Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*,*N*′,*N*′-Tetraethylnaphthalene-1,4-dicarboxamide

Lin-Hai Jing,* Li-Mei Zhou and Da-Bin Qin

Department of Chemistry, China West Normal University, Nanchong 637002, People's Republic of China
Correspondence e-mail: jlhjhr@yahoo.com.cn

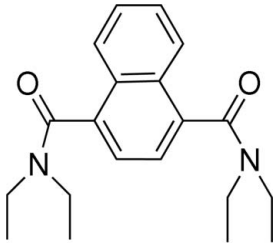
Received 1 October 2007; accepted 3 October 2007

Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.039; wR factor = 0.117; data-to-parameter ratio = 17.9.

In the title compound, $C_{20}H_{26}N_2O_2$, all bond lengths and angles are normal. The two amide groups are twisted away from the naphthalene mean plane by 86.29 (4) and 84.06 (4)°, respectively. Intermolecular C—H$\cdots\pi$ interactions contribute to the crystal packing stability. One ethyl group is disordered equally over two sites.

Related literature

For related crystal structures, see Jing *et al.* (2006*a*,*b*). For applications of 1,4-naphthalenedicarboxylic acid derivatives, see: Fukuzumi *et al.* (1994) and Tsukada *et al.* (1994).



Experimental

Crystal data

$C_{20}H_{26}N_2O_2$
M_r = 326.43
Monoclinic, $C2/c$
a = 23.1133 (14) Å
b = 12.6202 (8) Å
c = 12.9917 (9) Å
β = 107.293 (2)°
V = 3618.3 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 153 (2) K
0.58 × 0.52 × 0.51 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: none
16253 measured reflections
4142 independent reflections
3595 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.117
S = 1.00
4142 reflections
232 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

Cg is the centroid of the C5–C10 ring..

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C15—H15$B\cdots Cg^{i}$	0.98	2.78	3.643 (2)	147
C18—H18$B\cdots Cg^{ii}$	0.98	2.72	3.586 (2)	148

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

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank the Centre for Testing and Analysis, Cheng Du Branch of the Chinese Academy of Sciences, for analytical support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2315).

References

Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Fukuzumi, T., Tajiri, T., Tsukada, H. & Yoshida, J. (1994). Jpn Patent JP 06298919.
Jing, L.-H., Qin, D.-B., Gu, S.-J., Zhang, H.-X. & Lei, G. (2006*a*). *Acta Cryst.* C**62**, o561–o562.
Jing, L. H., Qin, D. B., Gu, S. J., Zhang, H. X. & Mao, Z. H. (2006*b*). *Z. Kristallogr. New Cryst. Struct.* **221**, 200–202.
Rigaku (2004). *RAPID-AUTO* and *CrystalStructure*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tsukada, H., Tajiri, T., Fukuzumi, T. & Yoshida, J. (1994). Jpn Patent JP 06298918.

 doi:10.1107/S1600536807048544

supplementary materials

Acta Cryst. (2007). E**63**, o4273 [**doi:10.1107/S1600536807048544**]

N,*N*,*N*',*N*'-Tetraethylnaphthalene-1,4-dicarboxamide

L.-H. Jing, L.-M. Zhou and D.-B. Qin

Comment

1,4-Naphthalenedicarboxylic acid derivatives are a class of intermediates important for applications as monomers in the preparation of polymers (Fukuzumi *et al.*, 1994; Tsukada *et al.*, 1994). Previously, we have reported the crystal structures of *N*,*N*'-bis(4-nitrophenyl)naphthalene-1,4-dicarboxamide dimethylsulfoxide disolvate (Jing *et al.*, 2006*b*) and *N*,*N*'-bis(2-methoxyphenyl)naphthalene-1,4-dicarboxamide (Jing *et al.*, 2006*a*). Herewith we report the crystal structure of the title compound, (I).

The naphthalene ring system in (I) is essentially planar, with a maximum deviation of 0.020 (1) Å for atoms C2 and C4. As a result of steric effects, two amide groups are twisted away from the naphthalene mean plane at 86.29 (4) and 84.06 (4)°, respectively (Fig. 1). The crystal packing is stabilized by intermolecular C—H···π interactions (Table 1).

Experimental

Naphthalene-1,4-dicarboxylic acid (2 mmol) and an excess of thionyl chloride (6 mmol) in dioxane (20 ml) were boiled under reflux for 6 h. The solution was distilled under reduced pressure and a yellow solid was formed. Diethylamine (4 mmol) in tetrahydrofuran (20 ml) was added to the yellow solid and boiled under reflux for 1 d. The solution was then cooled to ambient temperature and filtered to remove the tetrahydrofuran. The precipitate was dissolved in dimethylsulfoxide and allowed to stand for one month at ambient temperature to obtain white single crystals of (I) suitable for X-ray diffraction.

Refinement

The methyl group attached to atom C19 was treated as disordered between two postions with the occupancy factors fixed to 0.5. A ll H atoms were placed in calculated positions, with C—H = 0.95 and 0.98 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

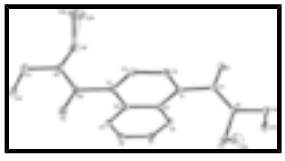


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids and atomic numbering. H atoms have been omitted for clarity.

N,*N*,*N*',*N*'-Tetraethylnaphthalene-1,4-dicarboxamide

Crystal data

$C_{20}H_{26}N_2O_2$ F_{000} = 1408

M_r = 326.43	D_x = 1.198 Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 23.1133 (14) Å	Cell parameters from 13310 reflections
b = 12.6202 (8) Å	θ = 3.2–27.5º
c = 12.9917 (9) Å	μ = 0.08 mm^{-1}
β = 107.293 (2)º	T = 153 (2) K
V = 3618.3 (4) Å^3	Block, white
Z = 8	0.58 × 0.52 × 0.51 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	3595 reflections with $I > 2\sigma(I)$
Radiation source: Rotating Anode	R_{int} = 0.020
Monochromator: graphite	θ_{max} = 27.5º
T = 153(2) K	θ_{min} = 3.2º
ω scans	h = −30→30
Absorption correction: none	k = −15→16
16253 measured reflections	l = −16→16
4142 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.039	H-atom parameters constrained
$wR(F^2)$ = 0.117	$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 1.926P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max} < 0.001$
4142 reflections	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
232 parameters	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
2 restraints	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0060 (5)

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 $F^2 > 2\text{sigma}(F^2)$ is used only for calculat-

ing *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}	Occ. (<1)
O1	0.34773 (4)	0.68029 (6)	0.68184 (6)	0.0331 (2)	
O2	0.35699 (4)	0.82048 (6)	0.14179 (6)	0.0341 (2)	
N1	0.35264 (4)	0.52131 (7)	0.60330 (7)	0.0250 (2)	
N2	0.35967 (4)	0.97548 (7)	0.23134 (7)	0.0279 (2)	
C1	0.35319 (5)	0.68534 (7)	0.50255 (8)	0.0218 (2)	
C2	0.30086 (5)	0.71488 (8)	0.42612 (8)	0.0248 (2)	
H2	0.2629	0.6929	0.4330	0.030*	
C3	0.30266 (5)	0.77771 (8)	0.33704 (8)	0.0253 (2)	
H3	0.2659	0.7991	0.2857	0.030*	
C4	0.35700 (5)	0.80788 (7)	0.32418 (8)	0.0224 (2)	
C5	0.46980 (5)	0.80461 (8)	0.38949 (9)	0.0272 (2)	
H5	0.4716	0.8444	0.3285	0.033*	
C6	0.52242 (5)	0.77531 (9)	0.46494 (10)	0.0322 (3)	
H6	0.5603	0.7946	0.4558	0.039*	
C7	0.52062 (5)	0.71644 (9)	0.55633 (10)	0.0329 (3)	
H7	0.5573	0.6971	0.6091	0.039*	
C8	0.46614 (5)	0.68711 (8)	0.56913 (9)	0.0274 (2)	
H8	0.4655	0.6470	0.6307	0.033*	
C9	0.41065 (4)	0.71556 (7)	0.49208 (8)	0.0215 (2)	
C10	0.41248 (5)	0.77666 (7)	0.40066 (8)	0.0218 (2)	
C11	0.35081 (4)	0.62789 (8)	0.60333 (8)	0.0228 (2)	
C12	0.36014 (5)	0.45706 (8)	0.51393 (9)	0.0297 (2)	
H12A	0.3924	0.4039	0.5431	0.036*	
H12B	0.3736	0.5035	0.4641	0.036*	
C13	0.30299 (7)	0.40049 (12)	0.45156 (11)	0.0508 (4)	
H13A	0.2885	0.3564	0.5008	0.061*	
H13B	0.3115	0.3556	0.3962	0.061*	
H13C	0.2719	0.4527	0.4171	0.061*	
C14	0.35801 (5)	0.46542 (9)	0.70497 (9)	0.0314 (3)	
H14A	0.3410	0.3931	0.6893	0.038*	
H14B	0.3345	0.5035	0.7458	0.038*	
C15	0.42378 (6)	0.45865 (10)	0.77230 (10)	0.0381 (3)	
H15A	0.4464	0.4164	0.7340	0.046*	
H15B	0.4265	0.4251	0.8416	0.046*	
H15C	0.4410	0.5301	0.7849	0.046*	
C16	0.35807 (5)	0.86896 (8)	0.22470 (8)	0.0241 (2)	
C17	0.36309 (6)	1.03641 (9)	0.13698 (9)	0.0331 (3)	
H17A	0.3455	1.1077	0.1387	0.040*	
H17B	0.3389	1.0003	0.0704	0.040*	
C18	0.42771 (6)	1.04733 (10)	0.13518 (11)	0.0409 (3)	
H18A	0.4509	1.0877	0.1984	0.049*	
H18B	0.4285	1.0846	0.0694	0.049*	

H18C	0.4457	0.9768	0.1365	0.049*	
C19	0.36776 (6)	1.03511 (9)	0.33181 (9)	0.0334 (3)	
H19A	0.4029	1.0830	0.3422	0.040*	
H19B	0.3777	0.9844	0.3927	0.040*	
C20	0.3140 (3)	1.1002 (6)	0.3370 (10)	0.0529 (18)	0.50
H20A	0.3067	1.1567	0.2829	0.064*	0.50
H20B	0.3222	1.1314	0.4089	0.064*	0.50
H20C	0.2781	1.0546	0.3224	0.064*	0.50
C20'	0.3074 (3)	1.0719 (6)	0.3415 (11)	0.0505 (17)	0.50
H20D	0.2849	1.1084	0.2751	0.061*	0.50
H20E	0.3141	1.1207	0.4026	0.061*	0.50
H20F	0.2841	1.0106	0.3530	0.061*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0496 (5)	0.0274 (4)	0.0282 (4)	0.0026 (3)	0.0206 (4)	−0.0021 (3)
O2	0.0510 (5)	0.0298 (4)	0.0235 (4)	−0.0028 (3)	0.0142 (3)	−0.0036 (3)
N1	0.0318 (5)	0.0210 (4)	0.0248 (4)	−0.0019 (3)	0.0124 (4)	0.0008 (3)
N2	0.0392 (5)	0.0224 (4)	0.0211 (4)	0.0019 (3)	0.0073 (4)	0.0028 (3)
C1	0.0283 (5)	0.0171 (4)	0.0225 (5)	0.0000 (3)	0.0112 (4)	−0.0014 (3)
C2	0.0249 (5)	0.0255 (5)	0.0259 (5)	−0.0024 (4)	0.0102 (4)	−0.0020 (4)
C3	0.0265 (5)	0.0257 (5)	0.0224 (5)	0.0007 (4)	0.0051 (4)	−0.0010 (4)
C4	0.0305 (5)	0.0173 (4)	0.0199 (4)	0.0003 (4)	0.0083 (4)	−0.0018 (3)
C5	0.0311 (5)	0.0234 (5)	0.0305 (5)	−0.0003 (4)	0.0143 (4)	0.0041 (4)
C6	0.0263 (5)	0.0310 (6)	0.0427 (6)	0.0002 (4)	0.0155 (5)	0.0060 (5)
C7	0.0256 (5)	0.0325 (6)	0.0393 (6)	0.0045 (4)	0.0077 (5)	0.0088 (5)
C8	0.0290 (5)	0.0244 (5)	0.0296 (5)	0.0032 (4)	0.0097 (4)	0.0071 (4)
C9	0.0262 (5)	0.0163 (4)	0.0238 (5)	0.0012 (3)	0.0100 (4)	−0.0003 (3)
C10	0.0275 (5)	0.0166 (4)	0.0234 (5)	0.0003 (3)	0.0104 (4)	−0.0006 (3)
C11	0.0239 (5)	0.0234 (5)	0.0235 (5)	−0.0003 (4)	0.0106 (4)	0.0007 (4)
C12	0.0392 (6)	0.0219 (5)	0.0303 (5)	0.0007 (4)	0.0138 (5)	−0.0032 (4)
C13	0.0576 (9)	0.0489 (8)	0.0423 (7)	−0.0142 (7)	0.0094 (6)	−0.0142 (6)
C14	0.0420 (6)	0.0247 (5)	0.0315 (6)	−0.0042 (4)	0.0174 (5)	0.0056 (4)
C15	0.0479 (7)	0.0330 (6)	0.0321 (6)	−0.0009 (5)	0.0100 (5)	0.0081 (5)
C16	0.0273 (5)	0.0239 (5)	0.0203 (5)	0.0002 (4)	0.0061 (4)	0.0007 (4)
C17	0.0454 (7)	0.0263 (5)	0.0251 (5)	0.0028 (5)	0.0065 (5)	0.0087 (4)
C18	0.0497 (8)	0.0346 (6)	0.0393 (6)	−0.0011 (5)	0.0146 (6)	0.0114 (5)
C19	0.0489 (7)	0.0226 (5)	0.0268 (5)	0.0010 (5)	0.0083 (5)	−0.0019 (4)
C20	0.076 (3)	0.045 (4)	0.039 (2)	0.030 (3)	0.018 (2)	−0.001 (3)
C20'	0.075 (3)	0.036 (3)	0.038 (2)	0.026 (2)	0.014 (2)	0.004 (3)

Geometric parameters (Å, °)

O1—C11	1.2352 (12)	C12—H12A	0.9900
O2—C16	1.2326 (12)	C12—H12B	0.9900
N1—C11	1.3458 (13)	C13—H13A	0.9800
N1—C12	1.4681 (13)	C13—H13B	0.9800
N1—C14	1.4697 (13)	C13—H13C	0.9800

N2—C16	1.3469 (14)	C14—C15	1.5142 (17)
N2—C17	1.4691 (13)	C14—H14A	0.9900
N2—C19	1.4697 (13)	C14—H14B	0.9900
C1—C2	1.3689 (14)	C15—H15A	0.9800
C1—C9	1.4265 (13)	C15—H15B	0.9800
C1—C11	1.5119 (13)	C15—H15C	0.9800
C2—C3	1.4137 (14)	C17—C18	1.5068 (18)
C2—H2	0.9500	C17—H17A	0.9900
C3—C4	1.3694 (14)	C17—H17B	0.9900
C3—H3	0.9500	C18—H18A	0.9800
C4—C10	1.4245 (14)	C18—H18B	0.9800
C4—C16	1.5113 (13)	C18—H18C	0.9800
C5—C6	1.3668 (16)	C19—C20	1.507 (3)
C5—C10	1.4196 (14)	C19—C20'	1.510 (3)
C5—H5	0.9500	C19—H19A	0.9900
C6—C7	1.4116 (16)	C19—H19B	0.9900
C6—H6	0.9500	C20—H20A	0.9800
C7—C8	1.3693 (15)	C20—H20B	0.9800
C7—H7	0.9500	C20—H20C	0.9800
C8—C9	1.4187 (14)	C20'—H20D	0.9800
C8—H8	0.9500	C20'—H20E	0.9800
C9—C10	1.4271 (13)	C20'—H20F	0.9800
C12—C13	1.5083 (17)		
C11—N1—C12	124.29 (8)	H13A—C13—H13C	109.5
C11—N1—C14	118.28 (8)	H13B—C13—H13C	109.5
C12—N1—C14	116.57 (8)	N1—C14—C15	110.38 (9)
C16—N2—C17	118.44 (9)	N1—C14—H14A	109.6
C16—N2—C19	124.18 (8)	C15—C14—H14A	109.6
C17—N2—C19	116.68 (9)	N1—C14—H14B	109.6
C2—C1—C9	120.33 (9)	C15—C14—H14B	109.6
C2—C1—C11	120.47 (9)	H14A—C14—H14B	108.1
C9—C1—C11	119.03 (9)	C14—C15—H15A	109.5
C1—C2—C3	120.79 (9)	C14—C15—H15B	109.5
C1—C2—H2	119.6	H15A—C15—H15B	109.5
C3—C2—H2	119.6	C14—C15—H15C	109.5
C4—C3—C2	120.47 (9)	H15A—C15—H15C	109.5
C4—C3—H3	119.8	H15B—C15—H15C	109.5
C2—C3—H3	119.8	O2—C16—N2	122.98 (9)
C3—C4—C10	120.40 (9)	O2—C16—C4	119.54 (9)
C3—C4—C16	119.66 (9)	N2—C16—C4	117.48 (8)
C10—C4—C16	119.84 (9)	N2—C17—C18	111.12 (9)
C6—C5—C10	121.20 (10)	N2—C17—H17A	109.4
C6—C5—H5	119.4	C18—C17—H17A	109.4
C10—C5—H5	119.4	N2—C17—H17B	109.4
C5—C6—C7	120.21 (10)	C18—C17—H17B	109.4
C5—C6—H6	119.9	H17A—C17—H17B	108.0
C7—C6—H6	119.9	C17—C18—H18A	109.5
C8—C7—C6	120.17 (10)	C17—C18—H18B	109.5
C8—C7—H7	119.9	H18A—C18—H18B	109.5

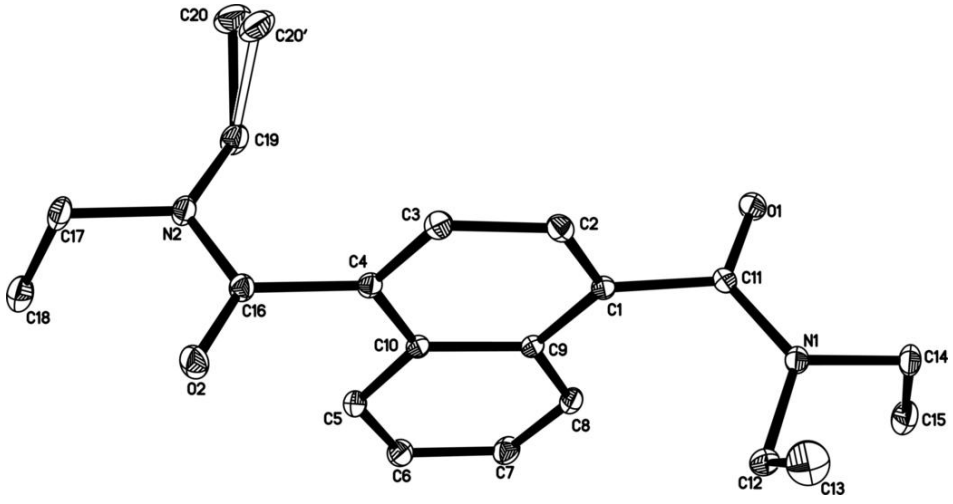
C6—C7—H7	119.9	C17—C18—H18C	109.5
C7—C8—C9	121.13 (10)	H18A—C18—H18C	109.5
C7—C8—H8	119.4	H18B—C18—H18C	109.5
C9—C8—H8	119.4	N2—C19—C20	115.4 (5)
C8—C9—C1	122.48 (9)	N2—C19—C20'	110.8 (5)
C8—C9—C10	118.67 (9)	C20—C19—C20'	15.2 (6)
C1—C9—C10	118.85 (9)	N2—C19—H19A	108.4
C5—C10—C4	122.26 (9)	C20—C19—H19A	108.4
C5—C10—C9	118.61 (9)	C20'—C19—H19A	122.8
C4—C10—C9	119.13 (9)	N2—C19—H19B	108.4
O1—C11—N1	123.01 (9)	C20—C19—H19B	108.4
O1—C11—C1	118.96 (9)	C20'—C19—H19B	97.7
N1—C11—C1	118.02 (8)	H19A—C19—H19B	107.5
N1—C12—C13	113.33 (10)	C19—C20—H20A	109.5
N1—C12—H12A	108.9	C19—C20—H20B	109.5
C13—C12—H12A	108.9	C19—C20—H20C	109.5
N1—C12—H12B	108.9	C19—C20'—H20D	109.5
C13—C12—H12B	108.9	C19—C20'—H20E	109.5
H12A—C12—H12B	107.7	H20D—C20'—H20E	109.5
C12—C13—H13A	109.5	C19—C20'—H20F	109.5
C12—C13—H13B	109.5	H20D—C20'—H20F	109.5
H13A—C13—H13B	109.5	H20E—C20'—H20F	109.5
C12—C13—H13C	109.5		
C9—C1—C2—C3	−1.47 (15)	C14—N1—C11—O1	−6.97 (15)
C11—C1—C2—C3	173.66 (9)	C12—N1—C11—C1	3.49 (14)
C1—C2—C3—C4	1.69 (15)	C14—N1—C11—C1	172.50 (9)
C2—C3—C4—C10	−0.22 (15)	C2—C1—C11—O1	−86.37 (12)
C2—C3—C4—C16	176.03 (9)	C9—C1—C11—O1	88.83 (12)
C10—C5—C6—C7	−0.20 (17)	C2—C1—C11—N1	94.14 (11)
C5—C6—C7—C8	0.91 (18)	C9—C1—C11—N1	−90.67 (11)
C6—C7—C8—C9	−0.50 (18)	C11—N1—C12—C13	−107.46 (12)
C7—C8—C9—C1	179.36 (10)	C14—N1—C12—C13	83.36 (12)
C7—C8—C9—C10	−0.59 (16)	C11—N1—C14—C15	−84.26 (12)
C2—C1—C9—C8	179.88 (9)	C12—N1—C14—C15	85.60 (12)
C11—C1—C9—C8	4.68 (14)	C17—N2—C16—O2	−2.88 (16)
C2—C1—C9—C10	−0.16 (14)	C19—N2—C16—O2	−172.93 (10)
C11—C1—C9—C10	−175.37 (8)	C17—N2—C16—C4	177.68 (9)
C6—C5—C10—C4	178.83 (10)	C19—N2—C16—C4	7.63 (15)
C6—C5—C10—C9	−0.88 (15)	C3—C4—C16—O2	−85.72 (12)
C3—C4—C10—C5	178.89 (9)	C10—C4—C16—O2	90.55 (12)
C16—C4—C10—C5	2.65 (14)	C3—C4—C16—N2	93.73 (12)
C3—C4—C10—C9	−1.40 (14)	C10—C4—C16—N2	−90.00 (12)
C16—C4—C10—C9	−177.64 (8)	C16—N2—C17—C18	−84.91 (12)
C8—C9—C10—C5	1.26 (14)	C19—N2—C17—C18	85.89 (12)
C1—C9—C10—C5	−178.69 (9)	C16—N2—C19—C20	−113.5 (4)
C8—C9—C10—C4	−178.46 (9)	C17—N2—C19—C20	76.3 (4)
C1—C9—C10—C4	1.58 (14)	C16—N2—C19—C20'	−97.8 (3)
C12—N1—C11—O1	−175.98 (10)	C17—N2—C19—C20'	92.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15B···Cg^{i}	0.98	2.78	3.643 (2)	147
C18—H18B···Cg^{ii}	0.98	2.72	3.586 (2)	148

Symmetry codes: (i) −*x*+1/2, *y*+1/2, −*z*−1/2; (ii) −*x*+1/2, *y*+3/2, −*z*+1/2.

Fig. 1


C20
C20'
C19
C17
N2
C3
C2
O1
C4
C11
C18
C16
C1
C10
C9
N1
C14
O2
C5
C8
C15
C6
C7
C12
C13