metal-organic compounds

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

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In the title compound, $(C_{16}H_{36}N)_2[Pt(C_4N_2S_2)_2]$, 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)°]. 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 $[Pt(i\text{-mnt})_2]^{2-}$ (*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).
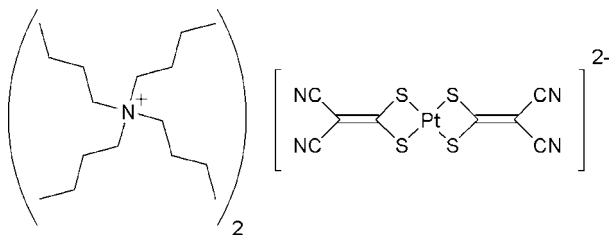
Experimental

Crystal data

$(C_{16}H_{36}N)_2[Pt(C_4N_2S_2)_2]$ M_r = 960.40

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

Z = 2
Mo $K\alpha$ radiation
μ = 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_{min} = 0.468, T_{max} = 0.612

22256 measured reflections
4087 independent reflections
3226 reflections with $I > 2\sigma(I)$
R_{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
$\Delta\rho_{max}$ = 1.02 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Data collection: *SMART* (Bruker,2003); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; 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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supporting information

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

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S1. Comment

Salts of metal complexes of [Pt(*i*-mnt)$_2$]$^{2-}$ (*i*-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 analagous 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 [*M*(mnt)$_2$]$^{2-}$ (*M*= Ni^{II}, Pd^{II}, Pt^{II}) which do exhibit reversible oxidation behavior, analagous *i*-mnt complexes of the form [*M*(*i*-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*-mnt complexes. Salts of [Pt(*i*-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 [Pt(*i*-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 (C$_{16}$H$_{36}$N)$_2$[Pt(S$_2$C$_4$N$_2$)$_2$] shows significant distortions from a square planar environment as forced by the four-membered chelate rings of the *i*-mnt ligands, with the *i*-mnt bite angle S(2)—Pt(1)—S(1) = 74.35 (4)°. As the Pt sits on the special position (1/2, 1/2, 1/2) in the space group *P*2$_1$/*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) Å. The bond lengths within coordinated *i*-mnt ligand, in particular the bonds C(1)—C(2) 1.361 (6) Å, C(2)—C(3) 1.429 (6) Å, and C(2)—C(4) 1.430 (6)Å 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.

S2. Experimental

The title compound (C$_{16}$H$_{36}$N)$_2$[Pt(S$_2$C$_4$N$_2$)$_2$] was prepared using a procedure similar to that described by Fackler and Coucouvanis (1966) subsituting 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 di-ethyl ether into a concentrated solution of the title compound dissolved in dichloromethane.

S3. Refinement

The H atoms were geometrically placed (C—H = 0.98–0.99 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).
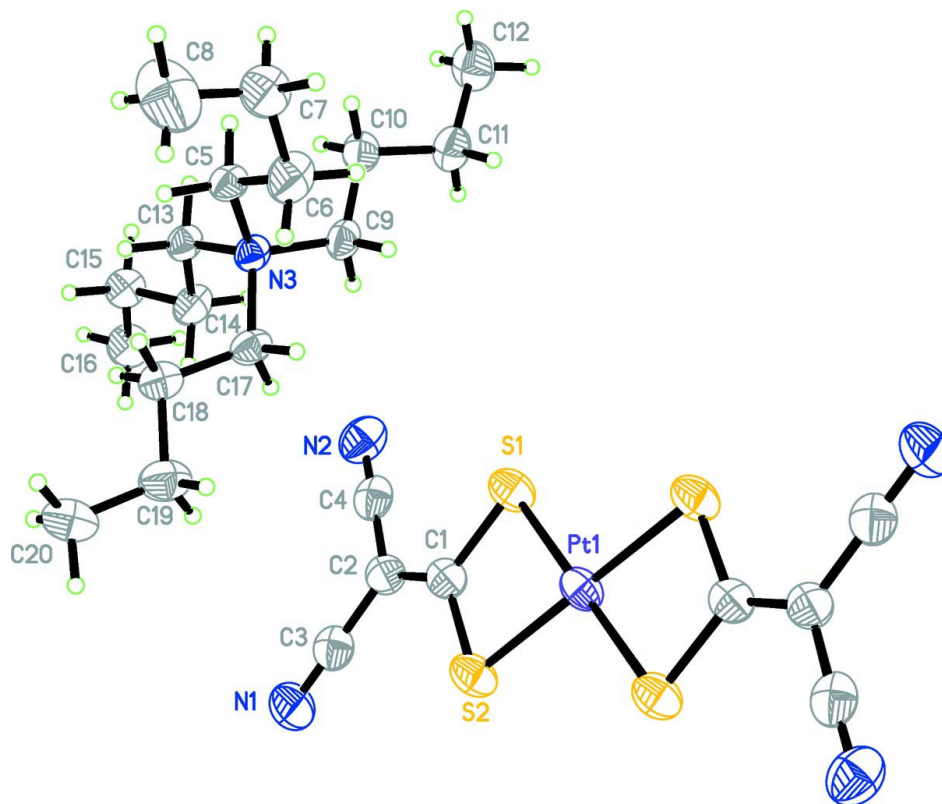
Figure 1

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.

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

Crystal data

$(C_{16}H_{36}N)_2[Pt(C_4N_2S_2)_2]$	$F(000) = 992$
$M_r = 960.40$	$D_x = 1.380$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Hall symbol: -P 2yn	Cell parameters from 3207 reflections
$a = 9.8687$ (6) Å	$\theta = 5.5–50.0°$
$b = 16.9556$ (11) Å	$\mu = 3.25$ mm^{-1}
$c = 13.8274$ (9) Å	$T = 173$ K
$\beta = 92.840$ (1)°	Plate, yellow
$V = 2310.9$ (3) Å^3	$0.4 \times 0.2 \times 0.15$ mm
$Z = 2$	

Data collection

Bruker SMART CCD area-detector diffractometer	22256 measured reflections
	4087 independent reflections
Radiation source: normal-focus sealed tube	3226 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.033$
φ scans	$\theta_{max} = 25.1°, \theta_{min} = 1.9°$
Absorption correction: multi-scan	$h = -11 \rightarrow 11$
(*SADABS*; Bruker 2003)	$k = -20 \rightarrow 20$
$T_{min} = 0.468, T_{max} = 0.612$	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.027$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.077$	
$S = 1.09$	H-atom parameters constrained
4087 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 3.6638P]$
236 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} = 0.001$
0 constraints	$\Delta\rho_{max} = 1.02$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{min} = -0.33$ e Å^{-3}

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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{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)
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 (Å²)

	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, º)

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
C9—H9B	0.9900	C20—H20B	0.9800
C10—C11	1.521 (6)	C20—H20C	0.9800
C10—H10A	0.9900		
S2—Pt1—S2ⁱ	180.0	C12—C11—H11A	108.8
S2—Pt1—S1	74.35 (4)	C10—C11—H11A	108.8
S2ⁱ—Pt1—S1	105.65 (4)	C12—C11—H11B	108.8
S2—Pt1—S1ⁱ	105.65 (4)	C10—C11—H11B	108.8
S2ⁱ—Pt1—S1ⁱ	74.35 (4)	H11A—C11—H11B	107.7
S1—Pt1—S1ⁱ	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 code: (i) −*x*+1, −*y*+1, −*z*+1.