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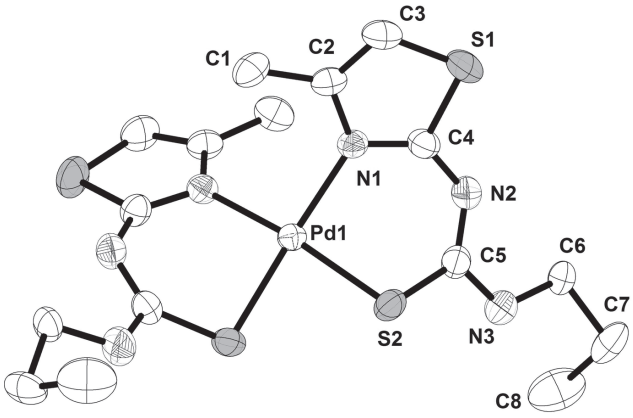
Crystal structure of bis(2-((allylcarbamothioyl) imino)-4-methylthiazol-3-ido-κ²*N*,*S*)palladium(II), $C_{16}H_{20}N_6PdS_4$



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Abstract

$C_{16}H_{20}N_6PdS_4$, monoclinic, *C*2/*c* (no. 15), $a = 13.2801(8)$ Å, $b = 18.5771(8)$ Å, $c = 10.2577(5)$ Å, $\beta = 121.906(2)°$, $V = 2148.29(19)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0300$, $wR_{ref}(F^2) = 0.0721$, $T = 293$ K.

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The crystal structure is shown in the figure. The disorder in the ally moiety is omitted for clarity. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of $K_2[PtCl_4]$ (0.001 mol in distilled water), 1-allyl-3-(4-methylthiazol-2(3*H*)-ylidene)thiourea (0.002 mol in ethanol), was heated and stirred for 3 h. Then the solution was cooled to room temperature, filtered and washed. The resulting compound crystallized and was dried in a final step.

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Table 1: Data collection and handling.

Crystal:	Block, colorless
Size:	0.34 × 0.27 × 0.11 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	1.27 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
$2\theta_{max}$, completeness:	33.2°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	49183, 4099, 0.033
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3838
$N(param)_{refined}$:	159
Programs:	Bruker programs [1], SHELX [2]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Pd1	0.5000	0.31839(2)	0.7500	0.03215(5)
S1	0.38995(6)	0.19783(3)	0.30890(7)	0.05980(14)
S2	0.48422(4)	0.40860(2)	0.58973(6)	0.04436(10)
N1	0.44970(12)	0.24457(7)	0.57476(16)	0.0367(3)
N2	0.54461(16)	0.30251(9)	0.45503(19)	0.0464(3)
N3	0.6317(2)	0.41207(11)	0.4937(2)	0.0566(4)
C1	0.33325(18)	0.16658(12)	0.6500(3)	0.0508(4)
H1A	0.2670	0.1342	0.5999	0.076*
H1B	0.3113	0.2083	0.6845	0.076*
H1C	0.3987	0.1429	0.7365	0.076*
C2	0.36847(16)	0.18883(9)	0.5399(2)	0.0413(3)
C3	0.3282(2)	0.15846(11)	0.4019(3)	0.0537(5)
H3A	0.2738	0.1209	0.3619	0.064*
C4	0.47004(16)	0.25548(10)	0.4628(2)	0.0413(3)
C5	0.55713(16)	0.36801(10)	0.5067(2)	0.0418(3)
C6[a]	0.6960(14)	0.3851(9)	0.4193(18)	0.0460(18)
H6A[a]	0.6418	0.3612	0.3229	0.055*
H6B[a]	0.7582	0.3516	0.4861	0.055*
C7[a]	0.7481(9)	0.4521(4)	0.3926(13)	0.060(2)
H7A[a]	0.695(8)	0.484(5)	0.325(10)	0.072*
C8[a]	0.8575(9)	0.4727(6)	0.5772(16)	0.098(4)
H8A[a]	0.8688	0.4439	0.6581	0.118*
H8B[a]	0.9056	0.5127	0.5966	0.118*
C8X[b]	0.8542(8)	0.4600(4)	0.4428(15)	0.146(4)
H8XA[b]	0.8296	0.4772	0.3452	0.175*
H8XB[b]	0.9308	0.4694	0.5244	0.175*
C7X[b]	0.7982(7)	0.4313(5)	0.4601(10)	0.099(2)
H7XA[b]	0.8412	0.4200	0.5642	0.118*
C6X[b]	0.6822(11)	0.3987(7)	0.4007(14)	0.083(3)
H6XA[b]	0.6282	0.4170	0.2981	0.099*
H6XB[b]	0.6890	0.3471	0.3928	0.099*
H1N3	0.627(3)	0.4521(16)	0.515(3)	0.061(8)*

Occupancies: [a]0.345(9), [b]0.655(9).

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Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Discussion

In recent years, thioureas and thiourea derivatives have gained unprecedented fame in medical and non-medical applications. Their characteristics as versatile ligands allow them to form stable complexes [3, 4]. Many reports have documented the ability of thioureas to coordinate transition metals such as Ni(II), Cu(II), Co(II), Fe(III) [5, 6], Zn(II) [7], Pd(II) [8], and Ru(II) [9]. Their diversified use has received attention by various scientific communities including medical [10], analytical chemistry and metallurgy fields [11]. To name a few, they have been used in antiviral [12, 13], anti-HIV [14], antimicrobial, antitumor, anti-inflammatory [15], and insecticidal substances [16].

In the title Pd(II) complex two ligands act as bidentate N, S-donor chelates [17]. Pd(II) is four-coordinated (PtN_2S_2) in a square planar geometry. The Pd1—N1 bond distance is 2.0710(14) Å, the bond angles of N1—Pd1—N1A, N1—Pd1—S2, N1A—Pd1—S2A are 97.06(8), 89.79(4), 89.79(4), respectively. The Pd1—S2 bond distance is 2.2783(4), the bond angles of S2—Pd1—S2A, S2—Pd1—S2A are 85.38(7)°, 85.30(3)°, respectively. Geometric parameters of the organic ligand is within the expectations [18].

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