

Tetra-*n*-butylammonium bis(1,1-dicyanoethylene-2,2-dithiolato)platinum(II)

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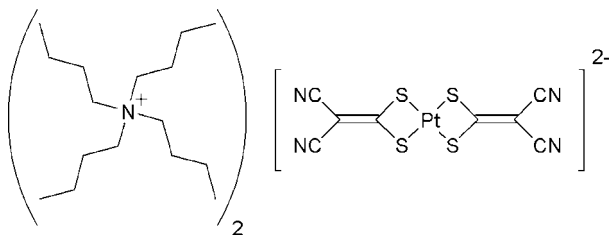
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.027; wR factor = 0.077; data-to-parameter ratio = 17.3.

In the title compound, $(\text{C}_{16}\text{H}_{36}\text{N})_2[\text{Pt}(\text{C}_4\text{N}_2\text{S}_2)_2]$, the Pt^{II} center adopts a distorted square-planar geometry due to the 4-membered chelate rings formed by coordination to the S atoms of the 1,1-dicyanoethylene-2,2-dithiolate (*i*-mnt) ligands [bite angle $74.35(4)^\circ$]. The bond distances in the coordinated *i*-mnt ligands indicate some delocalization of the π -system.

Related literature

For general background on the salts of metal complexes of $[\text{Pt}(\textit{i}\text{-mnt})_2]^{2-}$ (*i*-mnt=1,1-dicyanoethylene-2,2-dithiolate), see: Cummings & Eisenberg (1996); Fackler & Coucouvanis (1966); Werden *et al.* (1966). For related structures, see: Gao *et al.* (2005, 2006); Hummel (1987); Li *et al.* (2004); Sun *et al.* (2006).



Experimental

Crystal data

 $(\text{C}_{16}\text{H}_{36}\text{N})_2[\text{Pt}(\text{C}_4\text{N}_2\text{S}_2)_2]$
 $M_r = 960.40$

Monoclinic, $P2_1/n$
 $a = 9.8687(6)$ Å
 $b = 16.9556(11)$ Å
 $c = 13.8274(9)$ Å
 $\beta = 92.840(1)^\circ$
 $V = 2310.9(3)$ Å³

$Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 3.25$ mm⁻¹
 $T = 173(2)$ K
 $0.40 \times 0.20 \times 0.15$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Bruker 2003)
 $T_{\text{min}} = 0.468$, $T_{\text{max}} = 0.612$

22256 measured reflections
 4087 independent reflections
 3226 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.077$
 $S = 1.09$
 4087 reflections

236 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.02$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.33$ e Å⁻³

Data collection: *SMART* (Bruker,2003); cell refinement: *SAINTE* (Bruker, 2006); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2127).

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supplementary materials

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Tetra-*n*-butylammonium bis(1,1-dicyanoethylene-2,2-dithiolato)platinum(II)

N. Kanganga, K. R. Mann and D. E. Janzen

Comment

Salts of metal complexes of $[\text{Pt}(i\text{-mnt})_2]^{2-}$ ($i\text{-mnt}$ =1,1-dicyanoethylene-2,2-dithiolate) have been studied for their interesting electronic properties including their photoluminescence (Cummings & Eisenberg, 1996) and their redox behavior especially in relation to the analogous isomeric ligand 1,2-dicyanoethylene-1,2-dithiolate (mnt^{2-}) complexes (Fackler & Coucouvanis, 1966; Werden *et al.*, 1966). In sharp contrast to mnt complexes of the form $[\text{M}(\text{mnt})_2]^{2-}$ ($\text{M} = \text{Ni}^{\text{II}}, \text{Pd}^{\text{II}}, \text{Pt}^{\text{II}}$) which do exhibit reversible oxidation behavior, analogous $i\text{-mnt}$ complexes of the form $[\text{M}(i\text{-mnt})_2]^{2-}$ do not. This effect is attributed to better π -delocalization of the five-membered rings formed by complexation of mnt compared with four-membered chelate rings of $i\text{-mnt}$ complexes. Salts of $[\text{Pt}(i\text{-mnt})_2]^{2-}$ have also been studied as supramolecular linker groups in organic-inorganic hybrid coordination polymers (Gao *et al.* 2005, 2006; Li *et al.* 2004; Sun *et al.* 2006). While several x -ray structures of $[\text{Pt}(i\text{-mnt})_2]^{2-}$ with alkali metal-complexed crown ether salts have been reported, only one other simple non-coordinating cation salt (tetraethylammonium, Hummel 1987) has been structurally characterized.

The structure of the anion in the title compound $(\text{C}_{16}\text{H}_{36}\text{N})_2[\text{Pt}(\text{S}_2\text{C}_4\text{N}_2)_2]$ shows significant distortions from a square planar environment as forced by the four-membered chelate rings of the $i\text{-mnt}$ ligands, with the $i\text{-mnt}$ bite angle $\text{S}(2)\text{—Pt}(1)\text{—S}(1) = 74.35(4)^\circ$. As the Pt sits on the special position $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ in the space group $P2_1/n$, $Z=0.5$. The anion is quite planar, with a calculated r.m.s. deviation from a least-squares plane formed by all atoms of the complex anion of $0.042(3) \text{ \AA}$. The bond lengths within coordinated $i\text{-mnt}$ ligand, in particular the bonds $\text{C}(1)\text{—C}(2) 1.361(6) \text{ \AA}$, $\text{C}(2)\text{—C}(3) 1.429(6) \text{ \AA}$, and $\text{C}(2)\text{—C}(4) 1.430(6) \text{ \AA}$ are very similar to those observed in the tetraethylammonium salt, showing significant π -delocalization. No columnar stacking is observed amongst the complex anions. As expected, upon comparison of the structure of the title compound and the tetraethylammonium salt, little effect was observed on the intramolecular features of the complex anion.

Experimental

The title compound $(\text{C}_{16}\text{H}_{36}\text{N})_2[\text{Pt}(\text{S}_2\text{C}_4\text{N}_2)_2]$ was prepared using a procedure similar to that described by Fackler and Coucouvanis (1966) substituting the use of tetra-*n*-propylammonium iodide with tetra-*n*-butylammonium bromide. The title compound has been previously characterized by Werden *et al.* (1966). Spectroscopic analysis of the present sample obtained by this procedure was consistent with the data previously reported. Crystals were obtained by diffusion of diethyl ether into a concentrated solution of the title compound dissolved in dichloromethane.

Refinement

The H atoms were geometrically placed ($\text{C—H} = 0.98\text{--}0.99 \text{ \AA}$) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

Figures

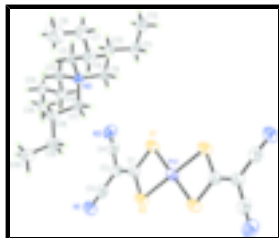


Fig. 1. The molecular structure of $(C_{16}H_{36}N)_2[Pt(S_2C_4N_2)_2]$ showing 50% displacement ellipsoids for the non-hydrogen atoms. Only the crystallographically independent atoms are labelled.

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Crystal data

$(C_{16}H_{36}N)_2[Pt(C_4N_2S_2)_2]$

$M_r = 960.40$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2yn$

$a = 9.8687\ (6)\ \text{\AA}$

$b = 16.9556\ (11)\ \text{\AA}$

$c = 13.8274\ (9)\ \text{\AA}$

$\beta = 92.840\ (1)^\circ$

$V = 2310.9\ (3)\ \text{\AA}^3$

$Z = 2$

$F_{000} = 992$

$D_x = 1.380\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71069\ \text{\AA}$

Cell parameters from 3207 reflections

$\theta = 5.5\text{--}50.0^\circ$

$\mu = 3.25\ \text{mm}^{-1}$

$T = 173\ (2)\ \text{K}$

Plate, yellow

$0.4 \times 0.2 \times 0.15\ \text{mm}$

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: normal-focus sealed tube

Monochromator: graphite

$T = 173\ (2)\ \text{K}$

φ scans

Absorption correction: multi-scan

(SADABS; Bruker 2003)

$T_{\min} = 0.468$, $T_{\max} = 0.612$

22256 measured reflections

4087 independent reflections

3226 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\max} = 25.1^\circ$

$\theta_{\min} = 1.9^\circ$

$h = -11 \rightarrow 11$

$k = -20 \rightarrow 20$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.077$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 3.6638P]$

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

$S = 1.09$ $(\Delta/\sigma)_{\max} = 0.001$
 4087 reflections $\Delta\rho_{\max} = 1.02 \text{ e } \text{\AA}^{-3}$
 236 parameters $\Delta\rho_{\min} = -0.33 \text{ e } \text{\AA}^{-3}$
 Primary atom site location: structure-invariant direct methods Extinction correction: none

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|-------------|----------------------------------|
| Pt1 | 0.5000 | 0.5000 | 0.5000 | 0.03643 (9) |
| S1 | 0.56122 (11) | 0.43791 (7) | 0.64610 (8) | 0.0434 (3) |
| S2 | 0.30447 (11) | 0.49674 (7) | 0.58620 (8) | 0.0439 (2) |
| C1 | 0.3957 (4) | 0.4489 (2) | 0.6793 (3) | 0.0365 (9) |
| C2 | 0.3440 (4) | 0.4241 (2) | 0.7636 (3) | 0.0395 (9) |
| C3 | 0.2028 (5) | 0.4321 (2) | 0.7797 (3) | 0.0432 (10) |
| C4 | 0.4294 (5) | 0.3889 (2) | 0.8383 (3) | 0.0419 (10) |
| N1 | 0.0899 (4) | 0.4381 (3) | 0.7927 (3) | 0.0585 (11) |
| N2 | 0.4951 (5) | 0.3608 (2) | 0.8982 (3) | 0.0558 (10) |
| N3 | 0.6156 (3) | 0.15041 (17) | 0.7976 (2) | 0.0311 (7) |
| C5 | 0.6718 (4) | 0.0849 (2) | 0.7366 (3) | 0.0325 (8) |
| H5A | 0.5998 | 0.0449 | 0.7250 | 0.039* |
| H5B | 0.7471 | 0.0592 | 0.7747 | 0.039* |
| C6 | 0.7239 (5) | 0.1092 (3) | 0.6392 (3) | 0.0513 (12) |
| H6A | 0.6473 | 0.1284 | 0.5965 | 0.062* |
| H6B | 0.7899 | 0.1528 | 0.6485 | 0.062* |
| C7 | 0.7915 (5) | 0.0399 (3) | 0.5914 (3) | 0.0530 (12) |
| H7A | 0.8370 | 0.0594 | 0.5338 | 0.064* |
| H7B | 0.8626 | 0.0185 | 0.6372 | 0.064* |
| C8 | 0.6986 (7) | -0.0250 (4) | 0.5610 (5) | 0.088 (2) |
| H8A | 0.7497 | -0.0664 | 0.5293 | 0.131* |
| H8B | 0.6276 | -0.0047 | 0.5156 | 0.131* |
| H8C | 0.6568 | -0.0470 | 0.6180 | 0.131* |
| C9 | 0.7213 (4) | 0.2133 (2) | 0.8215 (3) | 0.0364 (9) |
| H9A | 0.6795 | 0.2539 | 0.8620 | 0.044* |
| H9B | 0.7446 | 0.2391 | 0.7603 | 0.044* |
| C10 | 0.8523 (4) | 0.1859 (2) | 0.8736 (3) | 0.0407 (10) |

supplementary materials

| | | | | |
|------|------------|------------|------------|-------------|
| H10A | 0.8317 | 0.1624 | 0.9368 | 0.049* |
| H10B | 0.8954 | 0.1448 | 0.8346 | 0.049* |
| C11 | 0.9494 (5) | 0.2548 (3) | 0.8897 (3) | 0.0454 (10) |
| H11A | 0.9651 | 0.2796 | 0.8264 | 0.054* |
| H11B | 0.9063 | 0.2947 | 0.9305 | 0.054* |
| C12 | 1.0841 (5) | 0.2320 (3) | 0.9372 (4) | 0.0548 (12) |
| H12A | 1.1439 | 0.2781 | 0.9408 | 0.082* |
| H12B | 1.1256 | 0.1905 | 0.8991 | 0.082* |
| H12C | 1.0706 | 0.2124 | 1.0027 | 0.082* |
| C13 | 0.5705 (4) | 0.1106 (2) | 0.8892 (3) | 0.0321 (8) |
| H13A | 0.5059 | 0.0680 | 0.8703 | 0.039* |
| H13B | 0.6507 | 0.0855 | 0.9223 | 0.039* |
| C14 | 0.5040 (5) | 0.1638 (2) | 0.9614 (3) | 0.0416 (10) |
| H14A | 0.5685 | 0.2056 | 0.9834 | 0.050* |
| H14B | 0.4234 | 0.1896 | 0.9297 | 0.050* |
| C15 | 0.4618 (4) | 0.1166 (2) | 1.0474 (3) | 0.0389 (9) |
| H15A | 0.5434 | 0.0922 | 1.0794 | 0.047* |
| H15B | 0.4007 | 0.0736 | 1.0242 | 0.047* |
| C16 | 0.3900 (5) | 0.1654 (3) | 1.1214 (3) | 0.0499 (11) |
| H16A | 0.3599 | 0.1309 | 1.1729 | 0.075* |
| H16B | 0.3112 | 0.1916 | 1.0897 | 0.075* |
| H16C | 0.4526 | 0.2052 | 1.1492 | 0.075* |
| C17 | 0.4978 (4) | 0.1918 (2) | 0.7443 (3) | 0.0354 (9) |
| H17A | 0.4689 | 0.2363 | 0.7848 | 0.042* |
| H17B | 0.5309 | 0.2145 | 0.6839 | 0.042* |
| C18 | 0.3751 (4) | 0.1418 (2) | 0.7184 (3) | 0.0395 (9) |
| H18A | 0.3417 | 0.1178 | 0.7780 | 0.047* |
| H18B | 0.4014 | 0.0985 | 0.6750 | 0.047* |
| C19 | 0.2614 (5) | 0.1896 (3) | 0.6683 (3) | 0.0517 (12) |
| H19A | 0.2422 | 0.2362 | 0.7084 | 0.062* |
| H19B | 0.2914 | 0.2086 | 0.6052 | 0.062* |
| C20 | 0.1329 (5) | 0.1419 (3) | 0.6520 (4) | 0.0549 (12) |
| H20A | 0.0649 | 0.1735 | 0.6153 | 0.082* |
| H20B | 0.0979 | 0.1273 | 0.7146 | 0.082* |
| H20C | 0.1526 | 0.0941 | 0.6154 | 0.082* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|---------------|-------------|---------------|
| Pt1 | 0.03067 (12) | 0.04558 (14) | 0.03345 (13) | -0.00168 (10) | 0.00587 (8) | -0.00881 (11) |
| S1 | 0.0354 (5) | 0.0561 (6) | 0.0392 (6) | 0.0020 (5) | 0.0066 (4) | -0.0062 (5) |
| S2 | 0.0336 (5) | 0.0607 (7) | 0.0379 (5) | 0.0017 (5) | 0.0067 (4) | -0.0022 (5) |
| C1 | 0.037 (2) | 0.033 (2) | 0.040 (2) | 0.0008 (17) | 0.0046 (17) | -0.0123 (17) |
| C2 | 0.040 (2) | 0.034 (2) | 0.045 (2) | 0.0013 (18) | 0.0059 (19) | -0.0068 (18) |
| C3 | 0.049 (3) | 0.039 (2) | 0.043 (2) | -0.001 (2) | 0.009 (2) | -0.0047 (19) |
| C4 | 0.053 (3) | 0.032 (2) | 0.043 (3) | -0.0012 (19) | 0.014 (2) | -0.0088 (19) |
| N1 | 0.045 (2) | 0.063 (3) | 0.069 (3) | 0.001 (2) | 0.022 (2) | 0.004 (2) |
| N2 | 0.071 (3) | 0.047 (2) | 0.050 (2) | 0.006 (2) | 0.008 (2) | 0.0006 (19) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| N3 | 0.0361 (17) | 0.0295 (16) | 0.0282 (17) | 0.0022 (13) | 0.0071 (13) | 0.0044 (13) |
| C5 | 0.038 (2) | 0.0298 (19) | 0.031 (2) | 0.0043 (16) | 0.0081 (16) | -0.0007 (15) |
| C6 | 0.067 (3) | 0.047 (3) | 0.041 (3) | 0.003 (2) | 0.024 (2) | 0.007 (2) |
| C7 | 0.060 (3) | 0.056 (3) | 0.045 (3) | 0.002 (2) | 0.026 (2) | 0.000 (2) |
| C8 | 0.080 (4) | 0.102 (5) | 0.083 (4) | -0.016 (4) | 0.034 (4) | -0.046 (4) |
| C9 | 0.043 (2) | 0.030 (2) | 0.037 (2) | -0.0031 (17) | 0.0095 (18) | 0.0057 (17) |
| C10 | 0.041 (2) | 0.038 (2) | 0.043 (2) | -0.0033 (18) | 0.0023 (19) | 0.0032 (18) |
| C11 | 0.053 (3) | 0.041 (2) | 0.043 (2) | -0.007 (2) | 0.000 (2) | 0.0058 (19) |
| C12 | 0.054 (3) | 0.057 (3) | 0.052 (3) | -0.011 (2) | -0.008 (2) | -0.004 (2) |
| C13 | 0.039 (2) | 0.030 (2) | 0.028 (2) | 0.0020 (16) | 0.0077 (16) | 0.0059 (15) |
| C14 | 0.053 (3) | 0.033 (2) | 0.039 (2) | 0.0041 (18) | 0.0141 (19) | 0.0023 (18) |
| C15 | 0.047 (2) | 0.042 (2) | 0.028 (2) | 0.0022 (19) | 0.0080 (18) | -0.0009 (17) |
| C16 | 0.055 (3) | 0.055 (3) | 0.040 (3) | 0.003 (2) | 0.016 (2) | 0.000 (2) |
| C17 | 0.041 (2) | 0.034 (2) | 0.032 (2) | 0.0081 (17) | 0.0054 (17) | 0.0061 (16) |
| C18 | 0.042 (2) | 0.039 (2) | 0.037 (2) | 0.0074 (18) | 0.0019 (18) | 0.0018 (18) |
| C19 | 0.049 (3) | 0.055 (3) | 0.051 (3) | 0.012 (2) | -0.001 (2) | 0.008 (2) |
| C20 | 0.044 (3) | 0.068 (3) | 0.052 (3) | 0.012 (2) | -0.003 (2) | 0.001 (2) |

Geometric parameters (Å, °)

| | | | |
|---------------------|-------------|----------|-----------|
| Pt1—S2 | 2.3184 (10) | C10—H10B | 0.9900 |
| Pt1—S2 ⁱ | 2.3185 (10) | C11—C12 | 1.504 (6) |
| Pt1—S1 | 2.3310 (11) | C11—H11A | 0.9900 |
| Pt1—S1 ⁱ | 2.3310 (11) | C11—H11B | 0.9900 |
| S1—C1 | 1.729 (4) | C12—H12A | 0.9800 |
| S2—C1 | 1.735 (4) | C12—H12B | 0.9800 |
| C1—C2 | 1.361 (6) | C12—H12C | 0.9800 |
| C2—C3 | 1.429 (6) | C13—C14 | 1.519 (5) |
| C2—C4 | 1.430 (6) | C13—H13A | 0.9900 |
| C3—N1 | 1.142 (5) | C13—H13B | 0.9900 |
| C4—N2 | 1.132 (6) | C14—C15 | 1.509 (6) |
| N3—C9 | 1.516 (5) | C14—H14A | 0.9900 |
| N3—C5 | 1.516 (4) | C14—H14B | 0.9900 |
| N3—C17 | 1.518 (5) | C15—C16 | 1.517 (6) |
| N3—C13 | 1.522 (4) | C15—H15A | 0.9900 |
| C5—C6 | 1.522 (5) | C15—H15B | 0.9900 |
| C5—H5A | 0.9900 | C16—H16A | 0.9800 |
| C5—H5B | 0.9900 | C16—H16B | 0.9800 |
| C6—C7 | 1.518 (6) | C16—H16C | 0.9800 |
| C6—H6A | 0.9900 | C17—C18 | 1.508 (6) |
| C6—H6B | 0.9900 | C17—H17A | 0.9900 |
| C7—C8 | 1.480 (8) | C17—H17B | 0.9900 |
| C7—H7A | 0.9900 | C18—C19 | 1.522 (6) |
| C7—H7B | 0.9900 | C18—H18A | 0.9900 |
| C8—H8A | 0.9800 | C18—H18B | 0.9900 |
| C8—H8B | 0.9800 | C19—C20 | 1.511 (7) |
| C8—H8C | 0.9800 | C19—H19A | 0.9900 |
| C9—C10 | 1.521 (6) | C19—H19B | 0.9900 |
| C9—H9A | 0.9900 | C20—H20A | 0.9800 |

supplementary materials

| | | | |
|--------------------------------------|------------|---------------|-----------|
| C9—H9B | 0.9900 | C20—H20B | 0.9800 |
| C10—C11 | 1.521 (6) | C20—H20C | 0.9800 |
| C10—H10A | 0.9900 | | |
| S2—Pt1—S2 ⁱ | 180.0 | C12—C11—H11A | 108.8 |
| S2—Pt1—S1 | 74.35 (4) | C10—C11—H11A | 108.8 |
| S2 ⁱ —Pt1—S1 | 105.65 (4) | C12—C11—H11B | 108.8 |
| S2—Pt1—S1 ⁱ | 105.65 (4) | C10—C11—H11B | 108.8 |
| S2 ⁱ —Pt1—S1 ⁱ | 74.35 (4) | H11A—C11—H11B | 107.7 |
| S1—Pt1—S1 ⁱ | 180.0 | C11—C12—H12A | 109.5 |
| C1—S1—Pt1 | 88.49 (15) | C11—C12—H12B | 109.5 |
| C1—S2—Pt1 | 88.74 (14) | H12A—C12—H12B | 109.5 |
| C2—C1—S1 | 126.4 (3) | C11—C12—H12C | 109.5 |
| C2—C1—S2 | 125.2 (3) | H12A—C12—H12C | 109.5 |
| S1—C1—S2 | 108.4 (2) | H12B—C12—H12C | 109.5 |
| C1—C2—C3 | 120.9 (4) | C14—C13—N3 | 115.9 (3) |
| C1—C2—C4 | 121.0 (4) | C14—C13—H13A | 108.3 |
| C3—C2—C4 | 118.1 (4) | N3—C13—H13A | 108.3 |
| N1—C3—C2 | 179.6 (5) | C14—C13—H13B | 108.3 |
| N2—C4—C2 | 178.8 (5) | N3—C13—H13B | 108.3 |
| C9—N3—C5 | 111.7 (3) | H13A—C13—H13B | 107.4 |
| C9—N3—C17 | 106.4 (3) | C15—C14—C13 | 110.3 (3) |
| C5—N3—C17 | 111.2 (3) | C15—C14—H14A | 109.6 |
| C9—N3—C13 | 110.9 (3) | C13—C14—H14A | 109.6 |
| C5—N3—C13 | 105.6 (3) | C15—C14—H14B | 109.6 |
| C17—N3—C13 | 111.2 (3) | C13—C14—H14B | 109.6 |
| N3—C5—C6 | 116.3 (3) | H14A—C14—H14B | 108.1 |
| N3—C5—H5A | 108.2 | C14—C15—C16 | 113.5 (4) |
| C6—C5—H5A | 108.2 | C14—C15—H15A | 108.9 |
| N3—C5—H5B | 108.2 | C16—C15—H15A | 108.9 |
| C6—C5—H5B | 108.2 | C14—C15—H15B | 108.9 |
| H5A—C5—H5B | 107.4 | C16—C15—H15B | 108.9 |
| C7—C6—C5 | 110.5 (4) | H15A—C15—H15B | 107.7 |
| C7—C6—H6A | 109.5 | C15—C16—H16A | 109.5 |
| C5—C6—H6A | 109.5 | C15—C16—H16B | 109.5 |
| C7—C6—H6B | 109.5 | H16A—C16—H16B | 109.5 |
| C5—C6—H6B | 109.5 | C15—C16—H16C | 109.5 |
| H6A—C6—H6B | 108.1 | H16A—C16—H16C | 109.5 |
| C8—C7—C6 | 114.8 (5) | H16B—C16—H16C | 109.5 |
| C8—C7—H7A | 108.6 | C18—C17—N3 | 116.2 (3) |
| C6—C7—H7A | 108.6 | C18—C17—H17A | 108.2 |
| C8—C7—H7B | 108.6 | N3—C17—H17A | 108.2 |
| C6—C7—H7B | 108.6 | C18—C17—H17B | 108.2 |
| H7A—C7—H7B | 107.5 | N3—C17—H17B | 108.2 |
| C7—C8—H8A | 109.5 | H17A—C17—H17B | 107.4 |
| C7—C8—H8B | 109.5 | C17—C18—C19 | 112.0 (3) |
| H8A—C8—H8B | 109.5 | C17—C18—H18A | 109.2 |
| C7—C8—H8C | 109.5 | C19—C18—H18A | 109.2 |
| H8A—C8—H8C | 109.5 | C17—C18—H18B | 109.2 |

| | | | |
|----------------------------|--------------|-----------------|------------|
| H8B—C8—H8C | 109.5 | C19—C18—H18B | 109.2 |
| N3—C9—C10 | 116.6 (3) | H18A—C18—H18B | 107.9 |
| N3—C9—H9A | 108.1 | C20—C19—C18 | 112.2 (4) |
| C10—C9—H9A | 108.1 | C20—C19—H19A | 109.2 |
| N3—C9—H9B | 108.1 | C18—C19—H19A | 109.2 |
| C10—C9—H9B | 108.1 | C20—C19—H19B | 109.2 |
| H9A—C9—H9B | 107.3 | C18—C19—H19B | 109.2 |
| C11—C10—C9 | 110.5 (3) | H19A—C19—H19B | 107.9 |
| C11—C10—H10A | 109.6 | C19—C20—H20A | 109.5 |
| C9—C10—H10A | 109.6 | C19—C20—H20B | 109.5 |
| C11—C10—H10B | 109.6 | H20A—C20—H20B | 109.5 |
| C9—C10—H10B | 109.6 | C19—C20—H20C | 109.5 |
| H10A—C10—H10B | 108.1 | H20A—C20—H20C | 109.5 |
| C12—C11—C10 | 113.8 (4) | H20B—C20—H20C | 109.5 |
| S2—Pt1—S1—C1 | 0.38 (13) | C5—C6—C7—C8 | 67.3 (6) |
| S2 ⁱ —Pt1—S1—C1 | -179.62 (13) | C5—N3—C9—C10 | -57.1 (4) |
| S1—Pt1—S2—C1 | -0.38 (13) | C17—N3—C9—C10 | -178.6 (3) |
| S1 ⁱ —Pt1—S2—C1 | 179.62 (13) | C13—N3—C9—C10 | 60.4 (4) |
| Pt1—S1—C1—C2 | 179.1 (4) | N3—C9—C10—C11 | 178.2 (3) |
| Pt1—S1—C1—S2 | -0.52 (17) | C9—C10—C11—C12 | -177.5 (4) |
| Pt1—S2—C1—C2 | -179.1 (3) | C9—N3—C13—C14 | 61.4 (4) |
| Pt1—S2—C1—S1 | 0.52 (17) | C5—N3—C13—C14 | -177.5 (3) |
| S1—C1—C2—C3 | -175.8 (3) | C17—N3—C13—C14 | -56.8 (4) |
| S2—C1—C2—C3 | 3.8 (6) | N3—C13—C14—C15 | 178.8 (3) |
| S1—C1—C2—C4 | 3.9 (6) | C13—C14—C15—C16 | -178.0 (4) |
| S2—C1—C2—C4 | -176.6 (3) | C9—N3—C17—C18 | -176.2 (3) |
| C9—N3—C5—C6 | -59.8 (4) | C5—N3—C17—C18 | 62.0 (4) |
| C17—N3—C5—C6 | 58.9 (4) | C13—N3—C17—C18 | -55.3 (4) |
| C13—N3—C5—C6 | 179.6 (4) | N3—C17—C18—C19 | 178.0 (3) |
| N3—C5—C6—C7 | 173.5 (4) | C17—C18—C19—C20 | -173.8 (4) |

Symmetry codes: (i) $-x+1, -y+1, -z+1$.

Fig. 1

