Crystal structure of benzamide-2-thiolato(tri-*o*-tolylphosphine)gold(I), $C_{28}H_{27}AuNOPS$

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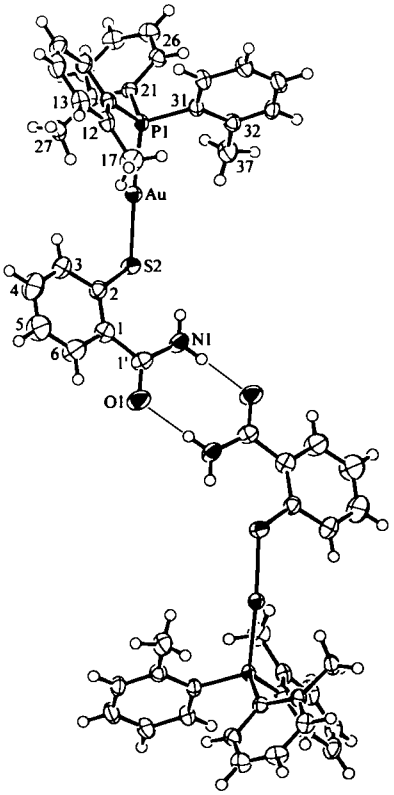

Abstract

$C_{28}H_{27}AuNOPS$, triclinic, $P\bar{1}$ (No. 2), $a = 11.731(2)$ Å, $b = 13.237(4)$ Å, $c = 9.245(3)$ Å, $\alpha = 105.06(2)°$, $\beta = 91.32(2)°$, $\gamma = 75.65(2)°$, $V = 1341.7$ Å^3, $Z = 2$, $R_{gt}(F) = 0.034$, $wR_{ref}(F^2) = 0.088$, $T = 173$ K.

Source of material

The title compound was prepared in 95% yield from the reaction between *o*-tol$_3$PAuCl and 2-mercaptobenzamide [1]. Colourless crystals were obtained from the slow evaporation of an acetonitrile solution of the compound (mp 437 K – 439 K).

Experimental details

The H atoms were placed in their geometrically calculated positions and included in the final refinement in the riding model approximation.

Discussion

The gold atom exists in the expected linear environment defined by the sulfur, d(Au—S) = 2.295(1) Å, and phosphorus, d(Au—P) = 2.271(1) Å, atoms which define an angle of 174.97(4)° at gold. Centrosymmetric molecules associate via hydrogen bonding interactions as shown in the figure. The parameters associated with these interactions are d(H1a···O1^i) = 1.97 Å, d(N1···O1^i) = 2.840(7) Å with an angle of 176° subtended at H1a for symmetry operation i: $-1-x$, $1-y$, $1-z$. The second amide hydrogen atom forms an intramolecular S···H interaction so that d(H1b···S) is 2.33 Å and the angle at H1b is 131°.

Table 1. Data collection and handling.

Crystal:	colourless plate, size 0.04 × 0.25 × 0.25 mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ:	56.58 cm^{-1}
Diffractometer, scan mode:	Rigaku AFC7R, $\omega/2\theta$
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6440, 6141
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 4823
$N(param)_{refined}$:	301
Programs:	teXsan [2], DIRDIF92 [3], SHELXL-97 [4], DIFABS [5], ORTEPII [6]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1a)	2*i*	–0.4080	0.4439	0.5327	0.046
H(1b)	2*i*	–0.2836	0.3794	0.4751	0.046
H(3)	2*i*	–0.0086	0.2643	0.0891	0.056
H(4)	2*i*	–0.0227	0.3836	–0.0570	0.085
H(5)	2*i*	–0.1870	0.5279	–0.0333	0.086
H(6)	2*i*	–0.3384	0.5541	0.1430	0.064
H(13)	2*i*	0.4006	0.3729	0.2863	0.048
H(14)	2*i*	0.5675	0.2473	0.1627	0.050
H(15)	2*i*	0.5901	0.0630	0.1388	0.049
H(16)	2*i*	0.4453	0.0063	0.2431	0.038
H(17a)	2*i*	0.2257	0.4228	0.4265	0.071
H(17b)	2*i*	0.2046	0.3422	0.5196	0.071
H(17c)	2*i*	0.1444	0.3418	0.3625	0.071
H(23)	2*i*	0.2788	–0.2491	0.0642	0.042
H(24)	2*i*	0.3713	–0.3421	0.2335	0.046
H(25)	2*i*	0.4064	–0.2470	0.4730	0.045
H(26)	2*i*	0.3417	–0.0592	0.5458	0.037
H(27a)	2*i*	0.2061	–0.0958	–0.0144	0.053
H(27b)	2*i*	0.2385	0.0132	0.0764	0.053
H(27c)	2*i*	0.1152	–0.0089	0.1111	0.053
H(33)	2*i*	0.1397	0.1417	0.9317	0.044
H(34)	2*i*	0.3002	0.2067	1.0190	0.049
H(35)	2*i*	0.4301	0.2322	0.8515	0.047
H(36)	2*i*	0.3971	0.1899	0.5942	0.039
H(37a)	2*i*	0.0349	0.0593	0.7446	0.068
H(37b)	2*i*	0.0895	0.0160	0.5763	0.068
H(37c)	2*i*	0.0031	0.1343	0.6313	0.068

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Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Au	2*i*	0.03792(2)	0.17399(2)	0.34937(2)	0.0269(1)	0.0271(1)	0.0283(1)	–0.00609(7)	–0.00153(7)	0.00679(7)
S(2)	2*i*	–0.1571(1)	0.2340(1)	0.3040(2)	0.0272(6)	0.0329(7)	0.0428(7)	–0.0046(5)	0.0006(5)	0.0120(5)
P(1)	2*i*	0.2258(1)	0.1067(1)	0.4075(1)	0.0273(6)	0.0270(6)	0.0210(5)	–0.0088(5)	–0.0011(4)	0.0083(5)
O(1)	2*i*	–0.4598(4)	0.5192(4)	0.3185(6)	0.050(3)	0.057(3)	0.073(3)	0.014(2)	0.021(2)	0.040(3)
N(1)	2*i*	–0.3510(4)	0.4231(4)	0.4630(5)	0.039(3)	0.030(2)	0.041(2)	–0.001(2)	0.011(2)	0.007(2)
C(1')	2*i*	–0.3666(5)	0.4578(4)	0.3397(7)	0.035(3)	0.025(3)	0.049(3)	–0.006(2)	0.003(2)	0.010(2)
C(1)	2*i*	–0.2638(5)	0.4264(4)	0.2266(6)	0.043(3)	0.029(3)	0.040(3)	–0.011(2)	0.002(2)	0.010(2)
C(2)	2*i*	–0.1663(5)	0.3356(5)	0.2084(6)	0.028(3)	0.043(3)	0.029(2)	–0.011(2)	0.001(2)	0.007(2)
C(3)	2*i*	–0.0763(6)	0.3232(5)	0.1011(7)	0.041(3)	0.057(4)	0.042(3)	–0.011(3)	0.008(3)	0.015(3)
C(4)	2*i*	–0.0846(7)	0.3940(7)	0.0140(9)	0.059(5)	0.099(6)	0.068(5)	–0.023(4)	0.020(4)	0.042(5)
C(5)	2*i*	–0.1813(7)	0.4797(7)	0.0283(9)	0.072(5)	0.074(5)	0.083(5)	–0.005(4)	0.018(4)	0.056(5)
C(6)	2*i*	–0.2710(6)	0.4953(5)	0.1340(8)	0.052(4)	0.045(4)	0.068(4)	–0.002(3)	0.014(3)	0.030(3)
C(11)	2*i*	0.3358(4)	0.1558(4)	0.3265(5)	0.028(2)	0.028(2)	0.023(2)	–0.012(2)	–0.004(2)	0.007(2)
C(12)	2*i*	0.3198(5)	0.2673(4)	0.3397(5)	0.040(3)	0.036(3)	0.024(2)	–0.019(2)	–0.004(2)	0.011(2)
C(13)	2*i*	0.4086(6)	0.2984(5)	0.2777(6)	0.057(4)	0.041(3)	0.032(3)	–0.030(3)	–0.006(2)	0.011(2)
C(14)	2*i*	0.5086(5)	0.2236(5)	0.2038(6)	0.046(3)	0.059(4)	0.033(3)	–0.032(3)	–0.002(2)	0.015(3)
C(15)	2*i*	0.5223(5)	0.1144(5)	0.1900(6)	0.034(3)	0.059(4)	0.034(3)	–0.019(3)	0.004(2)	0.011(3)
C(16)	2*i*	0.4360(5)	0.0811(4)	0.2518(5)	0.033(3)	0.034(3)	0.031(2)	–0.011(2)	0.002(2)	0.009(2)
C(17)	2*i*	0.2147(6)	0.3507(5)	0.4189(7)	0.059(4)	0.027(3)	0.058(4)	–0.012(3)	0.003(3)	0.011(3)
C(21)	2*i*	0.2735(4)	–0.0401(4)	0.3468(5)	0.024(2)	0.026(2)	0.028(2)	–0.008(2)	0.000(2)	0.009(2)
C(22)	2*i*	0.2546(4)	–0.0976(4)	0.1999(5)	0.031(3)	0.030(2)	0.026(2)	–0.009(2)	0.001(2)	0.011(2)
C(23)	2*i*	0.2917(5)	–0.2095(4)	0.1620(6)	0.040(3)	0.033(3)	0.034(3)	–0.013(2)	–0.001(2)	0.007(2)
C(24)	2*i*	0.3472(5)	–0.2654(4)	0.2625(7)	0.038(3)	0.025(3)	0.052(3)	–0.009(2)	–0.002(2)	0.010(2)
C(25)	2*i*	0.3670(5)	–0.2093(4)	0.4044(6)	0.042(3)	0.029(3)	0.046(3)	–0.010(2)	–0.002(2)	0.019(2)
C(26)	2*i*	0.3294(5)	–0.0975(4)	0.4469(6)	0.033(3)	0.034(3)	0.032(2)	–0.011(2)	–0.002(2)	0.016(2)
C(27)	2*i*	0.1987(5)	–0.0425(4)	0.0831(5)	0.046(3)	0.035(3)	0.023(2)	–0.007(2)	–0.002(2)	0.007(2)
C(31)	2*i*	0.2474(4)	0.1411(4)	0.6089(5)	0.034(3)	0.027(2)	0.021(2)	–0.006(2)	0.001(2)	0.007(2)
C(32)	2*i*	0.1688(5)	0.1258(4)	0.7105(5)	0.031(3)	0.033(3)	0.029(2)	–0.010(2)	–0.002(2)	0.011(2)
C(33)	2*i*	0.1918(5)	0.1514(4)	0.8622(6)	0.045(3)	0.038(3)	0.026(2)	–0.001(2)	0.008(2)	0.013(2)
C(34)	2*i*	0.2870(5)	0.1902(5)	0.9147(6)	0.054(4)	0.041(3)	0.023(2)	–0.006(3)	–0.007(2)	0.008(2)
C(35)	2*i*	0.3641(5)	0.2051(5)	0.8156(6)	0.043(3)	0.044(3)	0.031(3)	–0.015(3)	–0.008(2)	0.010(2)
C(36)	2*i*	0.3441(5)	0.1801(4)	0.6625(5)	0.040(3)	0.036(3)	0.026(2)	–0.014(2)	–0.003(2)	0.012(2)
C(37)	2*i*	0.0651(5)	0.0799(6)	0.6614(7)	0.039(3)	0.069(4)	0.042(3)	–0.028(3)	–0.001(2)	0.023(3)

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