trans-Bis(4-aminopyridine-κN)bis(quinoxaline-2,3-dithiolato-κ²S,S')platinum(IV) dimethyl sulfoxide monosolvate

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In the structure of the title solvated complex, [Pt(C₈H₄N₂S₂)(C₅H₆N₂)₂] C₃H₄OS or trans-[Pt(4-ap)₂(qdt)₂] dmso (4-ap = 4-aminopyridyl, C₅H₆N₂; qdt = quinoxaline-2,3-dithiolate, C₈H₄N₂S₂; dmso = dimethyl sulfoxide, C₂H₆OS) the centrosymmetric complex exhibits Pt—S distances in agreement with other PtIV—S bond lengths found in platinum(IV) dithiolene complexes. The qdt ligands have intermolecular interactions with an amine hydrogen atom on a 4-ap ligand (hydrogen bonding) and have sandwich π–π interactions with a neighboring qdt ligand.

Structure description

The title trans-[Pt(4-ap)₂(qdt)₂] ((4-ap = 4-aminopyridyl; qdt = quinoxaline-2,3-dithiolate) complex is located about an inversion center and has the central PtIV atom in a pseudo-octahedral N₂S₄ coordination environment (Fig. 1). In contrast to the shorter PtII—S distances in salts of [Pt(mnt)₂]²⁻ (mnt = maleonitriledithiolate), such as 2.295 (2) and 2.2958 (19) Å with the tetraphenylphosphine cation (Begum et al., 2014) or 2.290 (2) and 2.282 (2) Å with the tetrabutylammonium cation (Güntner et al., 1989), the PtIV—S distances of the title coordination compound are 2.3514 (11) Å (Pt₁—S₁) and 2.3495 (11) Å (Pt₁—S₂). These distances are similar to those in other platinum(IV) complexes containing bis(dithiolene) ligands and either trans-bis(NH₃) co-ligands, with Pt—S distances of 2.3434 (8) and 2.3461 (7) Å (Siddiqui et al., 2020), or trans-bis(PMe₃) co-ligands, with a Pt—S distance of 2.3619 (8) Å (Chandrasekaran et al., 2014). The Pt1—N1 distance in the title complex is 2.063 (4) Å, which is similar to the Pt—N distance of 2.055 (2) Å in the aforementioned trans-[Pt(NH₃)₂(mnt)₂] complex (Siddiqui et al., 2020).
The chelating qdt ligands of this platinum(IV) complex are slightly canted relative to the platinum-sulfur atoms, with a 15.59 (11)° angle between the plane of all the non-H atoms of the qdt ligand versus the plane containing Pt, S1, S2, S1 (1 – x, 1 – y, –z) and S2 (1 – x, 1 – y, –z). This tilt enables sandwich packing between intermolecular qdt ligands with a distance between centroids of the two qdt rings of 3.610 Å (Fig. 2), within the range of π–π interactions (Sinnokrot et al., 2002).

The basicity of the nitrogen atom on the coordinating qdt ligand (Cummings & Eisenberg, 1995b) makes it suitable for hydrogen bonding. This is observed between the amine hydrogen H4A and the N3 (x, y + 1, z) atom on a neighboring qdt ligand, with a distance of 2.23 Å (Table 1, Fig. 2). N—H···O hydrogen bonding is observed between the complex and the O atom of the dmso solvate molecule.

Synthesis and crystallization

An orange solution of the anionic qdt ligand was prepared by combining 9.3 mg of 2,3-quinoxalinedithiol (Cummings & Eisenberg, 1995a) and 7.7 mg of NaHCO3 with 25 ml of water and heating at 333 K for 5 h. Upon cooling to room temperature, the orange solution was added, via cannula, to a Schlenk flask containing 34.3 mg of [Pt(4-ap)4](BF4)2, prepared in a similar manner to [Pt(pyz)4](BF4)2 (Derry et al., 2008), and 7.9 mg of NaHCO3. The solution was stirred for 7 d with the exclusion of light. The resulting orange–brown solid was collected via vacuum filtration in air and washed with 3 × 10 ml of water and 15 ml of diethyl ether to give 7.4 mg (28% for [Pt(4-ap)4(qdt)])]. Oxidation of platinum(II) to platinum(IV) likely occurred upon prolonged air exposure of the

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**Table 1**

Hydrogen-bond geometry (Å, °).

|  | D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|---|
| N4—H4A···N3 | 0.87 | 2.30 | 3.085 (7) | 151 |
| N4—H4B···O1a | 0.87 | 2.28 | 3.045 (11) | 148 |

Symmetry codes: (i) x, y + 1, z; (ii) x – 1, y, z.

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**Table 2**

Experimental details.

| Crystal data | Chemical formula | [Pt(C8H4N2S2)2(C5H6N2)2]− C2H6OS |
|---|---|---|
| M1 | Crystal system, space group | Triclinic, P̅T |
| | Temperature (K) | 200 |
| | a, b, c (Å) | 7.7410 (18), 9.8690 (2), 10.47021 (18) |
| | α, β, γ (°) | 99.6963 (16), 102.9798 (17), 100.9394 (19) |
| V (Å³) | 746.43 (3) |
| Z | 1 |
| Radiation type | Cu Kα |
| μ (mm⁻¹) | 12.39 |
| Crystal size (mm) | 0.03 × 0.02 × 0.01 |

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**Figure 1**

The molecular structure of the title complex drawn with displacement ellipsoids at the 50% probability level. Non-labeled atoms are generated by symmetry operation –x + 1, –y + 1, –z. The disordered dmso solvate molecule is shown with only one orientation.

**Figure 2**

The packing of the complexes showing the hydrogen bonding between the H4A amine hydrogen atom and the N3 (x, y + 1, z) atom on a neighboring qdt ligand as well as the sandwich orientation between adjacent qdt ligands and the distance (Å) between centroids of two qdt rings. Displacement ellipsoids are drawn at the 50% probability level; the dmso solvate is omitted for clarity.
compound in solution (Geiger et al., 2001; Siddiqui et al., 2020).

Light-yellow crystals of the title compound were grown by slow diffusion of water into a dmso solution of the platinum complex.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The dmso solvent molecule is disordered about an inversion center and shows half occupancy.

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full crystallographic data

*IUCrData* (2022). 7, x220101  [https://doi.org/10.1107/S2414314622001018]

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**Crystal data**

\[
\text{[Pt(C}_8\text{H}_4\text{N}_2\text{S}_2)\text{](C}_5\text{H}_6\text{N}_2)}\cdot\text{C}_2\text{H}_6\text{OS}
\]

\[M_r = 845.96\]

Triclinic, \(P\)

\[a = 7.74108 \pm 18 \text{ Å} \]

\[b = 9.8690 \pm 2 \text{ Å} \]

\[c = 10.47021 \pm 18 \text{ Å} \]

\[α = 99.6963 \pm 16° \]

\[β = 102.9798 \pm 17° \]

\[γ = 100.9394 \pm 19° \]

\[V = 746.43 \pm 3 \text{ Å}^3 \]

\[Z = 1\]

\[F(000) = 416\]

\[D_r = 1.882 \text{ Mg m}^{-3}\]

Cu \(Kα\) radiation, \(λ = 1.54184 \text{ Å}\)

Cell parameters from 10134 reflections

\[θ = 4.7–77.2°\]

\[μ = 12.39 \text{ mm}^{-1}\]

\[T = 200 \text{ K}\]

Plate, clear light yellow

\[0.03 \times 0.02 \times 0.01 \text{ mm}\]

**Data collection**

XtaLAB Synergy, Dualflex, HyPix diffractometer

Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source

Mirror monochromator

Detector resolution: 10.0000 pixels mm\(^{-1}\)

\(ω\) scans

Absorption correction: multi-scan

(CrysAlisPro; Rigaku OD, 2019)

\[T_{\text{min}} = 0.671, T_{\text{max}} = 1.000\]

15557 measured reflections

3130 independent reflections

3097 reflections with \(I > 2σ(I)\)

\[R_{\text{int}} = 0.046\]

\[θ_{\text{max}} = 77.7°, θ_{\text{min}} = 4.4°\]

\[h = -9→9\]

\[k = -12→12\]

\[l = -11→13\]

**Refinement**

Refinement on \(F^2\)

Least-squares matrix: full

\[R(F^2 > 2σ(F^2)) = 0.033\]

\[wR(F^2) = 0.083\]

\[S = 1.11\]

3130 reflections

218 parameters

0 restraints

Hydrogen site location: mixed

H-atom parameters constrained

\[w = 1/\left[σ^2(F_o^2) + (0.0335P)^2 + 2.9739P\right]\]

where \(P = (F_o^2 + 2F_c^2)/3\)

\((Δ/σ)_{\text{max}} < 0.001\)

\[Δρ_{\text{max}} = 1.33 \text{ e Å}^{-3}\]

\[Δρ_{\text{min}} = -1.21 \text{ e Å}^{-3}\]

Extinction correction: SHELXL2018/3 (Sheldrick 2015),

\[Fc'' = kFc[1 + 0.001xFc^2\sin(2θ)]^{1/4}\]

Extinction coefficient: 0.00059 (15)
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.

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

|     | x     | y     | z     | Uiso*/Ueq | Occ. (<1) |
|-----|-------|-------|-------|-----------|-----------|
| Pt1 | 0.50  | 0.50  | 0.00  | 0.0264    | (11)      |
| S1  | 0.81  | 0.57  | 0.10  | 0.0312    | (2)       |
| S2  | 0.47  | 0.38  | 0.17  | 0.0317    | (2)       |
| N1  | 0.47  | 0.68  | 0.11  | 0.0302    | (8)       |
| N2  | 1.01  | 0.47  | 0.28  | 0.0340    | (9)       |
| N3  | 0.72  | 0.29  | 0.32  | 0.0326    | (9)       |
| N4  | 0.40  | 1.04  | 0.34  | 0.0487    | (12)      |
| H4A | 0.46  | 1.21  | 0.31  | 0.058    |           |
| H4B | 0.29  | 1.05  | 0.33  | 0.058    |           |
| C1  | 0.85  | 0.46  | 0.21  | 0.0286    | (9)       |
| C2  | 1.04  | 0.39  | 0.37  | 0.0344    | (10)      |
| C3  | 1.23  | 0.39  | 0.44  | 0.0429    | (12)      |
| H3  | 1.32  | 0.45  | 0.43  | 0.051    |           |
| C4  | 1.25  | 0.29  | 0.52  | 0.0485    | (14)      |
| H4  | 1.36  | 0.30  | 0.57  | 0.058    |           |
| C5  | 1.09  | 0.20  | 0.54  | 0.0475    | (14)      |
| H5  | 1.12  | 0.14  | 0.60  | 0.057    |           |
| C6  | 0.92  | 0.20  | 0.47  | 0.0441    | (13)      |
| H6  | 0.88  | 0.13  | 0.49  | 0.053    |           |
| C7  | 0.89  | 0.29  | 0.39  | 0.0344    | (10)      |
| C8  | 0.69  | 0.38  | 0.24  | 0.0297    | (9)       |
| C9  | 0.58  | 0.80  | 0.12  | 0.0392    | (12)      |
| H9  | 0.67  | 0.81  | 0.08  | 0.047    |           |
| C10 | 0.56  | 0.93  | 0.20  | 0.0419    | (12)      |
| H10 | 0.64  | 1.01  | 0.20  | 0.050    |           |
| C11 | 0.42  | 0.92  | 0.26  | 0.0377    | (11)      |
| C12 | 0.31  | 0.79  | 0.25  | 0.0408    | (12)      |
| H12 | 0.21  | 0.78  | 0.29  | 0.049    |           |
| C13 | 0.33  | 0.68  | 0.17  | 0.0344    | (10)      |
| H13 | 0.26  | 0.59  | 0.17  | 0.041    |           |
| S3  | 1.08  | 1.03  | 0.08  | 0.055    | (8)       |
| O1  | 1.00  | 0.99  | 0.19  | 0.058    |           |
| C1A | 1.00  | 0.89  | −0.05 | 0.072    | (5)       |
| H1AA| 1.06  | 0.82  | −0.04 | 0.108    | (5)       |
| H1AB| 1.03  | 0.92  | −0.13 | 0.108    | (5)       |
| H1AC| 0.88  | 0.86  | −0.07 | 0.108    | (5)       |
| C1B | 0.95  | 1.15  | 0.03  | 0.072    | (5)       |
| H1BA| 0.82  | 1.11  | 0.00  | 0.108    | (5)       |
| H1BB| 0.98  | 1.18  | −0.04 | 0.108    | (5)       |
**Atomic displacement parameters (Å²)**

|     | U₁₁     | U₂₂     | U₃₃     | U₁₂     | U₁₃     | U₂₃     |
|-----|---------|---------|---------|---------|---------|---------|
| Pt1 | 0.02549 (16) | 0.02164 (15) | 0.02864 (16) | 0.00156 (10) | 0.00498 (10) | 0.00351 (10) |
| S1  | 0.0253 (5)  | 0.0292 (5)  | 0.0350 (6)  | −0.0001 (4)  | 0.0036 (4)  | 0.0095 (4)  |
| S2  | 0.0294 (6)  | 0.0311 (6)  | 0.0341 (6)  | 0.0030 (4)  | 0.0081 (5)  | 0.0111 (5)  |
| N1  | 0.032 (2)   | 0.0230 (18) | 0.035 (2)   | 0.0056 (15) | 0.0114 (17) | 0.0015 (15) |
| N2  | 0.033 (2)   | 0.033 (2)   | 0.033 (2)   | 0.0061 (17) | 0.0046 (17) | 0.0048 (17) |
| N3  | 0.040 (2)   | 0.0248 (19) | 0.030 (2)   | 0.0051 (16) | 0.0079 (17) | 0.0045 (16) |
| N4  | 0.055 (3)   | 0.031 (2)   | 0.060 (3)   | 0.008 (2)   | 0.025 (3)   | 0.000 (2)   |
| C1  | 0.029 (2)   | 0.025 (2)   | 0.029 (2)   | 0.0064 (17) | 0.0039 (18) | 0.0018 (17) |
| C2  | 0.041 (3)   | 0.033 (2)   | 0.029 (2)   | 0.012 (2)   | 0.006 (2)   | 0.0035 (19) |
| C3  | 0.040 (3)   | 0.047 (3)   | 0.036 (3)   | 0.014 (2)   | 0.003 (2)   | 0.002 (2)   |
| C4  | 0.055 (4)   | 0.054 (3)   | 0.030 (3)   | 0.025 (3)   | −0.004 (2)  | 0.001 (2)   |
| C5  | 0.066 (4)   | 0.041 (3)   | 0.033 (3)   | 0.022 (3)   | −0.001 (3)  | 0.009 (2)   |
| C6  | 0.062 (4)   | 0.033 (3)   | 0.034 (3)   | 0.012 (2)   | 0.007 (3)   | 0.006 (2)   |
| C7  | 0.044 (3)   | 0.029 (2)   | 0.026 (2)   | 0.010 (2)   | 0.003 (2)   | 0.0031 (18) |
| C8  | 0.034 (2)   | 0.025 (2)   | 0.028 (2)   | 0.0053 (18) | 0.0069 (19) | 0.0029 (18) |
| C9  | 0.040 (3)   | 0.025 (2)   | 0.052 (3)   | 0.001 (2)   | 0.022 (2)   | 0.003 (2)   |
| C10 | 0.045 (3)   | 0.028 (2)   | 0.051 (3)   | 0.001 (2)   | 0.020 (3)   | 0.001 (2)   |
| C11 | 0.040 (3)   | 0.031 (2)   | 0.040 (3)   | 0.008 (2)   | 0.010 (2)   | 0.004 (2)   |
| C12 | 0.038 (3)   | 0.035 (3)   | 0.049 (3)   | 0.003 (2)   | 0.018 (2)   | 0.005 (2)   |
| C13 | 0.032 (2)   | 0.028 (2)   | 0.041 (3)   | 0.0019 (19) | 0.011 (2)   | 0.004 (2)   |
| S3  | 0.0454 (16) | 0.0553 (18) | 0.0601 (19) | −0.0016 (14) | 0.0131 (14) | 0.0125 (15) |
| O1  | 0.053 (5)   | 0.062 (6)   | 0.065 (6)   | 0.013 (4)   | 0.023 (4)   | 0.020 (5)   |
| C1A | 0.078 (13)  | 0.045 (9)   | 0.108 (16)  | 0.036 (8)   | 0.035 (11)  | 0.020 (9)   |
| C1B | 0.087 (13)  | 0.063 (11)  | 0.087 (12)  | 0.055 (10)  | 0.026 (10)  | 0.026 (9)   |

**Geometric parameters (Å, º)**

|     | C4—C5     | C9—C10    | C10—H10  |
|-----|------------|------------|-----------|
| Pt1—S1 | 2.3514 (11) | C4—C5     | 1.404 (10) |
| Pt1—S1' | 2.3514 (11) | C5—H5     | 0.9300    |
| Pt1—S2 | 2.3495 (11) | C5—C6     | 1.366 (9)  |
| Pt1—S2' | 2.3495 (11) | C6—H6     | 0.9300    |
| Pt1—N1 | 2.063 (4)  | C6—C7     | 1.413 (7)  |
| Pt1—N1' | 2.063 (4)  | C9—H9     | 0.9300    |
| S1—C1 | 1.743 (5)  | C9—C10    | 1.373 (7)  |
| S2—C8 | 1.741 (5)  | C10—H10   | 0.9300    |
| N1—C9 | 1.346 (6)  | C10—C11   | 1.393 (8)  |
| N1—C13 | 1.342 (6)  | C11—C12   | 1.407 (7)  |
| N2—C1 | 1.310 (6)  | C12—H12   | 0.9300    |
| N2—C2 | 1.371 (7)  | C12—C13   | 1.363 (7)  |
| N3—C7 | 1.369 (7)  | C13—H13   | 0.9300    |
| N3—C8 | 1.323 (6)  | S3—O1     | 1.505 (10) |
| N4—H4A | 0.8662    | S3—C1A    | 1.728 (19) |
| N4—H4B | 0.8665    | S3—C1B    | 1.752 (16) |
| Bond Pair   | Distance (Å) | Torsion Angle (°) | Bond Angle (°) |
|------------|-------------|-------------------|----------------|
| N4—C11     | 1.355 (7)   |                   |                |
| C1—C8      | 1.446 (7)   |                   |                |
| C2—C3      | 1.421 (8)   |                   |                |
| C2—C7      | 1.402 (8)   |                   |                |
| C3—H3      | 0.9300      |                   |                |
| C3—C4      | 1.370 (8)   |                   |                |
| C4—H4      | 0.9300      |                   |                |
| S1—Pt1—S1  | 180.0       |                   |                |
| S2—Pt1—S1  | 88.43 (4)   |                   |                |
| S2i—Pt1—S2i| 88.43 (4)   |                   |                |
| N1'—Pt1—S1 | 89.99 (12)  |                   |                |
| N1—Pt1—S1  | 90.01 (12)  |                   |                |
| N1—Pt1—S1' | 90.01 (12)  |                   |                |
| N1—Pt1—S2  | 90.33 (12)  |                   |                |
| N1—Pt1—S2' | 90.33 (12)  |                   |                |
| N1—Pt1—S2  | 89.67 (12)  |                   |                |
| N1—Pt1—S2' | 89.67 (12)  |                   |                |
| C1—S1—Pt1  | 103.03 (16) |                   |                |
| C8—S2—Pt1  | 102.34 (17) |                   |                |
| C9—N1—Pt1  | 120.7 (3)   |                   |                |
| C13—N1—Pt1 | 121.6 (3)   |                   |                |
| C13—N1—C9  | 117.7 (4)   |                   |                |
| C1—N2—C2  | 117.3 (4)   |                   |                |
| C8—N3—C7  | 117.1 (4)   |                   |                |
| H4A—N4—H4B| 108.6       |                   |                |
| C11—N4—H4A| 109.7       |                   |                |
| C11—N4—H4B| 110.6       |                   |                |
| N2—C1—S1  | 116.9 (4)   |                   |                |
| N2—C1—C8  | 121.8 (4)   |                   |                |
| C8—C1—S1  | 121.3 (4)   |                   |                |
| N2—C2—C3  | 119.6 (5)   |                   |                |
| N2—C2—C7  | 121.1 (5)   |                   |                |
| C7—C2—C3  | 119.3 (5)   |                   |                |
| C2—C3—H3  | 120.0       |                   |                |
| C4—C3—C2  | 120.0 (6)   |                   |                |
| C4—C3—H3  | 120.0       |                   |                |
| C3—C4—H4  | 119.8       |                   |                |
| C3—C4—C5  | 120.4 (6)   |                   |                |
| C5—C4—H4  | 119.8       |                   |                |
| C4—C5—H5  | 119.6       |                   |                |
| C6—C5—C4  | 120.7 (5)   |                   |                |
| C6—C5—H5  | 119.6       |                   |                |
data reports

Pt1—S1—C1—N2 173.6 (3)  C2—C3—C4—C5 0.6 (8)
Pt1—S1—C1—C8  −6.3 (4)  C3—C2—C7—N3 177.0 (5)
Pt1—S2—C8—N3  −166.6 (3)  C3—C2—C7—C6  −2.5 (7)
Pt1—S2—C8—C1  16.4 (4)  C3—C4—C5—C6  −0.9 (9)
Pt1—N1—C9—C10  −179.9 (5)  C4—C5—C6—C7  −0.5 (9)
Pt1—N1—C13—C12  179.8 (4)  C5—C6—C7—N3  −177.3 (5)
S1—C1—C8—S2  −7.3 (6)  C5—C6—C7—C2  2.2 (8)
S1—C1—C8—N3  175.8 (4)  C7—N3—C8—S2  −175.4 (3)
N1—C9—C10—C11  0.1 (10)  C7—N3—C8—C1  1.7 (7)
N2—C1—C8—N3  −4.1 (7)  C7—C2—C3—C4  1.1 (8)
N2—C1—C8—S2  −172.8 (4)  C8—C3—C4—C5  2.3 (7)
N2—C2—C3—C4  −177.7 (5)  C8—N3—C13—C12  0.7 (8)
N2—C2—C7—N3  −4.2 (7)  C9—N1—C13—C12  179.4 (6)
N2—C2—C7—C6  176.3 (5)  C9—C10—C11—N4  −0.6 (9)
N4—C11—C12—C13  −179.5 (6)  C9—C10—C11—C12  0.6 (9)
C1—N2—C2—C3  −179.4 (4)  C10—C11—C12—C13  −0.7 (9)
C1—N2—C2—C7  1.8 (7)  C11—C12—C13—N1  0.0 (9)
C2—N2—C1—S1  −177.8 (3)  C13—N1—C9—C10  −0.7 (8)
C2—N2—C1—C8  2.2 (7)

Symmetry code: (i) −x+1, −y+1, −z.

Hydrogen-bond geometry (Å, °)

|        | D—H···A | D—H   | H···A | D···A   | D—H···A |
|--------|---------|--------|-------|---------|---------|
| N4—H4A···N3ii | 0.87 | 2.30  | 3.085 (7) | 151      |
| N4—H4B···O1iii | 0.87 | 2.28  | 3.045 (11) | 148      |

Symmetry codes: (ii) x, y+1, z; (iii) x−1, y, z.