



Crystal structure of 4-{2-[4-(dimethyl-amino)phenyl]diazen-1-yl}-1-methyl-pyridinium iodide

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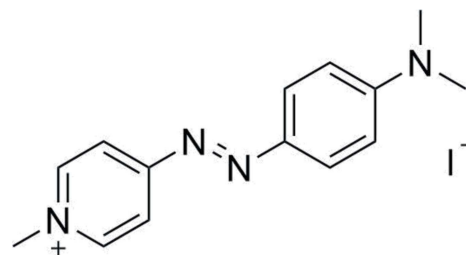
The molecular geometry of the ionic title compound, $C_{14}H_{17}N_4^+I^-$ or $DAZOP^+I^-$, is essentially featureless. Regarding the crystal structure, in addition to the obvious cation–anion Coulombic interactions, the packing is mostly directed by non-covalent interactions involving both ring systems, as well as the iodide anion. It consists of cationic molecules aligned along [101] and disposed in an antiparallel fashion while linked into π -bonded dimeric entities by a stacking contact involving symmetry-related phenyl rings, with a centroid–centroid distance of 3.468 (3) Å and a slippage of 0.951 Å. The dimers are, in addition, sustained by a number of $C-H\cdots I$ and $I\cdots\pi$ ($I\cdots$ centroid = 3.876 Å) interactions involving the anion. Finally, interdimeric contacts are of the $C-H\cdots I$ and $C-H\cdots\pi$ types.

Keywords: crystal structure; $[DAZOP^+][I^-]$; NLO; dye; π - π interaction; $C-H\cdots\pi$ interactions; $I\cdots\pi$ interaction.

CCDC reference: 1441443

1. Related literature

For the synthesis of precursors, see: Li *et al.* (1995). For spectroscopic properties of the title compound, see: Gonbeau *et al.* (1999). For general information on non-linear optical materials, see: Coradin *et al.* (1997); Mestechkin (2001); Nunzi *et al.* (2008). For general information on new photonic materials, see: Yu *et al.* (2013). For related structures, see: Cristian *et al.* (2004); Evans *et al.* (2001); Xu *et al.* (2012).



2. Experimental

2.1. Crystal data

$C_{14}H_{17}N_4^+I^-$	$V = 1476.60$ (19) Å ³
$M_r = 368.21$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 18.0508$ (14) Å	$\mu = 2.16$ mm ⁻¹
$b = 7.2790$ (5) Å	$T = 296$ K
$c = 11.3760$ (9) Å	$0.14 \times 0.08 \times 0.03$ mm
$\beta = 98.929$ (7)°	

2.2. Data collection

Agilent Xcalibur Sapphire3 Gemini diffractometer	5694 measured reflections
Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2009)	2591 independent reflections
$T_{\min} = 0.908$, $T_{\max} = 1.000$	1642 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.048$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$	132 restraints
$wR(F^2) = 0.065$	H-atom parameters constrained
$S = 0.78$	$\Delta\rho_{\max} = 1.00$ e Å ⁻³
2591 reflections	$\Delta\rho_{\min} = -0.51$ e Å ⁻³
175 parameters	

Table 1

Hydrogen-bond geometry (Å, °).

$Cg2$ is the centroid of the C12–C16/N17 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C1-H1A\cdots I1^i$	0.96	3.09	4.042 (6)	173
$C2-H2A\cdots I1^i$	0.96	3.15	4.102 (5)	169
$C15-H15A\cdots I1^{ii}$	0.93	2.99	3.907 (5)	171
$C7-H7A\cdots Cg2^{iii}$	0.93	2.71	3.505 (5)	143

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Supporting information for this paper is available from the IUCr electronic archives (Reference: BG2576).

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supporting information

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S1. Chemical context

Over the years, the spectroscopic properties of 4-[2-(4-dimethylaminophenyl)azo]-1-methylpyridinium iodide ([DAZOP⁺][I⁻]) have been widely studied (Gonbeau *et al.*, 1999). This dye with donor-acceptor character, belongs to the group of the so-called non-linear optical chromophores (NLO-phore) that are able to form J-type aggregates (Coradin *et al.*, 1997; Mestechkin, 2001; Nunzi *et al.*, 2008). The crystal structures of this kind of NLO dyes are a topic of interest in this context and also for studies related to the solvatochromic properties of these dyes in hydrogen-bond-donor (HBD) and hydrogen-bond-acceptor (HBA) solvents. Very recently, new 3D materials based on organic metalorganic frameworks (MOFs) with the capability to encapsulate dyes have been developed. All of these progress are aimed to the new photonic materials and devices design (Yu *et al.*, 2013).

S2. Structural commentary

The title ionic compound [DAZOP⁺][I⁻] (I) crystallizes in the monoclinic S.G. P21/c, and presents one single molecule in the asymmetric unit. The molecular geometry, presented in Fig. 1, is essentially featureless.

S3. Supramolecular features

In addition to the obvious cation-anion coulombian interactions, the crystal packing is mostly directed by non covalent interactions involving the ring systems Cg1 (C4→C9) and Cg2 (C12→C16,N17, as well as the Iodine anion).

It consists of cationic molecules aligned along the [101] direction and disposed in an antiparallel fashion while linked into π bonded dimeric entities (Fig. 1) by a stacking contact involving Cg2 and Cg2ⁱ [(i) : 1-x,1-y,2-z)], with d(Cg⁺⋯Cg) = 3.468 (3) Å and a slippage of 0.951 Å. The dimer is in addition sustained by a number of interactions involving I1, viz (a) I⁺⋯Cg1ⁱ, with d(I⁺⋯Cg) = 3.876 Å, (b) C1—H1A⋯I1ⁱ, with d(H⋯I) = 3.09 Å, <C—H⋯I> = 173°, (c) C2—H2A⋯I1ⁱ, with d(H⋯I) = 3.15 Å, <C—H⋯I> = 169°. The remaining non-covalent interactions serve to link these dimers with each other, either directly, viz., through a C7—H7⋯Cg2iii [(iii) : 1-x,1/2+y,3/2-z] contact, with d(H⋯Cg) = 2.71 Å, <C—H⋯Cg> = 143° or mediated by the external iodine (viz., C15—H15⋯I1ⁱⁱ [(ii) : x,3/2-y,-1/2+z], d(H⋯I): 2.99 Å; <C—H⋯I> = 171°).

S4. Database survey

There are in the literature a lot of crystal structures derived from DAZOP but none with iodine as counter ion. The most similar to (I) is the one with CSD code (Allen, 2002) HANKUD (Cristian *et al.*, 2004) which was solved using powder data and contains a molecule of hexafluorophosphate as counter ion. Thus although the molecules are practically the same, the differences between both structures are significant, mainly due to the absence of π - π interactions in HANKUD. Some similar structures of (DAZOP⁺) coordinated with metalorganic ions can be found in the CSD, viz., IFAHAY (J. S.

O. Evans *et al.*, 2001), RARTEL, RARTIP, RARTOV, (Xu *et al.*, 2012), etc.

S5. Synthesis and crystallization

Benzenamine, N,N-dimethyl-4- (4-pyridinylazo)- was obtained as described in the literature (Li *et al.*, 1995). It was then dissolved in acetonitrile and stirred while an excess of methyl iodide was added dropwise. The resultant mixture was refluxed for 3 h. After that, the orange precipitated obtained was further purified by column chromatography (1:4, methanol/ethyl acetate) with a yield of 59%. Single crystals were obtained by slow evaporation from a methanol solution using a Petri dish.

S6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1

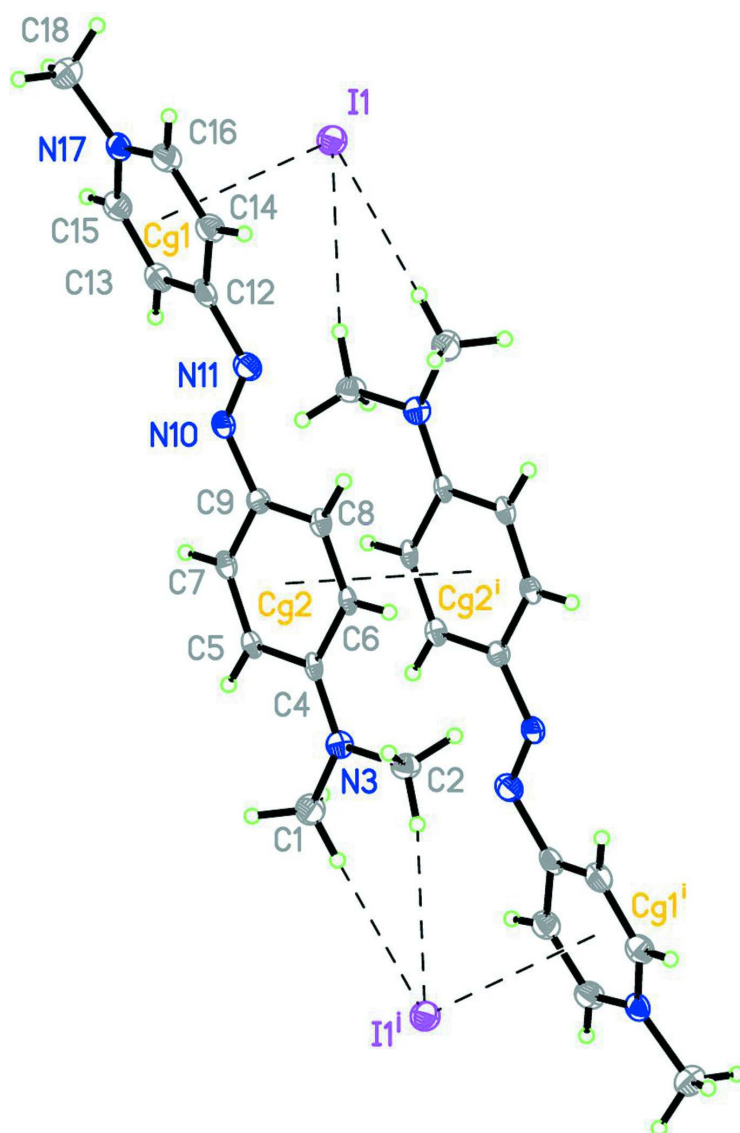


Figure 1

The molecular structure of (I), showing the atom-labelling scheme as well as the dimer formation. Displacement ellipsoids drawn at the 50% probability level. Symmetry codes: (i): 1 - x, 1 - y, 2 - z.

4-{2-[4-(Dimethylamino)phenyl]diazene-1-yl}-1-methylpyridinium iodide

Crystal data

$C_{14}H_{17}N_4^+I^-$	$F(000) = 728$
$M_r = 368.21$	$D_x = 1.656 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 18.0508 (14) \text{ \AA}$	Cell parameters from 2009 reflections
$b = 7.2790 (5) \text{ \AA}$	$\theta = 2.3\text{--}29.8^\circ$
$c = 11.3760 (9) \text{ \AA}$	$\mu = 2.16 \text{ mm}^{-1}$
$\beta = 98.929 (7)^\circ$	$T = 296 \text{ K}$
$V = 1476.60 (19) \text{ \AA}^3$	Plate, orange
$Z = 4$	$0.14 \times 0.08 \times 0.03 \text{ mm}$

Data collection

Agilent Xcalibur Sapphire3 Gemini diffractometer	5694 measured reflections
Radiation source: Enhance (Mo) X-ray Source	2591 independent reflections
Detector resolution: $16.0267 \text{ pixels mm}^{-1}$	1642 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.048$
Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2009)	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.3^\circ$
$T_{\text{min}} = 0.908$, $T_{\text{max}} = 1.000$	$h = -21 \rightarrow 17$
	$k = -6 \rightarrow 8$
	$l = -13 \rightarrow 10$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.035$	$w = 1/[\sigma^2(F_o^2) + (0.0256P)^2]$
$wR(F^2) = 0.065$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.78$	$(\Delta/\sigma)_{\text{max}} = 0.001$
2591 reflections	$\Delta\rho_{\text{max}} = 1.00 \text{ e \AA}^{-3}$
175 parameters	$\Delta\rho_{\text{min}} = -0.51 \text{ e \AA}^{-3}$
132 restraints	

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.7113 (3)	0.4360 (7)	0.9607 (5)	0.0253 (13)
H1A	0.7574	0.4185	1.0140	0.038*
H1B	0.6980	0.5639	0.9585	0.038*
H1C	0.7173	0.3960	0.8824	0.038*
C2	0.6716 (3)	0.2294 (6)	1.1152 (5)	0.0200 (13)
H2A	0.7244	0.2417	1.1432	0.030*
H2B	0.6593	0.1018	1.1030	0.030*
H2C	0.6439	0.2796	1.1732	0.030*
N3	0.6522 (2)	0.3295 (6)	1.0020 (4)	0.0184 (9)
C4	0.5810 (3)	0.3369 (6)	0.9457 (4)	0.0129 (9)

C5	0.5610 (3)	0.4377 (6)	0.8383 (4)	0.0152 (9)
H5A	0.5978	0.5008	0.8058	0.018*
C6	0.5211 (3)	0.2442 (6)	0.9920 (5)	0.0141 (10)
H6A	0.5316	0.1782	1.0627	0.017*
C7	0.4886 (3)	0.4430 (6)	0.7824 (4)	0.0155 (10)
H7A	0.4773	0.5105	0.7125	0.019*
C8	0.4502 (3)	0.2522 (6)	0.9340 (5)	0.0152 (10)
H8A	0.4127	0.1908	0.9660	0.018*
C9	0.4305 (3)	0.3502 (6)	0.8265 (4)	0.0131 (9)
N10	0.3607 (2)	0.3636 (5)	0.7569 (4)	0.0180 (9)
N11	0.3082 (2)	0.2693 (5)	0.7907 (4)	0.0215 (9)
C12	0.2413 (3)	0.2902 (7)	0.7100 (4)	0.0198 (10)
C13	0.2268 (3)	0.4246 (7)	0.6216 (5)	0.0219 (11)
H13A	0.2625	0.5145	0.6150	0.026*
C14	0.1827 (3)	0.1655 (7)	0.7185 (5)	0.0220 (11)
H14A	0.1880	0.0799	0.7799	0.026*
C15	0.1614 (3)	0.4251 (7)	0.5455 (5)	0.0211 (11)
H15A	0.1527	0.5167	0.4881	0.025*
C16	0.1185 (3)	0.1683 (7)	0.6385 (5)	0.0226 (10)
H16A	0.0813	0.0819	0.6441	0.027*
N17	0.1081 (2)	0.2955 (6)	0.5508 (4)	0.0184 (8)
C18	0.0410 (3)	0.2872 (7)	0.4591 (5)	0.0260 (13)
H18A	0.0347	0.4024	0.4178	0.039*
H18B	-0.0023	0.2629	0.4961	0.039*
H18C	0.0469	0.1908	0.4037	0.039*
I1	0.10101 (2)	0.68987 (5)	0.81084 (3)	0.02305 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0259 (19)	0.028 (3)	0.022 (3)	-0.0084 (19)	0.004 (2)	0.003 (2)
C2	0.018 (3)	0.021 (3)	0.0204 (17)	-0.001 (2)	0.0039 (14)	0.0044 (16)
N3	0.0204 (12)	0.016 (2)	0.0187 (16)	-0.0011 (11)	0.0036 (10)	0.0014 (15)
C4	0.0196 (12)	0.009 (2)	0.0116 (15)	0.0006 (11)	0.0060 (10)	-0.0040 (14)
C5	0.0206 (11)	0.013 (2)	0.0132 (15)	0.0011 (13)	0.0063 (11)	-0.0014 (15)
C6	0.0208 (13)	0.010 (2)	0.0125 (18)	-0.0006 (11)	0.0069 (10)	-0.0044 (15)
C7	0.0208 (11)	0.012 (2)	0.015 (2)	0.0010 (12)	0.0056 (10)	-0.0012 (17)
C8	0.0212 (13)	0.009 (2)	0.0159 (15)	-0.0013 (13)	0.0056 (12)	-0.0028 (14)
C9	0.0213 (11)	0.005 (2)	0.0140 (15)	0.0020 (11)	0.0076 (11)	-0.0056 (13)
N10	0.0219 (11)	0.017 (2)	0.0161 (17)	0.0021 (11)	0.0066 (10)	-0.0039 (14)
N11	0.0231 (11)	0.022 (2)	0.0211 (18)	0.0007 (11)	0.0073 (11)	-0.0010 (14)
C12	0.0221 (12)	0.0215 (19)	0.0178 (17)	0.0026 (12)	0.0092 (12)	-0.0038 (15)
C13	0.0215 (18)	0.024 (2)	0.0211 (19)	0.0008 (14)	0.0074 (14)	-0.0008 (16)
C14	0.0211 (13)	0.023 (2)	0.023 (2)	0.0027 (14)	0.0053 (13)	0.0022 (16)
C15	0.0223 (16)	0.019 (2)	0.023 (2)	0.0016 (13)	0.0062 (13)	-0.0021 (16)
C16	0.0214 (16)	0.024 (2)	0.0232 (18)	0.0021 (14)	0.0048 (14)	0.0031 (16)
N17	0.0208 (15)	0.0174 (17)	0.0178 (17)	0.0030 (13)	0.0056 (12)	-0.0027 (13)
C18	0.0255 (18)	0.027 (3)	0.024 (2)	-0.0005 (19)	0.0002 (16)	0.001 (2)

I1	0.0222 (2)	0.0228 (2)	0.0241 (2)	-0.0007 (2)	0.00320 (14)	-0.0028 (2)
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Geometric parameters (Å, °)

C1—N3	1.454 (6)	C8—H8A	0.9300
C1—H1A	0.9600	C9—N10	1.383 (6)
C1—H1B	0.9600	N10—N11	1.277 (5)
C1—H1C	0.9600	N11—C12	1.408 (6)
C2—N3	1.474 (6)	C12—C13	1.398 (7)
C2—H2A	0.9600	C12—C14	1.408 (7)
C2—H2B	0.9600	C13—C15	1.351 (7)
C2—H2C	0.9600	C13—H13A	0.9300
N3—C4	1.344 (6)	C14—C16	1.358 (7)
C4—C5	1.423 (7)	C14—H14A	0.9300
C4—C6	1.442 (6)	C15—N17	1.355 (6)
C5—C7	1.361 (6)	C15—H15A	0.9300
C5—H5A	0.9300	C16—N17	1.352 (6)
C6—C8	1.348 (7)	C16—H16A	0.9300
C6—H6A	0.9300	N17—C18	1.471 (6)
C7—C9	1.405 (6)	C18—H18A	0.9600
C7—H7A	0.9300	C18—H18B	0.9600
C8—C9	1.413 (7)	C18—H18C	0.9600
N3—C1—H1A	109.5	N10—C9—C7	115.2 (4)
N3—C1—H1B	109.5	N10—C9—C8	128.0 (5)
H1A—C1—H1B	109.5	C7—C9—C8	116.8 (5)
N3—C1—H1C	109.5	N11—N10—C9	116.2 (4)
H1A—C1—H1C	109.5	N10—N11—C12	110.4 (4)
H1B—C1—H1C	109.5	C13—C12—N11	126.2 (5)
N3—C2—H2A	109.5	C13—C12—C14	116.2 (5)
N3—C2—H2B	109.5	N11—C12—C14	117.6 (5)
H2A—C2—H2B	109.5	C15—C13—C12	120.6 (5)
N3—C2—H2C	109.5	C15—C13—H13A	119.7
H2A—C2—H2C	109.5	C12—C13—H13A	119.7
H2B—C2—H2C	109.5	C16—C14—C12	121.1 (5)
C4—N3—C1	121.2 (4)	C16—C14—H14A	119.5
C4—N3—C2	121.1 (4)	C12—C14—H14A	119.5
C1—N3—C2	117.3 (4)	C13—C15—N17	121.7 (5)
N3—C4—C5	121.8 (4)	C13—C15—H15A	119.1
N3—C4—C6	121.5 (4)	N17—C15—H15A	119.1
C5—C4—C6	116.7 (5)	N17—C16—C14	120.7 (5)
C7—C5—C4	120.9 (5)	N17—C16—H16A	119.6
C7—C5—H5A	119.6	C14—C16—H16A	119.6
C4—C5—H5A	119.6	C16—N17—C15	119.4 (5)
C8—C6—C4	120.7 (5)	C16—N17—C18	120.0 (4)
C8—C6—H6A	119.7	C15—N17—C18	120.6 (4)
C4—C6—H6A	119.7	N17—C18—H18A	109.5
C5—C7—C9	122.4 (5)	N17—C18—H18B	109.5

C5—C7—H7A	118.8	H18A—C18—H18B	109.5
C9—C7—H7A	118.8	N17—C18—H18C	109.5
C6—C8—C9	122.5 (5)	H18A—C18—H18C	109.5
C6—C8—H8A	118.7	H18B—C18—H18C	109.5
C9—C8—H8A	118.7		
C1—N3—C4—C5	4.8 (7)	C8—C9—N10—N11	-3.6 (7)
C2—N3—C4—C5	178.0 (4)	C9—N10—N11—C12	-177.8 (4)
C1—N3—C4—C6	-174.6 (4)	N10—N11—C12—C13	-14.3 (7)
C2—N3—C4—C6	-1.4 (7)	N10—N11—C12—C14	166.1 (4)
N3—C4—C5—C7	179.8 (4)	N11—C12—C13—C15	176.8 (5)
C6—C4—C5—C7	-0.8 (7)	C14—C12—C13—C15	-3.6 (7)
N3—C4—C6—C8	-179.6 (4)	C13—C12—C14—C16	5.2 (7)
C5—C4—C6—C8	1.0 (7)	N11—C12—C14—C16	-175.2 (5)
C4—C5—C7—C9	-0.3 (7)	C12—C13—C15—N17	-0.8 (8)
C4—C6—C8—C9	-0.1 (7)	C12—C14—C16—N17	-2.3 (8)
C5—C7—C9—N10	-177.6 (4)	C14—C16—N17—C15	-2.2 (7)
C5—C7—C9—C8	1.1 (7)	C14—C16—N17—C18	174.9 (5)
C6—C8—C9—N10	177.6 (4)	C13—C15—N17—C16	3.9 (7)
C6—C8—C9—C7	-0.9 (7)	C13—C15—N17—C18	-173.3 (5)
C7—C9—N10—N11	175.0 (4)		

Hydrogen-bond geometry (\AA , $^\circ$)

Cg2 is the centroid of the C12–C16/N17 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1—H1A \cdots I1 ⁱ	0.96	3.09	4.042 (6)	173
C2—H2A \cdots I1 ⁱ	0.96	3.15	4.102 (5)	169
C15—H15A \cdots I1 ⁱⁱ	0.93	2.99	3.907 (5)	171
C7—H7A \cdots Cg2 ⁱⁱⁱ	0.93	2.71	3.505 (5)	143

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $x, -y+3/2, z-1/2$; (iii) $-x+1, y+1/2, -z+3/2$.