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Tetrazolyl and tetrazolylidene complexes of gold: a synthetic and structural study

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Crystal data, data collection and structure refinement for compound **5.**

Compound	**5**
Empirical formula	$C_{29}H_{27}AuF_3N_4O_3PS$
M_r	796.54
Temp. (K)	100(2) K
Wavelength (Å)	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
a (Å)	22.829(2)
b (Å)	12.0611(12)
c (Å)	23.755(2)
α (°)	90
β (°)	112.286(2)
γ (°)	90
Volume (Å^3)	6052.3(10)
Z	8
d_{calcd} (g/cm^3)	1.748
Absorption coefficient (μ, mm^{-1})	5.039
F(000)	3120
Crystal size (mm^3)	0.20 x 0.10 x 0.10
No. of reflections collected	31715
No. independent reflections	11034 [R(int) = 0.0454]
Data/restraints/parameters	11034 / 19 / 253
Goof on F^2	1.035
$R1$ [I≥2σ(I)]	R_1 = 0.1114
$wR2$ [a]	wR_2 = 0.2840
Largest diff. peak and hole (e.A^{-3})	3.542 and -4.652
Weighing scheme	a = 0.1046 / b = 276.2091

[a] $wR2= \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; $w = 1/[\sigma^2(F_o^2)+(ap)^2+bp]$; $p = (F_o^2+ 2F_c^2)/3$.

Due to the low quality of the crystals only gold, sulfur and phosphorous atoms were refined anisotropically. Five- and six-membered rings were restrained to be ideal penta- or hexagons respectively. This structure is only intended to give an idea of the connectivity of the compound. Any more detailed discussion of the geometric features is subject to extreme caution.