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Crystal structure of 1,1′-(1,4-phenylenebis(methylene))bis(pyridin-1-ium) bis(1,2-dicyanoethene-1,2-dithiolato-κ^2*S*,*S*) platinum(II), $C_{26}H_{18}N_6PtS_4$

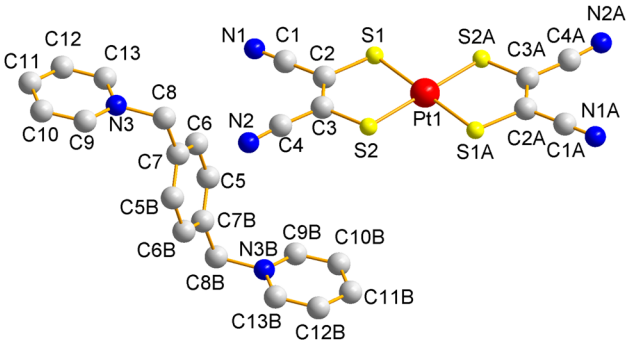

Table 1: Data collection and handling.

Crystal:	Red block
Size:	0.22 × 0.20 × 0.18 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	5.62 mm^{-1}
Diffractometer, scan mode:	*φ* and *ω*
θ_{max}, completeness:	28.3°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4773, 3258, 0.116
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3048
$N(param)_{refined}$:	169
Programs:	SHELX [1], Bruker [2]

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Abstract

$C_{26}H_{18}N_6PtS_4$, triclinic, $P\bar{1}$ (no. 2), a = 8.2661(5) Å, b = 9.1519(6) Å, c = 9.4673(6) Å, α = 70.473(1)°, β = 80.770(1)°, γ = 83.340(1)°, V = 664.77(7) Å^3, Z = 1, $R_{gt}(F)$ = 0.0477, $wR_{ref}(F^2)$ = 0.1168, T = 296(2) K.

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The salt-type title structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

All reagents and chemicals were purchased from commercial sources and used without further purification. The starting materials disodium maleonitriledithiolate and 1,4-bis(methylpyridinium benzene bromide were synthesized following the literature procedures [3, 4]. An aqueous solution (10 mL) of 1,4-bis(methylpyridinium benzene bromide (0.084 g, 0.2 mmol) was added slowly to an aqueous solution (20 mL) of disodium maleonitriledithiolate (0.074 g, 0.4 mmol) and K_2PtCl_4 (0.166 g, 0.4 mmol), and the mixture was stirred at room temperature for several minutes. A red precipitate which formed, was filtered off, washed by water and dried under vacuum. The precipitate was solved in DMF with ether diffusion to yield red crystals.

Experimental details

Absorption corrections were applied by using multi-scan program. The structure was refined based on F^2 with the SHELXL software package. Hydrogen atoms attached to C of the title complex located in difference electron density maps, and treated as riding atoms. The U_{iso} values of the hydrogen atoms were set to 1.2U_{eq} (C).

Comment

Coordination compounds have always been the focus of research because of their fascinating structures and great potential in diversified applications, such as magnetic

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2393 (9)	0.4945 (8)	0.5363 (8)	0.0536 (15)
C2	0.1419 (8)	0.4698 (8)	0.6811 (8)	0.0488 (14)
C3	0.0392 (8)	0.3521 (8)	0.7402 (8)	0.0476 (14)
C4	0.0248 (9)	0.2467 (9)	0.6605 (9)	0.0553 (16)
C5	0.6302 (9)	0.0678 (9)	0.5220 (10)	0.0618 (18)
H5	0.7183 (9)	0.1145 (9)	0.5351 (10)	0.074 (2)*
C6	0.5153 (10)	0.1570 (9)	0.4324 (10)	0.0618 (18)
H6	0.5253 (10)	0.2633 (9)	0.3878 (10)	0.074 (2)*
C7	0.3836 (8)	0.0886 (8)	0.4080 (8)	0.0488 (14)
C8	0.2611 (9)	0.1831 (10)	0.3085 (9)	0.0601 (18)
H8a	0.2516 (9)	0.2888 (10)	0.3113 (9)	0.072 (2)*
H8b	0.1545 (9)	0.1406 (10)	0.3459 (9)	0.072 (2)*
C9	0.2415 (10)	0.0913 (9)	0.0954 (10)	0.0634 (19)
H9	0.1604 (10)	0.0282 (9)	0.1576 (10)	0.076 (2)*
C10	0.2889 (14)	0.0879 (12)	−0.0473 (13)	0.084 (3)
H10	0.2443 (14)	0.0189 (12)	−0.0812 (13)	0.100 (3)*
C11	0.4016 (13)	0.1853 (14)	−0.1413 (11)	0.088 (3)
H11	0.4300 (13)	0.1881 (14)	−0.2412 (11)	0.106 (4)*
C12	0.4722 (13)	0.2786(14)	−0.0860(13)	0.092 (4)
H12	0.5537 (13)	0.3421 (14)	−0.1467 (13)	0.111 (4)*
C13	0.4234 (11)	0.2788 (10)	0.0573(11)	0.071(2)
H13	0.4690 (11)	0.3454 (10)	0.0935 (11)	0.085 (3)*
N1	0.3180 (9)	0.5159 (9)	0.4227 (8)	0.0709 (18)
N2	0.0123 (9)	0.1550 (9)	0.6054 (9)	0.0709 (19)
N3	0.3105 (7)	0.1845 (7)	0.1474 (7)	0.0507 (13)
Pt1	0.0	0.5	1.0	0.04262 (14)
S1	0.1667 (2)	0.5965 (2)	0.7778 (2)	0.0528 (4)
S2	−0.0818 (2)	0.3185 (2)	0.9135 (2)	0.0549 (4)

materials, luminescence, catalysis, gas adsorption and separation, and so on [5–10]. Continuous attention has been paid to the compounds with the maleonitriledithiolate (mnt) ligand owing to their special structures and diversity in physical and chemical properties. The ligand possesses a planar conjugate structures and contains N & S atoms, so it is easy to form accumulation of hydrogen bonds. As can be seen from previous reports [11–15], different counter-cations could induce versatile anion stack modes and bis(maleonitriledithiolate) complexes exhibit various weak interactions and a diversity of magnetic changes. Herein, we choose 1,4-bis(methylpyridinium benzene) as organic divalent cation [1,4–BMPB]$^{2+}$, to generate new platinum(II) complex.

X-ray crystallography analyses reveal that the title complex shows 3D framework linked through extensive hydrogen bonding interactions. The asymmetric units comprises one half of a $[Pt(mnt)_2]^{2-}$ anion and one half of 1,4-bis(methylpyridinium benzene) dication. Pt(II) ion is coordinated by four sulfur atoms, and exhibits a square-planar coordination geometry. The Pt–S distances as well as the S–Pt–S angle are normal, which are comparable to the reported $[Pt(mnt)_2]^{2-}$ complex [16] and the title structure is isomorphous to the corresponding Ni(II) salt [14]. The anions and cations are formed segregated columns. The C–H···N interactions are observed in complex [17]. A supramolecular network structure is thus constructed through hydrogen bonding interactions.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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