Crystal structure of methyltriphenylphosphonium bromo(pentafluorophenyl)aurate(I), $[\text{MePh}_3\text{P}]^+[\text{Br}(\text{C}_6\text{F}_5)\text{Au}]^-$

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Source of material: The title compound crystallised fortuitously from a reaction mixture in which it was a starting material.

Bond lengths and angles at gold: Au–C11 2.009(5) Å, Au–Br 2.4137(7) Å, C11–Au–Br 177.90(13)°. For a structure containing the related anion $[\text{Cl}(\text{C}_6\text{F}_5)\text{Au}]^-$ see ref. 1.

$\text{C}_{25}\text{H}_{18}\text{AuBrF}_5\text{P}$, monoclinic, $P12_1/n1$ (No. 14), $a = 8.875(1)$ Å, $b = 14.901(2)$ Å, $c = 18.001(2)$ Å, $\beta = 94.729(8)^\circ$, $V = 2372.5$ Å³, $Z = 4$, $R(F) = 0.028$, $R_w(F^2) = 0.045$.

Table 1. Parameters used for the X-ray data collection

Crystal:	colorless, equidimensional, size 0.40 x 0.40 x 0.40 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	80.03 cm ⁻¹
Diffractometer:	Siemens P4
Scan mode:	ω
$T_{\text{measurement}}$:	173 K
$2\theta_{\text{max}}$:	50°
$N(hkl)_{\text{unique}}$:	4174
Criterion for I_o :	Refined on F^2 for all reflections
$N(\text{param})_{\text{refined}}$:	300
Program:	SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{iso}
H(1A)	4e	0.2279	0.6100	0.9696	0.038
H(1B)	4e	0.3870	0.5645	0.9955	0.038
H(1C)	4e	0.2419	0.5031	0.9742	0.038
H(22)	4e	0.0478	0.6349	0.8695	0.042
H(23)	4e	-0.1626	0.6422	0.7841	0.047
H(24)	4e	-0.1696	0.5633	0.6736	0.051
H(25)	4e	0.0382	0.4780	0.6445	0.053
H(26)	4e	0.2503	0.4692	0.7297	0.042
H(32)	4e	0.3550	0.6685	0.7404	0.037
H(33)	4e	0.5010	0.7909	0.7127	0.048
H(34)	4e	0.6819	0.8482	0.8010	0.046
H(35)	4e	0.7135	0.7838	0.9182	0.049
H(36)	4e	0.5670	0.6617	0.9483	0.040
H(42)	4e	0.2933	0.3675	0.8792	0.043
H(43)	4e	0.4479	0.2412	0.8775	0.053
H(44)	4e	0.7021	0.2569	0.8558	0.048
H(45)	4e	0.7992	0.3982	0.8336	0.042
H(46)	4e	0.6454	0.5245	0.8324	0.036

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Au	4e	0.40685(2)	0.67925(2)	0.55160(1)	0.0343(1)	0.0315(1)	0.0266(1)	-0.0046(1)	0.00134(8)	-0.0033(1)
Br	4e	0.45315(6)	0.83753(4)	0.53631(3)	0.0403(3)	0.0338(4)	0.0498(4)	-0.0076(3)	0.0114(3)	-0.0032(3)
P	4e	0.3400(2)	0.55550(9)	0.86803(7)	0.0281(8)	0.0238(8)	0.0202(7)	0.0020(7)	0.0001(6)	-0.0010(6)
C(1)	4e	0.2940(6)	0.5586(3)	0.9624(3)	0.035(3)	0.032(3)	0.027(3)	0.003(3)	0.002(3)	0.003(3)
C(11)	4e	0.3669(5)	0.5471(3)	0.5602(2)	0.036(3)	0.023(3)	0.024(3)	0.003(2)	0.006(2)	-0.009(2)
C(12)	4e	0.2586(6)	0.5030(4)	0.5144(3)	0.047(4)	0.036(3)	0.027(3)	0.002(3)	-0.005(3)	0.005(3)
C(13)	4e	0.2300(6)	0.4129(4)	0.5186(3)	0.044(4)	0.036(3)	0.036(3)	-0.011(3)	0.005(3)	-0.005(3)
C(14)	4e	0.3125(6)	0.3607(4)	0.5705(3)	0.049(4)	0.022(3)	0.043(4)	0.001(3)	0.022(3)	-0.001(3)

Table 3. (Continued)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(15)	4e	0.4238(6)	0.4012(4)	0.6167(3)	0.039(3)	0.042(4)	0.037(3)	0.014(3)	0.013(3)	0.014(3)
C(16)	4e	0.4470(6)	0.4920(4)	0.6107(3)	0.030(3)	0.045(3)	0.026(3)	−0.001(3)	−0.001(2)	−0.008(3)
F(1)	4e	0.1746(4)	0.5490(2)	0.4621(2)	0.079(3)	0.041(2)	0.057(2)	−0.007(2)	−0.037(2)	0.007(2)
F(2)	4e	0.1229(4)	0.3734(2)	0.4722(2)	0.077(3)	0.047(2)	0.066(2)	−0.018(2)	−0.024(2)	−0.008(2)
F(3)	4e	0.2862(4)	0.2728(2)	0.5751(2)	0.071(3)	0.030(2)	0.066(2)	0.001(2)	0.021(2)	0.005(2)
F(4)	4e	0.5047(4)	0.3511(2)	0.6680(2)	0.068(2)	0.059(3)	0.058(2)	0.018(2)	−0.008(2)	0.024(2)
F(5)	4e	0.5560(4)	0.5272(2)	0.6593(2)	0.047(2)	0.062(2)	0.047(2)	−0.002(2)	−0.014(2)	0.001(2)
C(21)	4e	0.1711(6)	0.5518(3)	0.8072(2)	0.026(3)	0.025(3)	0.024(3)	0.003(2)	0.002(2)	0.002(2)
C(22)	4e	0.0465(6)	0.6030(3)	0.8238(3)	0.035(3)	0.036(4)	0.034(3)	0.001(3)	0.003(3)	−0.005(3)
C(23)	4e	−0.0781(6)	0.6068(4)	0.7733(3)	0.024(3)	0.037(4)	0.055(4)	0.005(3)	0.000(3)	0.002(3)
C(24)	4e	−0.0821(6)	0.5605(4)	0.7077(3)	0.035(3)	0.052(4)	0.039(3)	−0.009(3)	−0.012(3)	0.011(3)
C(25)	4e	0.0406(6)	0.5095(4)	0.6905(3)	0.043(4)	0.058(4)	0.031(3)	−0.009(3)	−0.005(3)	−0.011(3)
C(26)	4e	0.1664(6)	0.5049(4)	0.7407(3)	0.036(3)	0.045(4)	0.024(3)	−0.004(3)	0.005(2)	−0.008(3)
C(31)	4e	0.4463(5)	0.6522(3)	0.8468(2)	0.025(3)	0.022(3)	0.022(3)	0.006(2)	0.001(2)	−0.001(2)
C(32)	4e	0.4279(5)	0.6917(3)	0.7771(3)	0.032(3)	0.032(3)	0.027(3)	−0.005(3)	−0.004(2)	0.000(3)
C(33)	4e	0.5147(6)	0.7641(4)	0.7607(3)	0.048(4)	0.045(4)	0.027(3)	−0.010(3)	−0.004(3)	0.010(3)
C(34)	4e	0.6216(6)	0.7983(4)	0.8130(3)	0.036(3)	0.033(4)	0.045(3)	−0.005(3)	0.002(3)	−0.001(3)
C(35)	4e	0.6401(7)	0.7601(4)	0.8821(3)	0.044(4)	0.036(4)	0.039(3)	−0.009(3)	−0.015(3)	−0.008(3)
C(36)	4e	0.5536(6)	0.6876(4)	0.9000(3)	0.043(3)	0.028(3)	0.028(3)	0.001(3)	−0.007(2)	−0.004(3)
C(41)	4e	0.4536(5)	0.4582(3)	0.8568(2)	0.027(3)	0.028(3)	0.018(3)	0.002(3)	−0.002(2)	0.002(2)
C(42)	4e	0.3965(6)	0.3740(4)	0.8697(3)	0.031(3)	0.034(3)	0.042(3)	−0.001(3)	0.008(3)	0.003(3)
C(43)	4e	0.4883(7)	0.2990(4)	0.8690(3)	0.055(4)	0.030(3)	0.048(4)	0.002(3)	0.005(3)	0.003(3)
C(44)	4e	0.6385(6)	0.3082(4)	0.8558(3)	0.040(3)	0.039(3)	0.039(3)	0.021(3)	−0.001(3)	−0.001(3)
C(45)	4e	0.6958(6)	0.3920(4)	0.8426(3)	0.031(3)	0.039(3)	0.035(3)	0.009(3)	0.000(3)	−0.007(3)
C(46)	4e	0.6052(6)	0.4671(4)	0.8424(3)	0.031(3)	0.032(3)	0.026(3)	0.005(3)	0.004(2)	0.001(2)

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