C5 <sup>a</sup>	0.2601 (7)	0.7160 (6)	1.3664 (6)	0.0357 (13)
H5 <sup>a</sup>	0.262979	0.643259	1.414265	0.043*
C6 <sup>a</sup>	0.1804 (8)	0.7435 (6)	1.2856 (6)	0.0380 (14)
H6 <sup>a</sup>	0.124105	0.689208	1.280712	0.046*
C7 <sup>a</sup>	0.1806 (7)	0.8466 (6)	1.2131 (6)	0.0357 (14)
H7 <sup>a</sup>	0.124676	0.863203	1.159500	0.043*
C2 <sup>b</sup>	0.2638 (7)	0.9264 (5)	1.2191 (5)	0.0309 (13)
C3 <sup>b</sup>	0.3376 (8)	0.9039 (6)	1.3020 (6)	0.0366 (14)
H3 <sup>b</sup>	0.390074	0.959564	1.309723	0.044*
C4 <sup>b</sup>	0.3340 (7)	0.8001 (6)	1.3726 (6)	0.0355 (13)
H4 <sup>b</sup>	0.385450	0.785588	1.428875	0.043*
C5 <sup>b</sup>	0.2601 (7)	0.7160 (6)	1.3664 (6)	0.0357 (13)
H5 <sup>b</sup>	0.262979	0.643259	1.414265	0.043*
C6 <sup>b</sup>	0.1804 (8)	0.7435 (6)	1.2856 (6)	0.0380 (14)
F1 <sup>b</sup>	0.090 (2)	0.6796 (17)	1.288 (2)	0.061 (7)
C7 <sup>b</sup>	0.1806 (7)	0.8466 (6)	1.2131 (6)	0.0357 (14)
H7 <sup>b</sup>	0.124676	0.863203	1.159500	0.043*
C8	0.2945 (8)	1.2199 (6)	0.9894 (7)	0.0449 (17)
H8A	0.286604	1.239819	1.062243	0.067*
H8B	0.197896	1.210239	0.985174	0.067*
H8C	0.328077	1.283297	0.932088	0.067*
C11	0.8548 (7)	0.9020 (6)	0.6092 (5)	0.0334 (13)
H11	0.942359	0.914068	0.546327	0.040*
C12	0.8797 (8)	0.7734 (6)	0.6632 (6)	0.0366 (15)
H12A	0.971851	0.756233	0.688163	0.044*
H12B	0.797494	0.762801	0.729406	0.044*
C13	0.8902 (9)	0.6854 (8)	0.5877 (7)	0.053 (2)
H13A	0.899100	0.604906	0.629242	0.064*
H13B	0.979437	0.688279	0.525817	0.064*
C14	0.7545 (10)	0.7131 (9)	0.5423 (7)	0.060 (2)
H14A	0.766255	0.658701	0.488901	0.072*
H14B	0.666770	0.701091	0.603405	0.072*
C15	0.7316 (12)	0.8383 (10)	0.4859 (8)	0.067 (3)
H15A	0.641013	0.854794	0.459018	0.081*
H15B	0.815773	0.848129	0.421007	0.081*
C16	0.7179 (8)	0.9266 (7)	0.5631 (7)	0.0465 (18)
H16A	0.629053	0.921570	0.624933	0.056*
H16B	0.706104	1.007456	0.522255	0.056*
C21	1.0218 (8)	0.9802 (10)	0.7340 (7)	0.059 (2)
H21	1.040992	0.892354	0.751361	0.070*
C22	1.0266 (9)	1.0070 (14)	0.8374 (7)	0.085 (4)
H22A	0.959596	0.963389	0.896914	0.102*
H22B	0.986571	1.092101	0.839788	0.102*
C23	1.1723 (7)	0.9804 (6)	0.8632 (6)	0.0368 (14)

Table 2: (continued)

Atom	x	y	z	$U_{iso}^*/U_{eq}$
H23A	1.187765	0.898385	0.900961	0.044*
H23B	1.169731	1.032711	0.916089	0.044*
C24	1.3027 (9)	0.9936 (14)	0.7669 (8)	0.090 (4)
H24A	1.319512	1.075207	0.756898	0.108*
H24B	1.390416	0.940374	0.786406	0.108*
C25	1.2948 (8)	0.9704 (11)	0.6641 (8)	0.069 (3)
H25A	1.339600	0.886446	0.658863	0.083*
H25B	1.358903	1.017404	0.605670	0.083*
C26	1.1483 (7)	0.9924 (6)	0.6354 (6)	0.0346 (13)
H26A	1.130782	1.072824	0.594644	0.042*
H26B	1.152629	0.936003	0.585681	0.042*
C31 <sup>c</sup>	0.7819 (12)	1.1511 (6)	0.6493 (6)	0.078 (4)
H31 <sup>c</sup>	0.692503	1.140334	0.630071	0.094*
C32 <sup>c</sup>	0.7069 (16)	1.2391 (9)	0.7256 (8)	0.045 (3)
H32A <sup>c</sup>	0.781506	1.264643	0.751039	0.054*
H32B <sup>c</sup>	0.640521	1.202330	0.791258	0.054*
C33 <sup>c</sup>	0.6154 (9)	1.3490 (6)	0.6691 (7)	0.059 (2)
H33A <sup>c</sup>	0.536737	1.325656	0.646679	0.071*
H33B <sup>c</sup>	0.568956	1.407820	0.720702	0.071*
C34 <sup>c</sup>	0.7247 (18)	1.4019 (9)	0.5659 (10)	0.051 (4)
H34A <sup>c</sup>	0.674005	1.476726	0.531240	0.061*
H34B <sup>c</sup>	0.808261	1.418194	0.587625	0.061*
C35 <sup>c</sup>	0.7809 (17)	1.3114 (9)	0.4840 (8)	0.039 (3)
H35A <sup>c</sup>	0.696466	1.295650	0.462970	0.047*
H35B <sup>c</sup>	0.847987	1.344051	0.416272	0.047*
C36 <sup>c</sup>	0.8626 (6)	1.1965 (5)	0.5351 (5)	0.0377 (14)
H36A <sup>c</sup>	0.880769	1.135758	0.486552	0.045*
H36B <sup>c</sup>	0.959726	1.208810	0.538022	0.045*
C31 <sup>c</sup>	0.7819 (12)	1.1511 (6)	0.6493 (6)	0.078 (4)
H31C <sup>c</sup>	0.834931	1.186112	0.688446	0.094*
C32 <sup>c</sup>	0.6357 (13)	1.2144 (9)	0.6981 (11)	0.042 (3)
H32C <sup>c</sup>	0.615248	1.194065	0.779438	0.050*
H32D <sup>c</sup>	0.561946	1.187030	0.673391	0.050*
C33 <sup>c</sup>	0.6154 (9)	1.3490 (6)	0.6691 (7)	0.059 (2)
H33C <sup>c</sup>	0.674378	1.379919	0.705459	0.071*
H33D <sup>c</sup>	0.510376	1.385177	0.695488	0.071*
C34 <sup>c</sup>	0.6667 (15)	1.3806 (12)	0.5415 (11)	0.056 (5)
H34C <sup>c</sup>	0.610642	1.346940	0.504906	0.067*
H34D <sup>c</sup>	0.648877	1.467209	0.520648	0.067*
C35 <sup>c</sup>	0.8315 (14)	1.3299 (10)	0.5047 (13)	0.051 (5)
H35C <sup>c</sup>	0.866195	1.350320	0.423670	0.062*
H35D <sup>c</sup>	0.886851	1.365542	0.540234	0.062*
C36 <sup>c</sup>	0.8626 (6)	1.1965 (5)	0.5351 (5)	0.0377 (14)
H36C <sup>c</sup>	0.836234	1.160547	0.481142	0.045*
H36D <sup>c</sup>	0.969863	1.169917	0.528034	0.045*
Au2	0.93580 (2)	0.39019 (2)	0.87113 (2)	0.02961 (7)
S1A	1.0989 (2)	0.32835 (14)	0.71298 (14)	0.0380 (4)
P1A	0.75511 (17)	0.42992 (14)	1.02503 (13)	0.0305 (3)
O1A	1.1869 (5)	0.5211 (4)	0.7141 (4)	0.0331 (9)
N1A	1.2592 (7)	0.4590 (5)	0.5450 (5)	0.0341 (12)
C1A	1.1908 (7)	0.4434 (5)	0.6470 (5)	0.0282 (12)
C2A <sup>d</sup>	1.2616 (7)	0.3788 (6)	0.4748 (6)	0.0334 (13)
C3A <sup>d</sup>	1.1758 (8)	0.4133 (6)	0.3987 (6)	0.0364 (14)
H3A <sup>d</sup>	1.111909	0.487951	0.396442	0.044*
C4A <sup>d</sup>	1.1854 (8)	0.3370 (6)	0.3265 (6)	0.0377 (14)
F1A <sup>d</sup>	1.1005 (7)	0.3731 (5)	0.2528 (5)	0.0481 (19)

Table 2: (continued)

Atom	x	y	z	$U_{iso}^*/U_{eq}$
C5A <sup>d</sup>	1.2738 (9)	0.2282 (6)	0.3252 (6)	0.0414 (16)
H5A <sup>d</sup>	1.276318	0.177440	0.274924	0.050*
C6A <sup>d</sup>	1.3606 (9)	0.1950 (7)	0.4018 (6)	0.0450 (17)
H6A <sup>d</sup>	1.424345	0.120176	0.403097	0.054*
C7A <sup>d</sup>	1.3555 (8)	0.2692 (6)	0.4758 (6)	0.0406 (15)
H7A <sup>d</sup>	1.415624	0.245297	0.526810	0.049*
C2A <sup>re</sup>	1.2616 (7)	0.3788 (6)	0.4748 (6)	0.0334 (13)
C3A <sup>re</sup>	1.1758 (8)	0.4133 (6)	0.3987 (6)	0.0364 (14)
H3A <sup>re</sup>	1.111909	0.487951	0.396442	0.044*
C4A <sup>re</sup>	1.1854 (8)	0.3370 (6)	0.3265 (6)	0.0377 (14)
H4A <sup>re</sup>	1.126932	0.361656	0.274451	0.045*
C5A <sup>re</sup>	1.2738 (9)	0.2282 (6)	0.3252 (6)	0.0414 (16)
H5A <sup>re</sup>	1.276318	0.177440	0.274924	0.050*
C6A <sup>re</sup>	1.3606 (9)	0.1950 (7)	0.4018 (6)	0.0450 (17)
F1A <sup>re</sup>	1.461 (2)	0.1001 (15)	0.4013 (17)	0.060 (7)
C7A <sup>re</sup>	1.3555 (8)	0.2692 (6)	0.4758 (6)	0.0406 (15)
H7A <sup>re</sup>	1.415624	0.245297	0.526810	0.049*
C8A	1.2601 (8)	0.6179 (6)	0.6603 (6)	0.0393 (15)
H8A1	1.215334	0.661523	0.600553	0.059*
H8A2	1.364811	0.587750	0.629733	0.059*
H8A3	1.250011	0.670397	0.714010	0.059*
C11A	0.5766 (8)	0.4848 (6)	0.9849 (7)	0.0453 (17)
H11A	0.567661	0.421607	0.946347	0.054*
C12A	0.4395 (8)	0.4957 (7)	1.0788 (6)	0.0453 (16)
H12C	0.442299	0.554223	1.123947	0.054*
H12D	0.435915	0.418881	1.126793	0.054*
C13A	0.3006 (9)	0.5343 (9)	1.0338 (9)	0.068 (3)
H13C	0.289714	0.469254	0.999749	0.082*
H13D	0.213018	0.549094	1.096210	0.082*
C14A	0.3044 (9)	0.6415 (8)	0.9511 (7)	0.0522 (19)
H14C	0.297913	0.709964	0.987772	0.063*
H14D	0.217902	0.656553	0.919450	0.063*
C15A	0.4447 (10)	0.6291 (9)	0.8587 (8)	0.064 (3)
H15C	0.441149	0.571272	0.813044	0.077*
H15D	0.449357	0.705807	0.810788	0.077*
C16A	0.5809 (10)	0.5901 (10)	0.9000 (9)	0.080 (4)
H16C	0.666547	0.572761	0.836849	0.096*
H16D	0.595746	0.655553	0.931458	0.096*
C21A	0.7316 (6)	0.2951 (5)	1.1207 (5)	0.0284 (12)
H21A	0.645801	0.314476	1.184413	0.034*
C22A	0.8688 (8)	0.2430 (6)	1.1654 (7)	0.0413 (16)
H22C	0.956326	0.230279	1.102558	0.050*
H22D	0.884072	0.300141	1.206707	0.050*
C23A	0.8550 (10)	0.1269 (7)	1.2410 (7)	0.053 (2)
H23C	0.947197	0.094883	1.265164	0.064*
H23D	0.773277	0.140555	1.307471	0.064*
C24A	0.8256 (11)	0.0383 (7)	1.1820 (7)	0.050 (2)
H24C	0.910783	0.019875	1.118833	0.060*
H24D	0.813699	-0.035615	1.233328	0.060*
C25A	0.6870 (9)	0.0867 (6)	1.1406 (7)	0.0483 (18)
H25C	0.600772	0.098952	1.204388	0.058*
H25D	0.671606	0.028480	1.100441	0.058*
C26A	0.6981 (7)	0.2029 (5)	1.0640 (6)	0.0353 (14)
H26C	0.604065	0.234222	1.042171	0.042*
H26D	0.777257	0.188824	0.996139	0.042*
C31A	0.7938 (12)	0.5279 (7)	1.1046 (6)	0.063 (3)

Table 2: (continued)

Atom	x	y	z	$U_{iso}^*/U_{eq}$
H31B	0.881580	0.478027	1.128721	0.076*
C32A	0.8562 (14)	0.6321 (9)	1.0397 (6)	0.082 (4)
H32E	0.782067	0.683847	1.002715	0.099*
H32F	0.943530	0.604551	0.981237	0.099*
C33A <sup>f</sup>	0.9011 (8)	0.7037 (6)	1.1054 (6)	0.0467 (17)
H33E <sup>f</sup>	0.920249	0.779115	1.059125	0.056*
H33F <sup>f</sup>	0.994234	0.660795	1.123999	0.056*
C34A <sup>f</sup>	0.7850 (13)	0.7301 (9)	1.2121 (7)	0.051 (4)
H34E <sup>f</sup>	0.829267	0.762620	1.258268	0.061*
H34F <sup>f</sup>	0.702497	0.791205	1.193418	0.061*
C35A <sup>f</sup>	0.7253 (13)	0.6248 (9)	1.2776 (6)	0.084 (4)
H35E <sup>f</sup>	0.635432	0.652171	1.334077	0.100*
H35F <sup>f</sup>	0.798813	0.576742	1.317128	0.100*
C33B <sup>g</sup>	0.9011 (8)	0.7037 (6)	1.1054 (6)	0.0467 (17)
H33G <sup>g</sup>	1.009564	0.696566	1.080979	0.056*
H33H <sup>g</sup>	0.857389	0.787460	1.086494	0.056*
C34B <sup>g</sup>	0.860 (2)	0.674 (2)	1.2274 (9)	0.023 (8)
H34G <sup>g</sup>	0.943101	0.616247	1.249470	0.027*
H34H <sup>g</sup>	0.849355	0.745937	1.259913	0.027*
C35B <sup>g</sup>	0.7253 (13)	0.6248 (9)	1.2776 (6)	0.084 (4)
H35G <sup>g</sup>	0.641442	0.691474	1.291669	0.100*
H35H <sup>g</sup>	0.733944	0.579368	1.350204	0.100*
C36A	0.6875 (8)	0.5468 (6)	1.2138 (5)	0.0443 (16)
H36E	0.681220	0.469174	1.259814	0.053*
H36F	0.588582	0.581487	1.201151	0.053*

<sup>a</sup>Occupancy: 0.763(14).<sup>b</sup>Occupancy: 0.237(14).<sup>c</sup>Occupancy: 0.5.<sup>d</sup>Occupancy: 0.741(14).<sup>e</sup>Occupancy: 0.259(14).<sup>f</sup>Occupancy: 0.77 (3).<sup>g</sup>Occupancy: 0.23(3).

coordinated by phosphane-P [Au1–P1 = 2.2638(15) Å; Au2–P1a = 2.2674(15) Å] and thiolate-S [Au1–S1 = 2.2987(15) Å; Au2–S1a = 2.3043(15) Å] atoms with the equivalent bonds being experimentally indistinguishable. The P- and S-donor atoms define an almost linear geometry with the P1–Au1–S1 angle of 177.25(6)° being significantly greater than the P1a–Au2–S1a angle of 170.98(6)°. In each case, the thiolato ligand is orientated so the O atom is directed towards the Au atom with the Au1···O1 and Au2···O1a separations being 2.993(5) and 3.164(5) Å, respectively. These separations indicate there is no direct correlation between the magnitude of the Au···O interaction and the deviation from the ideal linear angle. In some related structures an alternate conformation of the thiolate ligand is observed where the O atom is directed away from the Au atom, an orientation which allows for the formation of an intramolecular Au···π(phenyl) contact instead. Calculations (DFT) indicate that Au···π interactions are approximately 6 kcal/mol more stable than Au···O contacts [9, 10] but, the

former are susceptible to steric effects [11]. In this regard, it is noteworthy that none of the known Cy<sub>3</sub>PAu[SC(OR)=NAr] structures feature intramolecular Au···π interactions, an observation that is ascribed to the bulky nature of the cyclohexyl substituents [11]. The major conformational difference in the molecules is apparent in the relative disposition of the fluorophenyl groups with respect to the central CNOS plane, as seen in the dihedral angles formed between the plane through the C1, N1, O1 and S1 atoms and that through the fluorophenyl ring of 87.9(2)° for the Au1-molecule, which is clearly closer to orthogonal compared to the equivalent angle of 75.1(2)° for the Au2-molecule.

In the molecular packing for (I), layers of molecules assemble in the *ab*-plane with the cyclohexyl and fluorophenyl rings projecting to either side. These stack along the *c*-axis so the latter rings occupy channels. Yet, there are no close interactions between the rings. A more detailed analysis of the packing is not warranted owing to the disorder in several of the residues.

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