An acetonitrile solvatomorph of dichlorido(1,10-phenanthroline-5,6-dione)platinum(II)

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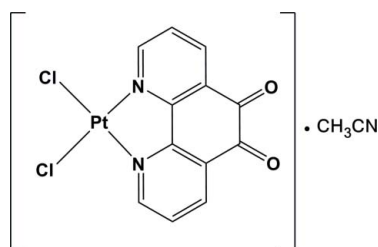Correspondence e-mail: rawji@southwestern.edu

In the title complex, $[PtCl_2(C_{12}H_6N_2O_2)]\cdot CH_3CN$, the Pt^{II} atom lies in a slightly distorted square-planar arrangement defined by an N_2Cl_2 donor set. In the packed structure, columns of complex moieties are stacked such that the neighboring units are oriented at 180° and laterally displaced with respect to each other. This prevents any overlap of the phenanthroline rings and thus there is no possibility of any π–π interactions between aromatic rings.

Related literature

For condensation of the free and complexed phendione ligand with primary amines, see: Dickerson & Summers (1970); MacDonnell & Bodige (1996); Moucheron et al. (1997); Westerlund et al. (2005); Williams et al. (2012). For use of the ligand in the construction of multinuclear homo- and hetero-metallic complexes as well as dendritic polynuclear metal structures, see: Fox et al. (1991); MacDonnell & Bodige (1996); Paw & Eisenberg (1997); Calderazzo et al. (1999); Campagna et al. (1999); Calucci et al. (2006). For antimicrobial activity of the free ligand and the title complex, see: Roy et al. (2008). For previous structural studies related to the title complex, see: Granger et al. (2005); Okamura et al. (2006); Roy et al. (2008). For synthesis of Pt(DMSO)$_2$Cl$_2$, see: Romeo & Scolaro (1998).

Experimental

Crystal data

$[PtCl_2(C_{12}H_6N_2O_2)]\cdot C_2H_3N$	$V = 1471.32\ (7)$ Å^3
$M_r = 517.23$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 6.7285\ (2)$ Å	$\mu = 9.91$ mm^{-1}
$b = 22.6380\ (6)$ Å	$T = 298$ K
$c = 9.7561\ (3)$ Å	$0.40 \times 0.06 \times 0.05$ mm
$\beta = 98.0740\ (17)°$	

Data collection

Nonius KappaCCD diffractometer	11801 measured reflections
Absorption correction: gaussian (XPREP in SHELXL/PC; Sheldrick, 2008)	3345 independent reflections
	2837 reflections with $I > 2\sigma(I)$
$T_{min} = 0.174$, $T_{max} = 0.629$	$R_{int} = 0.081$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$	201 parameters
$wR(F^2) = 0.094$	H-atom parameters constrained
$S = 1.16$	$\Delta\rho_{max} = 1.48$ e Å^{-3}
3345 reflections	$\Delta\rho_{min} = -1.30$ e Å^{-3}

Data collection: COLLECT (Nonius, 1998); cell refinement: COLLECT; data reduction: DENZO and SCALEPACK (Otwinowski & Minor, 1997); program(s) used to solve structure: SIR97 (Altomare et al., 1999); program(s) used to refine structure: SHELXL2013 (Sheldrick, 2008); molecular graphics: XP in SHELXTL/PC (Sheldrick, 2008); software used to prepare material for publication: publCIF (Westrip, 2010).

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supporting information

An acetonitrile solvatomorph of dichlorido(1,10-phenanthroline-5,6-dione)platinum(II)

Amanda Hamala, Carissa Fritz, Gulnar Rawji and Vincent Lynch

S1. Comment

1,10-phenanthroline-5,6-dione (phendione), a versatile electroactive ligand with dual functionalities (diquinoid and di-imine), has been widely used in condensation with primary amines either as a free phendione entity (Dickerson & Summers, 1970) or one coordinated to a metal center (MacDonnell & Bodige, 1996; Moucheron *et al.*, 1997; Westerlund *et al.*, 2005; Williams *et al.*, 2012). Because of its dual functionalities, the phendione ligand has been used as a bridging ligand in homo- and heterometallic multinuclear complexes and polymetallic dendritic structures (Fox *et al.*, 1991; MacDonnell & Bodige, 1996; Paw & Eisenberg, 1997; Calderazzo *et al.*, 1999; Campagna *et al.*, 1999; Calucci *et al.*, 2006). The antimicrobial properties of this complex and the free ligand have also been investigated (Roy *et al.*, 2008). In our studies, this ligand and the title complex have been used in the synthesis of metallointercalators of DNA.

Three structural studies of dichloro(phendione)platinum(II) have been reported (Granger *et al.*, 2005; Okamura *et al.*, 2006; Roy *et al.*, 2008). In all three studies, the complex was obtained as a DMSO solvate in the Cc space group. Two of these studies appear to be preliminary (Granger *et al.*, 2005; Okamura *et al.*, 2006) and the structural data were not submitted to the Cambridge Structural Database (CSD). The third study is thorough and its deposited data (CCDC 678530) are available for comparison (Roy *et al.*, 2008). The structure reported here is an acetonitrile solvate belonging to a different monoclinic space group, $P2_1/c$, resulting in a very different three dimensional packing arrangement compared to that in the reported study.

The title complex is essentially planar with three of the four bond angles about the Pt atom deviating slightly from the idealized square planar geometry. The N12—Pt1—N1 angle is significantly reduced to ~81° due to the constraints of the phendione ligand and two of the remaining bond angles are ~95° (Fig. 1). The unit cell contains four molecules each of the complex and the solvent, acetonitrile. Intermolecular interactions are responsible for the observed three dimensional array which may be described as consisting of zigzagging columns of stacked complex moieties, oriented 180° and laterally displaced with respect to each other. The separation between the stacked moieties alternates between 3.360 Å and 3.364 Å but due to the relative orientation of the stacked units, π-π stacking is not possible. The solvent molecules lie between the columns in the space created by the zigzagging (Fig. 2).

The three dimensional array of the title complex is clearly different from that of the reported structure (Roy *et al.*, 2008). A major contributing factor to the different packing arrangements observed in the two studies is the relative orientation of the stacked complex moieties with respect to each other, 180° (current study) versus ~120° (reported (Roy *et al.*, 2008)). The 120° orientation allows a partial overlap of the end rings of the stacked phendione ligands thereby increasing the potential for π-π interaction. Therefore, the structural study reported here is consistent with a solvate polymorph of [Pt(phendione)Cl$_2$] in which acetonitrile as the solvent leads to a different packing arrangement than in the DMSO solvate structure.

S2. Experimental

S2.1. Synthesis and crystallization

The phendione ligand, K_2PtCl_4, and other reagents used in the syntheses were purchased from Sigma-Aldrich. [Pt(DMSO)$_2$Cl] was prepared from K_2PtCl_4 and DMSO according to the literature (Romeo & Scolaro, 1998). The title complex was synthesized by adding the solid ligand in a 1:1 molar ratio to a stirred acetonitrile solution of [Pt(DMSO)$_2$Cl$_2$] at maintained at 343 K. The pale yellow mixture was kept stirred at this temperature for ~2 hours while replenishing the solvent as necessary. During this time, as the color darkened, orange needles began to precipitate. The mixture was removed from heat and left covered at room temperature for slow crystallization. Good quality light orange needle-shaped crystals suitable for a crystal structure were obtained after ~6 hours. Yield: 40%.

S2.2. Refinement

The H atoms were placed in idealized positions (aromatic C—H distances of 0.93 Å and methyl C—H distances of 0.96 Å) with displacement parameters U_{iso}(H)set to $1.2U_{eq}$(C) for aromatic and $1.5U_{eq}$(C) for methyl protons.
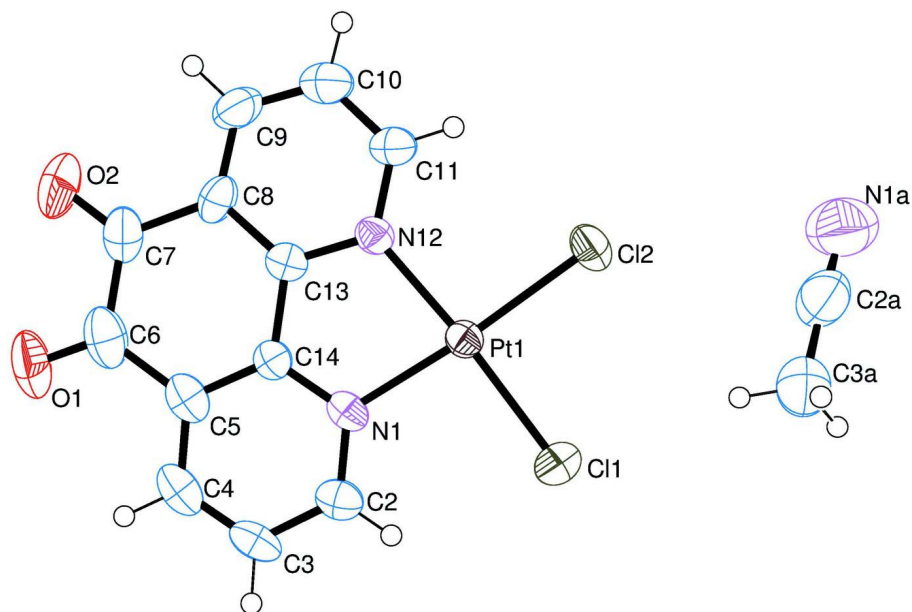

Figure 1

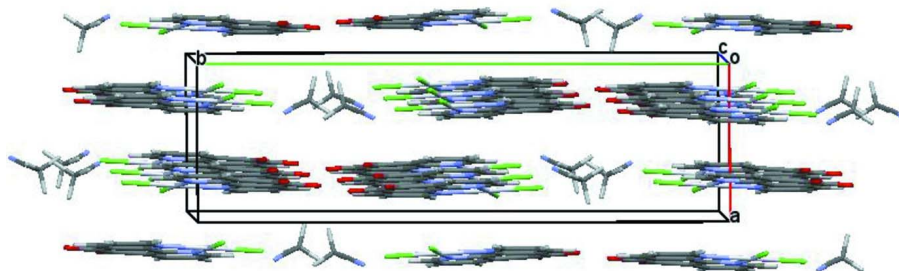An ORTEP diagram of the title complex showing 50% probability displacement elipsoids.

Figure 2

A packing diagram of the title complex viewed down the c axis.

Dichlorido(1,10-phenanthroline-5,6-dione-κ^2N,N')platinum(II) acetonitrile monosolvate

Crystal data

[PtCl$_2$(C$_{12}$H$_6$N$_2$O$_2$)]·C$_2$H$_3$N	$F(000) = 968$
$M_r = 517.23$	$D_x = 2.335$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 6.7285$ (2) Å	Cell parameters from 3185 reflections
$b = 22.6380$ (6) Å	$\theta = 1.0–27.5°$
$c = 9.7561$ (3) Å	$\mu = 9.91$ mm^{-1}
$\beta = 98.0740$ (17)°	$T = 298$ K
$V = 1471.32$ (7) Å^3	Needle, yellow
$Z = 4$	$0.40 \times 0.06 \times 0.05$ mm

Data collection

Nonius KappaCCD diffractometer	3345 independent reflections
Radiation source: sealed tube	2837 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.081$
Absorption correction: gaussian (*XPREP* in *SHELXL*/PC; Sheldrick, 2008)	$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
	$h = -7 \rightarrow 8$
$T_{min} = 0.174$, $T_{max} = 0.629$	$k = -29 \rightarrow 26$
11801 measured reflections	$l = -12 \rightarrow 9$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.039$	$w = 1/[\sigma^2(F_o^2) + (0.0216P)^2 + 7.4291P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.094$	
$S = 1.16$	$(\Delta/\sigma)_{max} = 0.002$
3345 reflections	$\Delta\rho_{max} = 1.48$ e Å^{-3}
201 parameters	$\Delta\rho_{min} = -1.30$ e Å^{-3}
0 restraints	Extinction correction: *SHELXL2013* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.0038 (4)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	y	z	$U_{iso}*/U_{eq}$
Pt1	0.22275 (4)	0.538338 (12)	0.35597 (3)	0.03226 (13)
Cl1	0.2456 (3)	0.63727 (10)	0.4031 (2)	0.0535 (5)
Cl2	0.1736 (3)	0.55973 (11)	0.12469 (18)	0.0490 (5)
O1	0.2795 (12)	0.3386 (4)	0.8277 (7)	0.078 (2)
O2	0.2372 (13)	0.2739 (4)	0.5941 (9)	0.088 (2)
N1	0.2643 (8)	0.5130 (3)	0.5574 (5)	0.0332 (13)
C2	0.2906 (10)	0.5475 (4)	0.6672 (8)	0.0413 (18)

H2A	0.2927	0.5882	0.6548	0.050*
C3	0.3157 (11)	0.5248 (4)	0.8018 (8)	0.047 (2)
H3A	0.3346	0.5501	0.8777	0.057*
C4	0.3120 (12)	0.4655 (4)	0.8204 (8)	0.050 (2)
H4A	0.3290	0.4496	0.9093	0.060*
C5	0.2831 (11)	0.4291 (4)	0.7071 (8)	0.0437 (19)
C6	0.2705 (13)	0.3630 (5)	0.7205 (10)	0.060 (3)
C7	0.2476 (13)	0.3264 (5)	0.5856 (10)	0.055 (2)
C8	0.2270 (12)	0.3572 (4)	0.4480 (9)	0.0442 (18)
C9	0.2042 (13)	0.3274 (4)	0.3234 (9)	0.055 (2)
H9A	0.2025	0.2864	0.3205	0.066*
C10	0.1843 (13)	0.3600 (5)	0.2043 (9)	0.056 (2)
H10A	0.1715	0.3409	0.1192	0.067*
C11	0.1828 (11)	0.4203 (4)	0.2087 (8)	0.0428 (18)
H11A	0.1639	0.4414	0.1262	0.051*
N12	0.2080 (8)	0.4498 (3)	0.3291 (6)	0.0339 (13)
C13	0.2300 (10)	0.4186 (4)	0.4489 (7)	0.0342 (15)
C14	0.2592 (11)	0.4543 (3)	0.5756 (7)	0.0335 (16)
N1A	0.328 (2)	0.6730 (6)	−0.1587 (14)	0.109 (4)
C2A	0.2973 (18)	0.6945 (6)	−0.0552 (13)	0.076 (3)
C3A	0.2662 (19)	0.7226 (6)	0.0677 (12)	0.085 (3)
H3A1	0.3414	0.7588	0.0775	0.127*
H3A2	0.3099	0.6972	0.1448	0.127*
H3A3	0.1259	0.7312	0.0650	0.127*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.03263 (17)	0.03434 (19)	0.03048 (17)	−0.00009 (12)	0.00674 (10)	−0.00010 (11)
Cl1	0.0700 (14)	0.0367 (11)	0.0542 (11)	−0.0022 (10)	0.0102 (9)	−0.0047 (9)
Cl2	0.0597 (12)	0.0558 (13)	0.0317 (9)	−0.0014 (10)	0.0069 (8)	0.0063 (8)
O1	0.095 (5)	0.081 (6)	0.060 (4)	0.013 (4)	0.015 (4)	0.039 (4)
O2	0.127 (7)	0.042 (5)	0.094 (6)	0.005 (4)	0.018 (5)	0.027 (4)
N1	0.024 (3)	0.048 (4)	0.029 (3)	−0.003 (3)	0.006 (2)	−0.001 (3)
C2	0.033 (4)	0.051 (5)	0.041 (4)	−0.002 (3)	0.010 (3)	−0.007 (3)
C3	0.041 (4)	0.071 (7)	0.030 (4)	0.003 (4)	0.009 (3)	−0.010 (4)
C4	0.040 (4)	0.076 (7)	0.034 (4)	0.006 (4)	0.006 (3)	0.009 (4)
C5	0.031 (4)	0.062 (6)	0.039 (4)	0.005 (4)	0.008 (3)	0.007 (4)
C6	0.050 (5)	0.074 (7)	0.057 (5)	0.012 (5)	0.009 (4)	0.024 (5)
C7	0.056 (5)	0.050 (6)	0.060 (5)	0.007 (4)	0.017 (4)	0.018 (4)
C8	0.045 (4)	0.030 (4)	0.058 (5)	0.009 (3)	0.009 (3)	0.008 (3)
C9	0.068 (6)	0.036 (5)	0.063 (5)	−0.002 (4)	0.012 (4)	−0.010 (4)
C10	0.061 (5)	0.056 (6)	0.051 (5)	−0.003 (5)	0.010 (4)	−0.015 (4)
C11	0.042 (4)	0.044 (5)	0.042 (4)	−0.005 (4)	0.007 (3)	−0.009 (3)
N12	0.035 (3)	0.037 (4)	0.031 (3)	0.001 (3)	0.007 (2)	−0.001 (2)
C13	0.028 (3)	0.040 (4)	0.035 (3)	0.002 (3)	0.005 (3)	−0.003 (3)
C14	0.033 (3)	0.037 (4)	0.033 (3)	0.000 (3)	0.005 (3)	0.001 (3)
N1A	0.131 (10)	0.094 (10)	0.105 (9)	−0.019 (8)	0.023 (7)	−0.019 (7)

C2A	0.090 (8)	0.056 (7)	0.086 (8)	−0.001 (6)	0.021 (6)	0.003 (6)
C3A	0.106 (9)	0.074 (9)	0.076 (8)	0.006 (7)	0.019 (6)	0.010 (6)

Geometric parameters (Å, º)

Pt1—N12	2.022 (7)	C7—C8	1.503 (12)
Pt1—N1	2.028 (5)	C8—C9	1.380 (12)
Pt1—Cl2	2.2860 (18)	C8—C13	1.389 (11)
Pt1—Cl1	2.287 (2)	C9—C10	1.367 (13)
O1—C6	1.177 (11)	C9—H9A	0.9300
O2—C7	1.192 (13)	C10—C11	1.365 (13)
N1—C2	1.318 (10)	C10—H10A	0.9300
N1—C14	1.341 (10)	C11—N12	1.341 (9)
C2—C3	1.398 (11)	C11—H11A	0.9300
C2—H2A	0.9300	N12—C13	1.356 (9)
C3—C4	1.356 (13)	C13—C14	1.466 (10)
C3—H3A	0.9300	N1A—C2A	1.166 (16)
C4—C5	1.370 (12)	C2A—C3A	1.399 (17)
C4—H4A	0.9300	C3A—H3A1	0.9600
C5—C14	1.395 (11)	C3A—H3A2	0.9600
C5—C6	1.506 (14)	C3A—H3A3	0.9600
C6—C7	1.545 (15)		
N12—Pt1—N1	81.0 (2)	C9—C8—C7	123.0 (8)
N12—Pt1—Cl2	94.83 (17)	C13—C8—C7	117.4 (8)
N1—Pt1—Cl2	175.8 (2)	C10—C9—C8	118.1 (9)
N12—Pt1—Cl1	175.87 (16)	C10—C9—H9A	121.0
N1—Pt1—Cl1	94.9 (2)	C8—C9—H9A	121.0
Cl2—Pt1—Cl1	89.27 (8)	C11—C10—C9	120.8 (8)
C2—N1—C14	118.9 (7)	C11—C10—H10A	119.6
C2—N1—Pt1	127.2 (6)	C9—C10—H10A	119.6
C14—N1—Pt1	113.8 (5)	N12—C11—C10	121.6 (8)
N1—C2—C3	122.0 (9)	N12—C11—H11A	119.2
N1—C2—H2A	119.0	C10—C11—H11A	119.2
C3—C2—H2A	119.0	C11—N12—C13	118.7 (7)
C4—C3—C2	119.2 (8)	C11—N12—Pt1	127.2 (5)
C4—C3—H3A	120.4	C13—N12—Pt1	114.0 (5)
C2—C3—H3A	120.4	N12—C13—C8	121.1 (7)
C3—C4—C5	119.4 (8)	N12—C13—C14	115.0 (7)
C3—C4—H4A	120.3	C8—C13—C14	123.9 (7)
C5—C4—H4A	120.3	N1—C14—C5	121.6 (7)
C4—C5—C14	118.9 (8)	N1—C14—C13	116.1 (6)
C4—C5—C6	122.0 (8)	C5—C14—C13	122.3 (7)
C14—C5—C6	119.1 (8)	N1A—C2A—C3A	177.3 (14)
O1—C6—C5	123.2 (10)	C2A—C3A—H3A1	109.5
O1—C6—C7	119.4 (11)	C2A—C3A—H3A2	109.5
C5—C6—C7	117.4 (7)	H3A1—C3A—H3A2	109.5
O2—C7—C8	121.7 (10)	C2A—C3A—H3A3	109.5

O2—C7—C6	118.4 (9)	H3A1—C3A—H3A3	109.5
C8—C7—C6	119.8 (9)	H3A2—C3A—H3A3	109.5
C9—C8—C13	119.6 (8)		
N12—Pt1—N1—C2	−179.6 (6)	C10—C11—N12—C13	−1.8 (11)
Cl1—Pt1—N1—C2	0.9 (6)	C10—C11—N12—Pt1	177.0 (6)
N12—Pt1—N1—C14	−1.0 (5)	N1—Pt1—N12—C11	−178.5 (6)
Cl1—Pt1—N1—C14	179.4 (4)	Cl2—Pt1—N12—C11	1.6 (6)
C14—N1—C2—C3	0.8 (10)	N1—Pt1—N12—C13	0.3 (5)
Pt1—N1—C2—C3	179.3 (5)	Cl2—Pt1—N12—C13	−179.6 (4)
N1—C2—C3—C4	−0.3 (11)	C11—N12—C13—C8	0.1 (10)
C2—C3—C4—C5	−0.3 (12)	Pt1—N12—C13—C8	−178.9 (5)
C3—C4—C5—C14	0.3 (12)	C11—N12—C13—C14	179.3 (6)
C3—C4—C5—C6	−177.9 (7)	Pt1—N12—C13—C14	0.4 (7)
C4—C5—C6—O1	2.0 (13)	C9—C8—C13—N12	1.0 (11)
C14—C5—C6—O1	−176.2 (8)	C7—C8—C13—N12	−178.6 (7)
C4—C5—C6—C7	−177.2 (7)	C9—C8—C13—C14	−178.2 (7)
C14—C5—C6—C7	4.6 (11)	C7—C8—C13—C14	2.2 (11)
O1—C6—C7—O2	0.9 (14)	C2—N1—C14—C5	−0.8 (10)
C5—C6—C7—O2	−179.9 (9)	Pt1—N1—C14—C5	−179.4 (5)
O1—C6—C7—C8	177.3 (8)	C2—N1—C14—C13	−179.8 (6)
C5—C6—C7—C8	−3.5 (12)	Pt1—N1—C14—C13	1.5 (7)
O2—C7—C8—C9	−3.1 (14)	C4—C5—C14—N1	0.2 (11)
C6—C7—C8—C9	−179.4 (8)	C6—C5—C14—N1	178.5 (7)
O2—C7—C8—C13	176.5 (9)	C4—C5—C14—C13	179.2 (7)
C6—C7—C8—C13	0.1 (11)	C6—C5—C14—C13	−2.6 (11)
C13—C8—C9—C10	−0.4 (12)	N12—C13—C14—N1	−1.3 (9)
C7—C8—C9—C10	179.2 (8)	C8—C13—C14—N1	178.0 (7)
C8—C9—C10—C11	−1.3 (13)	N12—C13—C14—C5	179.7 (6)
C9—C10—C11—N12	2.4 (13)	C8—C13—C14—C5	−1.1 (11)