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trans-Bis(pyridine-κ*N*)bis(thiocyanato-κ*S*)-palladium(II)

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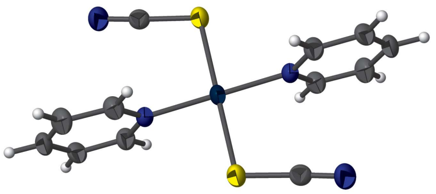
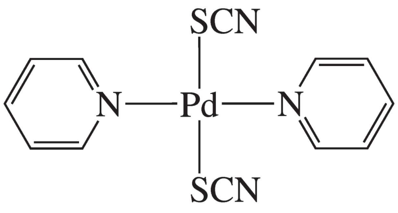
In the title complex, $[Pd(SCN)_2(C_5H_4N)_2]$, the Pd^{II} ion has a *trans*-N_2S_2 square-planar coordination sphere defined by two pyridine ligands and two S-bound SCN^- anions. The Pd^{II} cation lies on an inversion centre, thus the asymmetric unit contains one half of the complex, the PdN_2S_2 moiety is exactly planar and the two pyridine rings are parallel. In the crystal, the complex molecules are stacked in columns along the *a*-axis direction.

3D view



Chemical scheme



Structure description

With reference to the title complex, $[Pd(SCN)_2(py)_2]$, the crystal structures of related *trans*-dipyridine-Pd^{II} complexes $[PdX_2(py)_2]$ (X = Cl, Br, I; py = pyridine) have been determined previously. The chlorido complex $[PdCl_2(py)_2]$ has three polymorphic forms, crystallizing in space groups $C2/c$ (Viossat *et al.*, 1993), $P\overline{1}$ (Liao & Lee, 2006) and $P2_1/n$ (Lee & Liao, 2008). The bromido complex $[PdBr_2(py)_2]$ has one polymorph in space group $P\overline{1}$ (Ha, 2016), and the iodido complex $[PdI_2(py)_2]$ has two polymorphs in space groups $C2/m$ (Lord *et al.*, 2001; Grushin & Marshall, 2009) and $C2/c$ (Grushin & Marshall, 2009).

In the title complex, the central Pd^{II} ion has a *trans*-N_2S_2 square-planar coordination geometry defined by two N atoms from two pyridine ligands and two S atoms derived from two SCN^- anions (Fig. 1). The complex crystallizes in the triclinic space group $P\overline{1}$ and the asymmetric unit contains one half of the complex molecule: the Pd atom is located on an inversion centre. Therefore, the PdN_2S_2 moiety is exactly planar and the two pyridine rings are parallel. The dihedral angle between the PdS_2N_2 plane and the pyridine ring [maximum deviation = 0.008 (1) Å] is 89.32 (5)°. The thiocyanato ligand is almost linear displaying a S—C—N bond angle of 177.9 (2)°, and the S atoms are coordinated to the Pd^{II} cation with the nearly tetrahedral Pd—S—C bond angle of 104.89 (7)°, characteristic of an S-bonded conformation (Ha, 2013).

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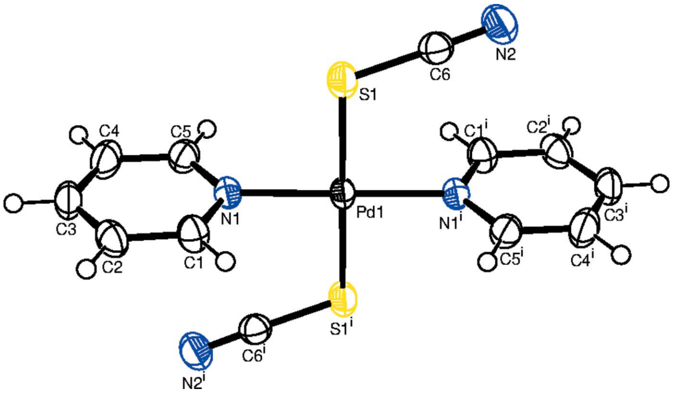

Figure 1
The molecular structure of the title complex showing the atom labelling and with displacement ellipsoids drawn at the 50% probability level for non-H atoms. [Symmetry code: (i) $2 - x$, $2 - y$, $-z$.]

In the crystal structure (Fig. 2), the complex molecules are stacked in columns along [100] with $d(\mathrm{Pd}\cdots\mathrm{Pd})$ = 5.2931 (4) Å, corresponding to the length of the *a* axis. In the columns, intermolecular π–π interactions between adjacent pyridine rings are present. For *Cg*1 (the centroid of ring N1–C5) and *Cg*1^{i} [symmetry code: (i) $2 - x$, $2 - y$, $1 - z$], the centroid–centroid distance is 5.116 (1) Å, the planes are parallel and shifted by 4.11 Å.

Synthesis and crystallization

A reaction mixture of $K_2Pd(SCN)_4$ (0.1835 g, 0.440 mmol) and pyridine (2 ml) in ethyl acetate (30 ml) was stirred for 1 h at room temperature. After evaporation of the solvent, the residue was washed with water and acetone, and dried at 323 K, to give a yellow powder (0.1141 g). Yellow crystals suitable for X-ray analysis were obtained by slow evaporation from a CH_3CN solution at room temperature.

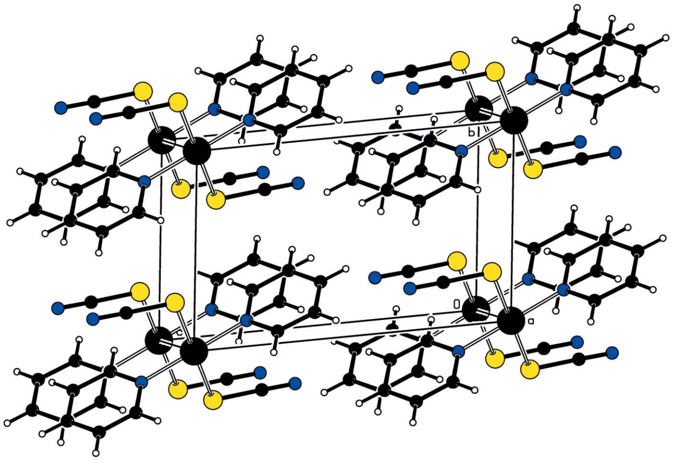

Figure 2
The packing in the crystal of the title complex, viewed approximately along the *a* axis.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Pd(SCN)_2(C_5H_5N)_2]$
M_r	380.76
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	223
a, *b*, *c* (Å)	5.2931 (4), 6.8101 (6), 10.5213 (9)
α, β, γ (°)	96.994 (3), 98.754 (3), 107.293 (3)
V (Å^3)	352.24 (5)
Z	1
Radiation type	Mo *K*α
μ (mm^{-1})	1.60
Crystal size (mm)	0.19 × 0.15 × 0.09
Data collection	
Diffractometer	Bruker PHOTON 100 CMOS detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
$T_{\min}$, $T_{\max}$	0.685, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8943, 1397, 1383
R_{int}	0.019
$(\sin \theta/\lambda)_{\max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.015, 0.040, 1.10
No. of reflections	1397
No. of parameters	88
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å^{-3})	0.38, −0.35

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

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Funding information

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full crystallographic data

IUCrData (2018). **3**, x181406 [https://doi.org/10.1107/S2414314618014062]

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trans-Bis(pyridine-*κN*)bis(thiocyanato-*κS*)palladium(II)

Crystal data

$[Pd(SCN)_2(C_5H_5N)_2]$
$M_r = 380.76$
Triclinic, $P\bar{1}$
$a = 5.2931\ (4)$ Å
$b = 6.8101\ (6)$ Å
$c = 10.5213\ (9)$ Å
$\alpha = 96.994\ (3)°$
$\beta = 98.754\ (3)°$
$\gamma = 107.293\ (3)°$
$V = 352.24\ (5)$ Å^3
$Z = 1$
$F(000) = 188$
$D_x = 1.795$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8652 reflections
$\theta = 3.2–28.4°$
$\mu = 1.60$ mm^{-1}
$T = 223$ K
Block, yellow
0.19 × 0.15 × 0.09 mm

Data collection

Bruker PHOTON 100 CMOS detector diffractometer
Radiation source: sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
$T_{min} = 0.685$, $T_{max} = 0.745$
8943 measured reflections
1397 independent reflections
1383 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 26.1°$, $\theta_{min} = 3.2°$
$h = -6 \rightarrow 6$
$k = -8 \rightarrow 8$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.015$
$wR(F^2) = 0.040$
$S = 1.10$
1397 reflections
88 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0212P)^2 + 0.1471P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Hydrogen atoms were positioned geometrically and allowed to ride on their respective parent atoms: C—H = 0.94 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
Pd1	1.0000	1.0000	0.0000	0.02642 (7)
S1	0.61794 (10)	0.72043 (8)	−0.10502 (5)	0.03935 (12)
N1	0.9587 (3)	0.8677 (2)	0.16016 (14)	0.0278 (3)
N2	0.5443 (4)	0.7580 (3)	−0.37129 (17)	0.0466 (4)
C1	0.8137 (4)	0.9263 (3)	0.24251 (18)	0.0347 (4)
H1	0.7276	1.0240	0.2219	0.042*
C2	0.7869 (4)	0.8482 (3)	0.35602 (18)	0.0372 (4)
H2	0.6825	0.8908	0.4116	0.045*
C3	0.9145 (4)	0.7075 (3)	0.38689 (19)	0.0401 (4)
H3	0.9014	0.6537	0.4647	0.048*
C4	1.0622 (4)	0.6460 (3)	0.3025 (2)	0.0427 (5)
H4	1.1507	0.5492	0.3219	0.051*
C5	1.0794 (4)	0.7273 (3)	0.18928 (18)	0.0344 (4)
H5	1.1782	0.6832	0.1312	0.041*
C6	0.5790 (4)	0.7453 (3)	−0.26277 (18)	0.0335 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.03078 (11)	0.03002 (11)	0.02182 (10)	0.01194 (8)	0.00732 (7)	0.00903 (7)
S1	0.0429 (3)	0.0392 (3)	0.0295 (2)	0.0031 (2)	0.0042 (2)	0.01138 (19)
N1	0.0295 (7)	0.0306 (7)	0.0237 (7)	0.0094 (6)	0.0051 (6)	0.0072 (6)
N2	0.0519 (10)	0.0501 (10)	0.0309 (9)	0.0071 (8)	0.0066 (8)	0.0070 (8)
C1	0.0367 (9)	0.0420 (10)	0.0311 (9)	0.0175 (8)	0.0104 (7)	0.0104 (8)
C2	0.0375 (10)	0.0444 (11)	0.0278 (9)	0.0079 (8)	0.0119 (8)	0.0064 (8)
C3	0.0459 (11)	0.0409 (10)	0.0289 (9)	0.0043 (9)	0.0058 (8)	0.0152 (8)
C4	0.0514 (12)	0.0395 (10)	0.0432 (11)	0.0191 (9)	0.0087 (9)	0.0191 (9)
C5	0.0394 (10)	0.0332 (9)	0.0350 (10)	0.0149 (8)	0.0110 (8)	0.0097 (7)
C6	0.0336 (9)	0.0302 (9)	0.0346 (10)	0.0080 (7)	0.0067 (7)	0.0040 (7)

Geometric parameters (Å, º)

Pd1—N1$^{\rm i}$	2.0159 (14)	C1—H1	0.9400
Pd1—N1	2.0159 (14)	C2—C3	1.369 (3)
Pd1—S1$^{\rm i}$	2.3353 (5)	C2—H2	0.9400
Pd1—S1	2.3353 (5)	C3—C4	1.375 (3)
S1—C6	1.6766 (19)	C3—H3	0.9400
N1—C5	1.338 (2)	C4—C5	1.377 (3)
N1—C1	1.341 (2)	C4—H4	0.9400
N2—C6	1.147 (3)	C5—H5	0.9400
C1—C2	1.375 (3)		
N1$^{\rm i}$—Pd1—N1	180.0	C3—C2—C1	118.98 (18)
N1$^{\rm i}$—Pd1—S1$^{\rm i}$	85.36 (4)	C3—C2—H2	120.5
N1—Pd1—S1$^{\rm i}$	94.64 (4)	C1—C2—H2	120.5

N1^{i}—Pd1—S1	94.64 (4)	C2—C3—C4	119.03 (17)
N1—Pd1—S1	85.36 (4)	C2—C3—H3	120.5
S1^{i}—Pd1—S1	180.0	C4—C3—H3	120.5
C6—S1—Pd1	104.89 (7)	C3—C4—C5	119.52 (18)
C5—N1—C1	118.73 (15)	C3—C4—H4	120.2
C5—N1—Pd1	121.84 (12)	C5—C4—H4	120.2
C1—N1—Pd1	119.39 (12)	N1—C5—C4	121.49 (17)
N1—C1—C2	122.23 (17)	N1—C5—H5	119.3
N1—C1—H1	118.9	C4—C5—H5	119.3
C2—C1—H1	118.9	N2—C6—S1	177.86 (18)
C5—N1—C1—C2	0.5 (3)	C2—C3—C4—C5	0.2 (3)
Pd1—N1—C1—C2	−177.35 (14)	C1—N1—C5—C4	−1.3 (3)
N1—C1—C2—C3	0.7 (3)	Pd1—N1—C5—C4	176.46 (15)
C1—C2—C3—C4	−1.0 (3)	C3—C4—C5—N1	1.0 (3)

Symmetry code: (i) $-x+2, -y+2, -z$.