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(*E*)-1-[2-(3,4-Dimethylphenyl)diazen-2-ium-1-yl]-naphthalen-2-olate

Souheyla Chetioui,[a]* Mehdi Boutebdja,[a] Mhamed Boudraa,[a] Rachid Touzani[b,c] and Hocine Merazig[a]

[a]Unité de Recherche de Chimie de l'Environnement et Moléculaire Structurale (CHEMS), Faculté des Sciences Exactes, Département de Chimie, Université des Frères Mentouri Constantine, Constantine 25000, Algeria, [b]Laboratoire de Chimie Appliquée et Environnement, LCAE-URAC18, COSTE, Faculté des Sciences, Université Mohamed Premier, BP524, 60000, Oujda, Morocco, and [c]Faculté Pluridisciplinaire Nador BP 300, Selouane, 62702, Nador, Morocco. *Correspondence e-mail: souheilachetioui@yahoo.fr

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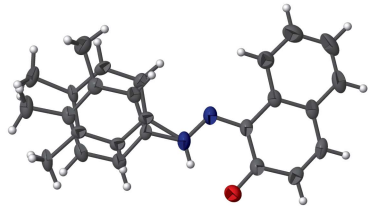
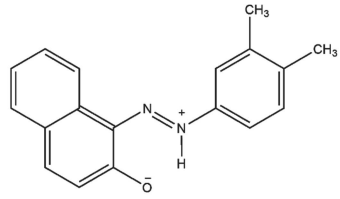
Structural data: full structural data are available from iucrdata.iucr.org

The title zwitterion, $C_{18}H_{16}N_2O$, features an intramolecular N—H···O hydrogen bond. The dimethylbenzene ring is rotationally disordered about the N—C bond over two adjacent orientations in a 0.75:0.25 ratio. The dihedral angle between the major orientation of the benzene ring and the naphthalene ring system is 6.06 (2)°. In the crystal, aromatic π–π stacking occurs [shortest centroid–centroid distance = 3.574 (3) Å] and C—H···O interactions are also observed.

3D view



Chemical scheme



Structure description

For general background to azo compounds and their use in dyes, pigments and advanced materials, see: Navarro & Sanz (1999); Tao *et al.* (1999).

The title azo dye adopts the zwitterionic form in the crystal (Fig. 1), with proton transfer from the phenol group to the azo group, which allows for the formation of an intramolecular N—H···O hydrogen bond (Table 1). The dimethyl benzene ring is disordered by ~180° rotation about the N2—C11 bond over two adjacent orientations in a 0.75:0.25 ratio. The dihedral angle between the major orientation of the benzene ring and the naphthalene ring system is 6.06 (2)°.

In the crystal, molecules are linked by aromatic π–π stacking between the benzene rings and the naphthalene ring systems of adjacent molecules, the centroid–centroid distances of 3.574 (3) and 3.5754 (12) Å, respectively, between the C5–C10 and C11*B*–C16*B*(x, $y-1$, z) rings and between the C5–C10 and C11*A*–C16*A*(x, $y-1$, z) rings. C—

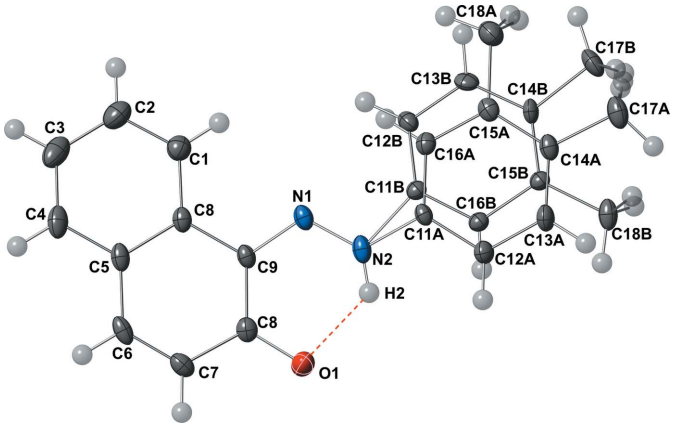


Figure 1
The molecular structure of the title compound, with 50% probability displacement ellipsoids.

H—O hydrogen bonds are also observed, forming chains running parallel to the *a*-axis direction (Table 1, Fig. 2).

Synthesis and crystallization

The title compound was synthesized according to a literature method (Wang *et al.*, 2003), *viz.* the diazotization of 3,4-dimethylaniline followed by a coupling reaction with 2-naphthol. Red prisms were obtained by slow evaporation of an acetone solution at room temperature (yield 88%).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

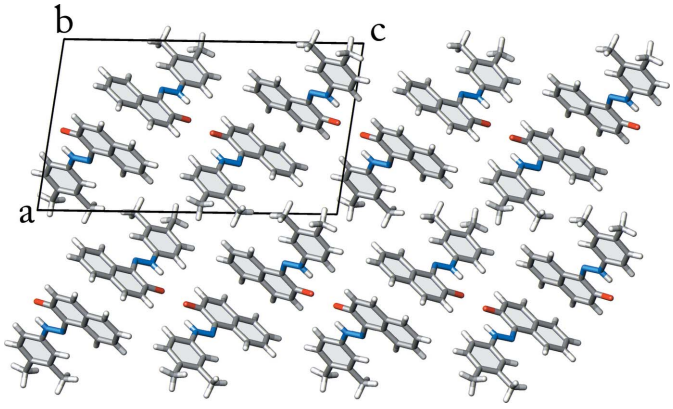


Figure 2
The crystal packing of the title compound, viewed along the *b*-axis direction.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1	0.86	1.82	2.5347 (15)	140
C12*A*—H12*A*···O1^{i}	0.93	2.54	3.325 (2)	143

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{16}N_2O$
M_r	276.33
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, *b*, *c* (Å)	11.6326 (5), 6.1866 (2), 20.1712 (8)
β (°)	98.023 (2)
V (Å^3)	1437.44 (10)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.15 × 0.08 × 0.08
Data collection	
Diffractometer	Bruker APEXII CCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13963, 3654, 2479
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.672
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.121, 1.04
No. of reflections	3654
No. of parameters	254
No. of restraints	7
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.23

Computer programs: *APEX2* and *SAINT* (Bruker, 2006), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008).

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full crystallographic data

IUCrData (2017). **2**, x170259 [https://doi.org/10.1107/S2414314617002590]

(*E*)-1-[2-(3,4-Dimethylphenyl)diazen-2-ium-1-yl]naphthalen-2-olate

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(*E*)-1-[2-(3,4-Dimethylphenyl)diazen-2-ium-1-yl]naphthalen-2-olate

Crystal data

$C_{18}H_{16}N_2O$
M_r = 276.33
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 11.6326 (5) Å
b = 6.1866 (2) Å
c = 20.1712 (8) Å
β = 98.023 (2)°
V = 1437.44 (10) Å^3
Z = 4
$F(000)$ = 584
D_x = 1.277 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3155 reflections
θ = 2.5–28.1°
μ = 0.08 mm^{-1}
T = 173 K
Prism, red
0.15 × 0.08 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
13963 measured reflections
3654 independent reflections
2479 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 28.5°, θ_{min} = 2.9°
h = −15→15
k = −8→8
l = −27→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.121
S = 1.04
3654 reflections
254 parameters
7 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0491P)^2 + 0.2765P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.53655 (9)	0.28137 (15)	0.04401 (5)	0.0423 (3)	
N1	0.71280 (9)	0.43066 (15)	0.14740 (5)	0.0306 (3)	
N2	0.69480 (9)	0.54119 (16)	0.09243 (6)	0.0330 (3)	
C1	0.75035 (12)	0.2025 (2)	0.26821 (7)	0.0410 (5)	
C2	0.77274 (15)	0.0808 (3)	0.32550 (8)	0.0542 (6)	
C3	0.71594 (15)	−0.1166 (3)	0.33086 (8)	0.0572 (6)	
C4	0.63748 (13)	−0.1890 (2)	0.27889 (8)	0.0450 (5)	
C5	0.61249 (11)	−0.0680 (2)	0.21974 (7)	0.0331 (4)	
C6	0.53071 (11)	−0.1422 (2)	0.16480 (7)	0.0353 (4)	
C7	0.50626 (11)	−0.0288 (2)	0.10759 (7)	0.0347 (4)	
C8	0.56216 (11)	0.17470 (19)	0.09888 (6)	0.0306 (4)	
C9	0.64717 (10)	0.25164 (18)	0.15195 (6)	0.0271 (3)	
C10	0.67092 (10)	0.13066 (19)	0.21396 (6)	0.0300 (4)	
C11A	0.75837 (19)	0.7234 (4)	0.08101 (11)	0.0240 (6)	0.750
C12A	0.73667 (19)	0.8278 (4)	0.01928 (10)	0.0317 (6)	0.750
C13A	0.7995 (2)	1.0103 (3)	0.00825 (12)	0.0358 (6)	0.750
C14A	0.8830 (2)	1.0934 (3)	0.05681 (16)	0.0308 (7)	0.750
C15A	0.9037 (2)	0.9908 (4)	0.11911 (16)	0.0308 (7)	0.750
C16A	0.8410 (3)	0.8045 (6)	0.13063 (13)	0.0296 (8)	0.750
C17A	0.94946 (19)	1.2939 (3)	0.04259 (12)	0.0460 (7)	0.750
C18A	0.98974 (19)	1.0814 (3)	0.17419 (11)	0.0488 (7)	0.750
C17B	0.9986 (5)	1.2864 (9)	0.0922 (4)	0.0434 (19)	0.250
C11B	0.7842 (8)	0.7320 (16)	0.1026 (4)	0.0278 (12)	0.250
C12B	0.8620 (9)	0.7828 (16)	0.1558 (4)	0.029 (2)	0.250
C13B	0.9316 (6)	0.9638 (11)	0.1505 (4)	0.0309 (19)	0.250
C14B	0.9186 (6)	1.0878 (11)	0.0925 (4)	0.0277 (19)	0.250
C15B	0.8400 (7)	1.0352 (11)	0.0381 (4)	0.0278 (12)	0.250
C16B	0.7699 (5)	0.8488 (11)	0.0447 (3)	0.0278 (12)	0.250
C18B	0.8259 (5)	1.1641 (8)	−0.0252 (3)	0.0397 (17)	0.250
H1	0.78830	0.33380	0.26540	0.0490*	
H16A	0.85510	0.73500	0.17190	0.0360*	0.750
H17A	0.94450	1.39880	0.07720	0.0690*	0.750
H17B	0.91670	1.35310	0.00010	0.0690*	0.750
H17C	1.02930	1.25720	0.04140	0.0690*	0.750
H18A	0.96720	1.22560	0.18440	0.0730*	0.750
H18B	1.06530	1.08450	0.16020	0.0730*	0.750
H18C	0.99190	0.99230	0.21330	0.0730*	0.750
H2	0.64080	0.49950	0.06150	0.0400*	
H2A	0.82600	0.12990	0.36100	0.0650*	
H3	0.73160	−0.19840	0.36980	0.0690*	

H4	0.60010	−0.32030	0.28270	0.0540*	
H6	0.49320	−0.27330	0.16880	0.0420*	
H7	0.45240	−0.08290	0.07320	0.0420*	
H12A	0.68040	0.77500	−0.01410	0.0380*	0.750
H13A	0.78520	1.07920	−0.03310	0.0430*	0.750
H12B	0.86920	0.70040	0.19470	0.0340*	0.250
H13B	0.98730	1.00200	0.18630	0.0370*	0.250
H16B	0.71430	0.80710	0.00940	0.0330*	0.250
H17D	0.95230	1.41420	0.08330	0.0650*	0.250
H17E	1.04770	1.26890	0.05800	0.0650*	0.250
H17F	1.04580	1.29960	0.13500	0.0650*	0.250
H18D	0.79660	1.30500	−0.01680	0.0600*	0.250
H18E	0.77250	1.09190	−0.05850	0.0600*	0.250
H18F	0.89980	1.17800	−0.04090	0.0600*	0.250

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0527 (6)	0.0378 (5)	0.0358 (5)	−0.0014 (5)	0.0037 (4)	0.0018 (4)
N1	0.0310 (6)	0.0229 (5)	0.0405 (6)	0.0030 (4)	0.0137 (5)	0.0008 (4)
N2	0.0350 (6)	0.0236 (5)	0.0429 (6)	0.0000 (4)	0.0146 (5)	0.0035 (5)
C1	0.0379 (8)	0.0428 (8)	0.0426 (8)	−0.0006 (6)	0.0067 (6)	0.0035 (6)
C2	0.0505 (10)	0.0671 (11)	0.0436 (9)	0.0047 (8)	0.0014 (7)	0.0092 (8)
C3	0.0562 (10)	0.0673 (11)	0.0509 (9)	0.0157 (9)	0.0169 (8)	0.0304 (8)
C4	0.0427 (8)	0.0402 (8)	0.0569 (9)	0.0067 (7)	0.0239 (7)	0.0183 (7)
C5	0.0315 (7)	0.0277 (6)	0.0442 (7)	0.0046 (5)	0.0197 (6)	0.0058 (6)
C6	0.0343 (7)	0.0210 (6)	0.0554 (9)	−0.0021 (5)	0.0233 (6)	−0.0022 (6)
C7	0.0338 (7)	0.0283 (6)	0.0438 (7)	−0.0032 (5)	0.0121 (6)	−0.0086 (6)
C8	0.0338 (7)	0.0256 (6)	0.0347 (7)	0.0023 (5)	0.0132 (5)	−0.0022 (5)
C9	0.0282 (6)	0.0207 (6)	0.0346 (6)	0.0012 (5)	0.0124 (5)	−0.0003 (5)
C10	0.0287 (6)	0.0268 (6)	0.0368 (7)	0.0044 (5)	0.0132 (5)	0.0029 (5)
C11A	0.0219 (11)	0.0186 (8)	0.0329 (13)	0.0009 (8)	0.0090 (8)	0.0007 (10)
C12A	0.0317 (11)	0.0314 (9)	0.0328 (11)	0.0002 (8)	0.0078 (8)	0.0052 (9)
C13A	0.0395 (12)	0.0331 (10)	0.0369 (11)	0.0019 (9)	0.0127 (9)	0.0109 (9)
C14A	0.0312 (13)	0.0248 (11)	0.0390 (14)	0.0043 (9)	0.0146 (10)	0.0043 (11)
C15A	0.0263 (12)	0.0271 (12)	0.0398 (14)	0.0049 (9)	0.0070 (11)	−0.0004 (12)
C16A	0.0292 (16)	0.0276 (11)	0.0326 (15)	0.0044 (10)	0.0065 (13)	0.0048 (13)
C17A	0.0479 (12)	0.0290 (9)	0.0653 (14)	−0.0034 (9)	0.0227 (11)	0.0082 (10)
C18A	0.0447 (12)	0.0417 (11)	0.0579 (13)	−0.0088 (10)	−0.0004 (10)	0.0026 (10)
C17B	0.038 (3)	0.026 (3)	0.067 (4)	−0.010 (2)	0.010 (3)	0.001 (3)
C11B	0.024 (2)	0.030 (2)	0.028 (2)	0.0008 (17)	−0.0014 (16)	−0.0009 (19)
C12B	0.023 (4)	0.023 (3)	0.039 (5)	−0.004 (3)	0.001 (4)	0.000 (4)
C13B	0.018 (3)	0.034 (3)	0.039 (4)	−0.002 (3)	−0.002 (3)	−0.005 (3)
C14B	0.032 (3)	0.022 (3)	0.032 (4)	0.002 (2)	0.015 (3)	0.011 (3)
C15B	0.024 (2)	0.030 (2)	0.028 (2)	0.0008 (17)	−0.0014 (16)	−0.0009 (19)
C16B	0.024 (2)	0.030 (2)	0.028 (2)	0.0008 (17)	−0.0014 (16)	−0.0009 (19)
C18B	0.045 (3)	0.027 (3)	0.052 (3)	−0.001 (2)	0.024 (3)	0.014 (2)

Geometric parameters (Å, º)

O1—C8	1.2873 (15)	C15A—C18A	1.497 (4)
N1—N2	1.2946 (15)	C15A—C16A	1.401 (4)
N1—C9	1.3555 (15)	C15B—C16B	1.429 (10)
N2—C11A	1.385 (3)	C15B—C18B	1.495 (10)
N2—C11B	1.568 (10)	C1—H1	0.9300
N2—H2	0.8600	C2—H2A	0.9300
C1—C2	1.373 (2)	C3—H3	0.9300
C1—C10	1.4023 (18)	C4—H4	0.9300
C2—C3	1.400 (3)	C6—H6	0.9300
C3—C4	1.366 (2)	C7—H7	0.9300
C4—C5	1.404 (2)	C12A—H12A	0.9300
C5—C10	1.4171 (17)	C12B—H12B	0.9300
C5—C6	1.4316 (19)	C13A—H13A	0.9300
C6—C7	1.3465 (19)	C13B—H13B	0.9300
C7—C8	1.4390 (17)	C16A—H16A	0.9300
C8—C9	1.4335 (17)	C16B—H16B	0.9300
C9—C10	1.4507 (17)	C17A—H17C	0.9600
C11A—C12A	1.394 (3)	C17A—H17A	0.9600
C11A—C16A	1.382 (4)	C17A—H17B	0.9600
C11B—C16B	1.364 (11)	C17B—H17E	0.9600
C11B—C12B	1.341 (12)	C17B—H17F	0.9600
C12A—C13A	1.380 (3)	C17B—H17D	0.9600
C12B—C13B	1.395 (12)	C18A—H18C	0.9600
C13A—C14A	1.379 (4)	C18A—H18A	0.9600
C13B—C14B	1.390 (11)	C18A—H18B	0.9600
C14A—C17A	1.510 (3)	C18B—H18D	0.9600
C14A—C15A	1.398 (4)	C18B—H18E	0.9600
C14B—C17B	1.542 (9)	C18B—H18F	0.9600
C14B—C15B	1.366 (11)		
N2—N1—C9	117.66 (10)	C2—C1—H1	120.00
N1—N2—C11A	123.10 (13)	C10—C1—H1	120.00
N1—N2—C11B	105.1 (3)	C1—C2—H2A	120.00
C11B—N2—H2	136.00	C3—C2—H2A	120.00
N1—N2—H2	118.00	C2—C3—H3	120.00
C11A—N2—H2	118.00	C4—C3—H3	120.00
C2—C1—C10	120.65 (13)	C3—C4—H4	120.00
C1—C2—C3	120.47 (15)	C5—C4—H4	119.00
C2—C3—C4	119.93 (15)	C5—C6—H6	119.00
C3—C4—C5	120.95 (13)	C7—C6—H6	119.00
C6—C5—C10	119.27 (12)	C6—C7—H7	119.00
C4—C5—C6	121.55 (12)	C8—C7—H7	120.00
C4—C5—C10	119.18 (12)	C11A—C12A—H12A	120.00
C5—C6—C7	122.30 (12)	C13A—C12A—H12A	120.00
C6—C7—C8	121.03 (12)	C11B—C12B—H12B	121.00
O1—C8—C7	119.95 (11)	C13B—C12B—H12B	121.00

O1—C8—C9	121.64 (11)	C12A—C13A—H13A	119.00
C7—C8—C9	118.41 (11)	C14A—C13A—H13A	119.00
N1—C9—C10	116.02 (10)	C14B—C13B—H13B	120.00
C8—C9—C10	120.07 (10)	C12B—C13B—H13B	120.00
N1—C9—C8	123.86 (11)	C15A—C16A—H16A	120.00
C1—C10—C9	122.33 (11)	C11A—C16A—H16A	120.00
C1—C10—C5	118.82 (11)	C11B—C16B—H16B	120.00
C5—C10—C9	118.85 (11)	C15B—C16B—H16B	120.00
N2—C11A—C12A	119.43 (19)	H17A—C17A—H17B	110.00
N2—C11A—C16A	120.6 (2)	H17A—C17A—H17C	110.00
C12A—C11A—C16A	120.0 (2)	C14A—C17A—H17A	109.00
N2—C11B—C12B	130.0 (8)	C14A—C17A—H17B	109.00
C12B—C11B—C16B	123.3 (9)	C14A—C17A—H17C	109.00
N2—C11B—C16B	106.7 (6)	H17B—C17A—H17C	109.00
C11A—C12A—C13A	119.3 (2)	C14B—C17B—H17D	110.00
C11B—C12B—C13B	117.5 (8)	H17D—C17B—H17E	109.00
C12A—C13A—C14A	121.8 (2)	H17D—C17B—H17F	110.00
C12B—C13B—C14B	120.8 (7)	H17E—C17B—H17F	109.00
C13A—C14A—C15A	119.0 (2)	C14B—C17B—H17E	109.00
C15A—C14A—C17A	121.0 (2)	C14B—C17B—H17F	110.00
C13A—C14A—C17A	120.0 (2)	H18B—C18A—H18C	109.00
C13B—C14B—C17B	116.6 (7)	H18A—C18A—H18B	109.00
C13B—C14B—C15B	121.8 (7)	H18A—C18A—H18C	110.00
C15B—C14B—C17B	121.6 (7)	C15A—C18A—H18A	109.00
C14A—C15A—C16A	119.6 (2)	C15A—C18A—H18B	110.00
C14A—C15A—C18A	120.7 (2)	C15A—C18A—H18C	109.00
C16A—C15A—C18A	119.7 (3)	C15B—C18B—H18D	109.00
C14B—C15B—C16B	116.4 (7)	C15B—C18B—H18E	109.00
C14B—C15B—C18B	122.7 (6)	C15B—C18B—H18F	109.00
C16B—C15B—C18B	120.9 (6)	H18D—C18B—H18E	110.00
C11A—C16A—C15A	120.3 (3)	H18D—C18B—H18F	109.00
C11B—C16B—C15B	120.3 (7)	H18E—C18B—H18F	109.00

C9—N1—N2—C11A	−178.13 (15)	O1—C8—C9—N1	−4.99 (19)
N2—N1—C9—C8	2.05 (17)	O1—C8—C9—C10	177.92 (11)
N2—N1—C9—C10	179.25 (10)	C7—C8—C9—N1	174.01 (11)
N1—N2—C11A—C12A	177.29 (17)	C7—C8—C9—C10	−3.08 (17)
N1—N2—C11A—C16A	−4.1 (3)	N1—C9—C10—C1	4.86 (17)
C10—C1—C2—C3	−0.4 (2)	N1—C9—C10—C5	−174.62 (11)
C2—C1—C10—C5	1.2 (2)	C8—C9—C10—C1	−177.83 (12)
C2—C1—C10—C9	−178.34 (13)	C8—C9—C10—C5	2.69 (17)
C1—C2—C3—C4	−0.1 (3)	N2—C11A—C12A—C13A	179.48 (19)
C2—C3—C4—C5	−0.1 (2)	C16A—C11A—C12A—C13A	0.8 (4)
C3—C4—C5—C6	179.81 (14)	N2—C11A—C16A—C15A	−179.0 (2)
C3—C4—C5—C10	0.8 (2)	C12A—C11A—C16A—C15A	−0.4 (4)
C4—C5—C6—C7	−179.60 (13)	C11A—C12A—C13A—C14A	−0.4 (3)
C10—C5—C6—C7	−0.6 (2)	C12A—C13A—C14A—C15A	−0.6 (3)
C4—C5—C10—C1	−1.30 (19)	C12A—C13A—C14A—C17A	−179.8 (2)

C4—C5—C10—C9	178.20 (12)	C13A—C14A—C15A—C16A	1.1 (4)
C6—C5—C10—C1	179.63 (12)	C13A—C14A—C15A—C18A	−177.2 (2)
C6—C5—C10—C9	−0.87 (18)	C17A—C14A—C15A—C16A	−179.7 (2)
C5—C6—C7—C8	0.1 (2)	C17A—C14A—C15A—C18A	2.0 (3)
C6—C7—C8—O1	−179.29 (12)	C14A—C15A—C16A—C11A	−0.6 (4)
C6—C7—C8—C9	1.69 (19)	C18A—C15A—C16A—C11A	177.7 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1	0.86	1.82	2.5347 (15)	140
C12*A*—H12*A*···O1^{i}	0.93	2.54	3.325 (2)	143

Symmetry code: (i) −*x*+1, −*y*+1, −*z*.