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N,*N*′-Bis(2-phenylethyl)naphthalene-1,8:4,5-bis(dicarboximide)

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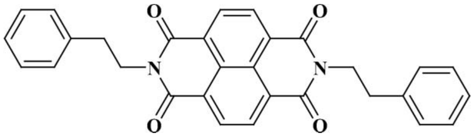
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.123; data-to-parameter ratio = 12.2.

The title compound, $C_{30}H_{22}N_2O_4$, is a derivative of the naphthalene–imide pigments that are characterized by significant overlap of the stacked molecules. The molecule has a centre of symmetry. Accordingly, the phenylethyl groups are arranged in a *trans* fashion across the skeleton. The phenyl rings are not parallel to the naphthaleneimide skeleton and are twisted in the same direction by 9.27 (7)°. The molecules are, however, stacked with insignificant overlap along the stacking axis, as characterized by appreciable slide in the direction of either the short or the long molecular axis, in marked contrast to the ordinary naphthalene–imide pigments.

Related literature

For perylene and perinone pigments, see: Herbst & Hunger (2004). Five structural studies of related compounds have been reported by Mizuguchi (2003*a*,*b*, 2004), Mizuguchi *et al.* (2005) and Tsukada *et al.* (2007). For ethyl phenylperylene-imide-related papers, see: Hädicke & Graser (1986), Mizuguchi (1998*a*,*b*, 2005*a*,*b*), Mizuguchi & Tojo (2002), Mizuguchi & Hino (2005), Mizuguchi *et al.* (2006). For related literature, see: Hino & Mizuguchi (2005); Mizuguchi (1981); Mizuguchi & Shimo (2006).



Experimental

Crystal data

$C_{30}H_{22}N_2O_4$
M_r = 474.50
Monoclinic, $P2_1/n$
a = 7.70264 (14) Å
b = 4.93695 (9) Å
c = 29.9857 (5) Å
β = 97.9096 (7)°
V = 1129.44 (3) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 0.76 mm^{-1}
T = 93 (1) K
0.5 × 0.14 × 0.06 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.790, T_{max} = 0.955
9315 measured reflections
1993 independent reflections
1723 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.124
S = 1.13
1993 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2006); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *CrystalStructure*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2244).

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N,*N*′-Bis(2-phenylethyl)naphthalene-1,8:4,5-bis(dicarboximide)

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S1. Comment

The title compound (PhENI) is a derivative of the naphthalene-imides which belongs to the category of perylene and perinone pigments (Herbst & Hunger, 2004). The difference between the perylene and perinone pigments is whether the central skeleton is perylene or naphthalene. Both pigments are typically characterized by close π-π stacks (Hädicke & Graser, 1986; Mizuguchi, 1998*a*, 2004; Mizuguchi & Shimo, 2006), giving rise to an additional absorption band in the visible region due to intermolecular excitonic interactions (Mizuguchi, 1998*b*). However, the present band disappears in the amorphous state where the molecules are randomly arranged. Accordingly, the color varies drastically from an amorphous phase to the crystalline one, as found in ethylphenylperyleneimide (EPhP), in which the naphthalene skeleton in PhENI is replaced by the perylene one (Mizuguchi, 1998*b*). Then, we struck on an idea that it would be ideal for electronic paper applications if the color change occurs in much shorter wavelength (for example, between colorless and blue) with a smaller chromphore such as PhENI. In this connection, an attempt has been made to synthesize PhENI and determine its crystal structure.

The title molecule is centrosymmetric (Fig. 1) and an asymmetric unit comprises a half of the molecule. Therefore, ethylphenyl groups are arranged in a *trans* fashion across the naphthaleneimide skeleton. The naphthalene-imide skeleton is entirely planar as indicated by a small deviation of 0.018 Å from the least-squares plane defined by atoms C1—C7/N1. The phenyl rings and the napthaleneimide skeleton are not in parallel, but twisted by 9.27 (7)°. Fig. 2 shows the molecular packing of PhENI. The molecules are stacked with insignificant overlap as characterized by significant slide in the direction of the short-molecular axis, quite in contrast to the ordinary naphthalene-imides (Mizuguchi, 2003*a*,b) and peryelene- imide pigments (Hädicke & Graser, 1986; Mizuguchi, 1998*a*, 2005*a*,b) where the molecules are directly stacked with an interplanar distance of about 3.3 - 3.5 Å. Since the π-π interactions are insignificant in PhENI, this compound gives no additional absorption band in the visible region and cannot be applied to electronic paper applications.

S2. Experimental

PhENI was synthesized by reaction of naphthalene-1,4,5,8-tetra-carboxylic-dianhydride with 2-phenylethylamine at 403 K for 5 h. Then, the products were purified two times by sublimation under vacuum, using a five-zone furnace (Mizuguchi, 1981). Single crystals of PhENI were grown from solution in dimethylsulfoxide. After 36 h, a number of single crystals were obtained in the form of needles.

S3. Refinement

All H atoms were placed in geometrically idealized position and constrained to ride on their parent atoms, with C—H = 0.95 and 0.99 Å, and $U_{iso}(H) = 1.2U_{eq}(C)$

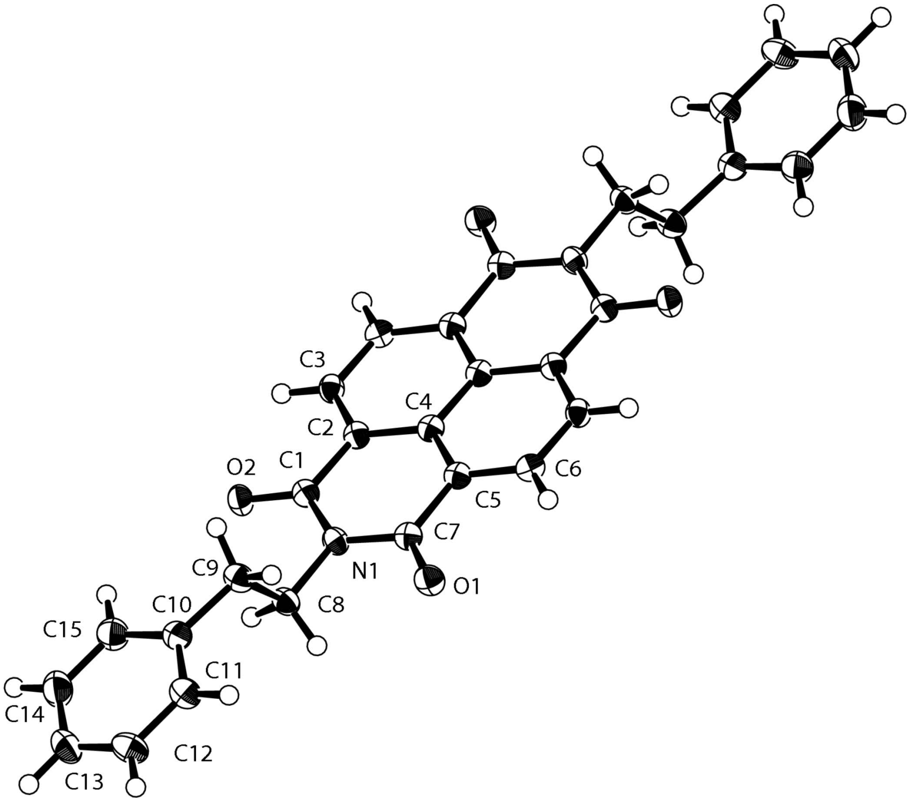

Figure 1

The molecular structure of (I) with the 50% displacement parameters. Unlabelled atoms are related by the symmetry code (1 - *x*, 1 - *y*, 1 - *z*).

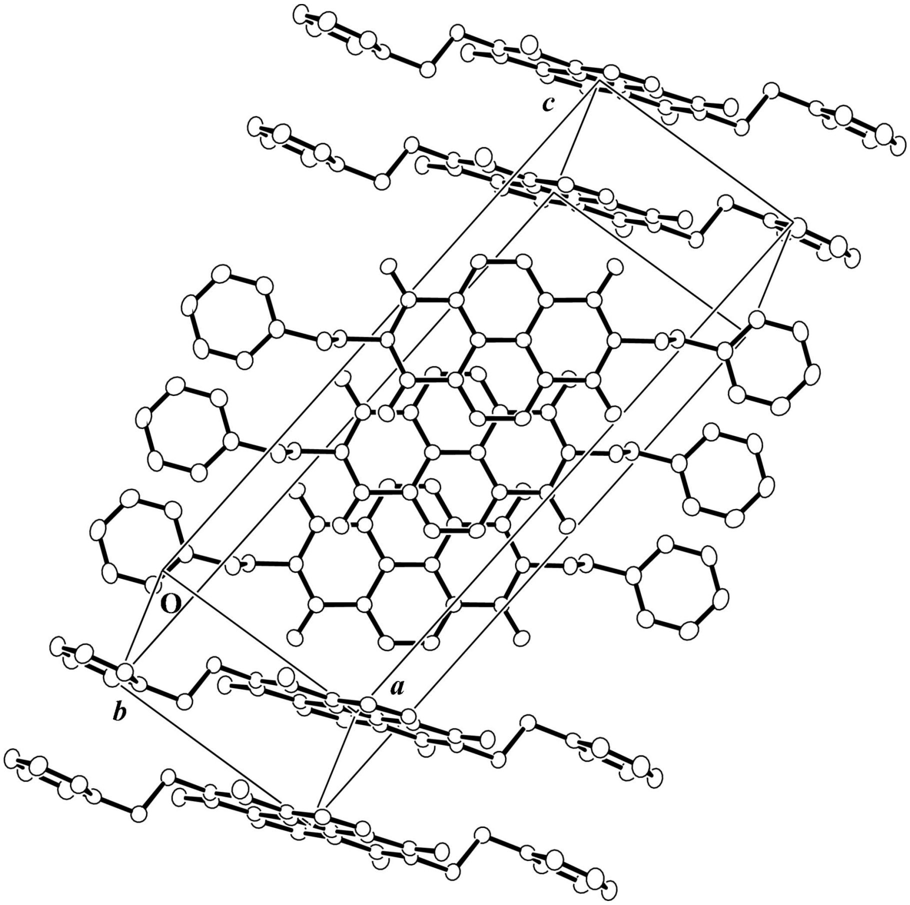

Figure 2

The crystal packing of PhENI. All H atoms have been omitted for clarity.

N,*N′*-Bis(2-phenylethyl)naphthalene-1,8:4,5-bis(dicarboximide)

Crystal data

$C_{30}H_{22}N_2O_4$
$M_r = 474.50$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.70264$ (14) Å
$b = 4.93695$ (9) Å
$c = 29.9857$ (5) Å
$\beta = 97.9096$ (7)°
$V = 1129.44$ (3) Å^3
$Z = 2$

$F(000) = 496.00$
$D_x = 1.395$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54187$ Å
Cell parameters from 7242 reflections
$\theta = 3.0$–68.2°
$\mu = 0.76$ mm^{-1}
$T = 93$ K
Needle, red
0.5 × 0.14 × 0.06 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.00 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)

$T_{min} = 0.790$, $T_{max} = 0.955$
9315 measured reflections
1993 independent reflections
1723 reflections with $F^2 > 2\sigma(F^2)$
$R_{int} = 0.033$
$\theta_{max} = 68.2°$

$h = -9 \rightarrow 9$
$k = -5 \rightarrow 5$
$l = -36 \rightarrow 36$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.124$
$S = 1.13$
1993 reflections
163 parameters
0 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.066P)^2 + 0.3352P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ 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^ > *σ*(*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	$U_{iso}*/U_{eq}$
O1	0.76514 (14)	0.4835 (2)	0.39308 (3)	0.0292 (3)
O2	0.47967 (13)	−0.2072 (2)	0.45229 (3)	0.0276 (3)
N1	0.62139 (16)	0.1417 (2)	0.42345 (4)	0.0229 (3)
C5	0.9302 (2)	0.2343 (3)	0.45209 (5)	0.0220 (3)
C4	0.92479 (19)	0.0265 (3)	0.48430 (5)	0.0208 (3)
C1	0.61317 (19)	−0.0739 (3)	0.45314 (5)	0.0229 (3)
C7	0.7696 (2)	0.3000 (3)	0.42016 (5)	0.0229 (3)
C2	0.77252 (19)	−0.1294 (3)	0.48570 (5)	0.0218 (3)
C6	1.0809 (2)	0.3834 (3)	0.45135 (5)	0.0235 (3)
C8	0.4594 (2)	0.2050 (3)	0.39298 (5)	0.0256 (3)
C10	0.2576 (2)	0.0767 (3)	0.32490 (5)	0.0261 (3)
C3	0.7698 (2)	−0.3308 (3)	0.51738 (5)	0.0232 (3)
C11	0.2122 (2)	0.2694 (3)	0.29170 (5)	0.0298 (4)
C12	0.0387 (2)	0.2994 (4)	0.27250 (6)	0.0351 (4)
C15	0.1263 (2)	−0.0841 (3)	0.33819 (6)	0.0341 (4)
C14	−0.0470 (2)	−0.0537 (4)	0.31927 (6)	0.0385 (4)
C9	0.4439 (2)	0.0522 (3)	0.34836 (5)	0.0273 (3)
C13	−0.0910 (2)	0.1393 (4)	0.28624 (6)	0.0360 (4)
H8b	0.4558	0.4020	0.3868	0.031*
H8a	0.3572	0.1598	0.4083	0.031*
H9b	0.5262	0.1294	0.3291	0.033*
H9a	0.4741	−0.1410	0.3539	0.033*
H11	0.3001	0.3814	0.2821	0.036*
H12	0.0090	0.4314	0.2497	0.042*

H15	0.1559	−0.2178	0.3607	0.041*
H14	−0.1353	−0.1651	0.3289	0.046*
H13	−0.2096	0.1616	0.2731	0.043*
H6	1.0838	0.5225	0.4296	0.028*
H3	0.6664	−0.4347	0.5181	0.028*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0300 (6)	0.0317 (7)	0.0252 (6)	−0.0004 (4)	0.0009 (4)	0.0065 (4)
O2	0.0227 (5)	0.0297 (7)	0.0301 (6)	−0.0049 (4)	0.0019 (4)	0.0004 (4)
N1	0.0213 (6)	0.0269 (8)	0.0199 (6)	−0.0006 (5)	0.0004 (4)	−0.0005 (5)
C5	0.0239 (8)	0.0232 (8)	0.0193 (7)	0.0007 (6)	0.0046 (5)	−0.0024 (6)
C4	0.0232 (7)	0.0218 (8)	0.0182 (7)	0.0002 (6)	0.0055 (5)	−0.0027 (5)
C1	0.0234 (7)	0.0251 (9)	0.0204 (7)	−0.0000 (6)	0.0041 (5)	−0.0034 (6)
C7	0.0256 (8)	0.0248 (9)	0.0187 (7)	0.0008 (6)	0.0038 (6)	−0.0023 (6)
C2	0.0230 (7)	0.0235 (9)	0.0194 (7)	−0.0006 (6)	0.0043 (5)	−0.0034 (5)
C6	0.0277 (8)	0.0235 (9)	0.0200 (7)	0.0005 (6)	0.0055 (6)	0.0014 (6)
C8	0.0221 (7)	0.0290 (9)	0.0248 (8)	0.0012 (6)	−0.0003 (6)	−0.0002 (6)
C10	0.0274 (8)	0.0287 (9)	0.0219 (7)	0.0019 (6)	0.0021 (6)	−0.0055 (6)
C3	0.0218 (7)	0.0248 (9)	0.0240 (7)	−0.0029 (6)	0.0063 (6)	−0.0028 (6)
C11	0.0287 (8)	0.0343 (10)	0.0262 (8)	0.0010 (7)	0.0037 (6)	0.0010 (7)
C12	0.0331 (9)	0.0436 (11)	0.0274 (8)	0.0083 (7)	0.0000 (6)	0.0055 (7)
C15	0.0346 (9)	0.0338 (10)	0.0327 (9)	−0.0009 (7)	0.0000 (7)	0.0047 (7)
C14	0.0325 (9)	0.0385 (11)	0.0437 (10)	−0.0077 (8)	0.0028 (7)	0.0013 (8)
C9	0.0261 (8)	0.0323 (9)	0.0230 (7)	0.0035 (7)	0.0014 (6)	−0.0014 (6)
C13	0.0252 (8)	0.0460 (11)	0.0348 (9)	−0.0001 (7)	−0.0029 (6)	−0.0049 (8)

Geometric parameters (Å, º)

O1—C7	1.2138 (19)	C8—H8a	0.990
O2—C1	1.2182 (18)	C10—C11	1.387 (2)
N1—C1	1.395 (2)	C10—C15	1.387 (2)
N1—C7	1.398 (2)	C10—C9	1.513 (2)
N1—C8	1.4749 (18)	C3—H3	0.950
C5—C4	1.414 (2)	C11—C12	1.388 (2)
C5—C7	1.492 (2)	C11—H11	0.950
C5—C6	1.377 (2)	C12—C13	1.380 (2)
C4—C4^{i}	1.4131 (19)	C12—H12	0.950
C4—C2	1.408 (2)	C15—C14	1.385 (2)
C1—C2	1.4849 (19)	C15—H15	0.950
C2—C3	1.377 (2)	C14—C13	1.383 (2)
C6—C3^{i}	1.405 (2)	C14—H14	0.950
C6—H6	0.950	C9—H9b	0.990
C8—C9	1.526 (2)	C9—H9a	0.990
C8—H8b	0.990	C13—H13	0.950
O1···O2^{ii}	3.3754 (15)	C7···C1^{ii}	3.509 (2)

O1···N1^{ii}	3.5905 (17)	C7···C2^{ii}	3.433 (2)
O1···C1^{ii}	3.1573 (19)	C7···C3^{ii}	3.438 (2)
O1···C2^{ii}	3.3654 (18)	C2···O1^{iii}	3.3654 (18)
O2···O1^{iii}	3.3754 (15)	C2···O2^{iv}	3.3145 (19)
O2···O2^{iv}	3.4962 (14)	C2···C5^{iii}	3.563 (2)
O2···N1^{iii}	3.5401 (17)	C2···C7^{iii}	3.433 (2)
O2···C1^{iv}	3.3222 (18)	C6···C5^{vi}	3.467 (2)
O2···C7^{iii}	3.5251 (19)	C6···C4^{ii}	3.581 (2)
O2···C2^{iv}	3.3145 (19)	C6···C4^{vi}	3.498 (2)
O2···C8^{iii}	3.396 (2)	C6···C6^{vi}	3.520 (2)
O2···C3^{v}	3.1941 (19)	C6···C3^{ii}	3.600 (2)
O2···C3^{iv}	3.4719 (19)	C8···O2^{ii}	3.396 (2)
N1···O1^{iii}	3.5905 (17)	C8···C3^{iv}	3.469 (2)
N1···O2^{ii}	3.5401 (17)	C3···O2^{v}	3.1941 (19)
C5···C2^{ii}	3.563 (2)	C3···O2^{iv}	3.4719 (19)
C5···C6^{vi}	3.467 (2)	C3···C5^{iii}	3.261 (2)
C5···C3^{ii}	3.261 (2)	C3···C4^{iii}	3.578 (2)
C4···C6^{iii}	3.581 (2)	C3···C7^{iii}	3.438 (2)
C4···C6^{vi}	3.498 (2)	C3···C6^{iii}	3.600 (2)
C4···C3^{ii}	3.578 (2)	C3···C8^{iv}	3.469 (2)
C1···O1^{iii}	3.1573 (19)	C11···C15^{ii}	3.581 (2)
C1···O2^{iv}	3.3222 (18)	C12···C14^{ii}	3.586 (2)
C1···C1^{iv}	3.580 (2)	C15···C11^{iii}	3.581 (2)
C1···C7^{iii}	3.509 (2)	C14···C12^{iii}	3.586 (2)
C7···O2^{ii}	3.5251 (19)		

C1—N1—C7	125.52 (11)	C11—C10—C15	118.49 (14)
C1—N1—C8	116.63 (12)	C11—C10—C9	121.22 (14)
C7—N1—C8	117.85 (12)	C15—C10—C9	120.19 (14)
C4—C5—C7	119.79 (13)	C2—C3—C6^{i}	120.32 (14)
C4—C5—C6	120.19 (13)	C2—C3—H3	119.8
C7—C5—C6	119.96 (14)	C6^{i}—C3—H3	119.8
C5—C4—C4^{i}	119.41 (13)	C10—C11—C12	120.30 (16)
C5—C4—C2	121.31 (12)	C10—C11—H11	119.8
C4^{i}—C4—C2	119.28 (13)	C12—C11—H11	119.9
O2—C1—N1	120.75 (12)	C11—C12—C13	120.66 (16)
O2—C1—C2	122.22 (14)	C11—C12—H12	119.7
N1—C1—C2	117.03 (12)	C13—C12—H12	119.7
O1—C7—N1	121.08 (13)	C10—C15—C14	121.36 (16)
O1—C7—C5	122.44 (14)	C10—C15—H15	119.3
N1—C7—C5	116.48 (13)	C14—C15—H15	119.3
C4—C2—C1	119.75 (13)	C15—C14—C13	119.69 (17)
C4—C2—C3	120.46 (13)	C15—C14—H14	120.2
C1—C2—C3	119.79 (13)	C13—C14—H14	120.2
C5—C6—C3^{i}	120.34 (14)	C8—C9—C10	108.83 (13)
C5—C6—H6	119.8	C8—C9—H9b	109.9
C3^{i}—C6—H6	119.8	C8—C9—H9a	109.9
N1—C8—C9	113.32 (13)	C10—C9—H9b	109.9

N1—C8—H8b	108.9	C10—C9—H9a	109.9
N1—C8—H8a	108.9	H9b—C9—H9a	108.3
C9—C8—H8b	108.9	C12—C13—C14	119.50 (15)
C9—C8—H8a	108.9	C12—C13—H13	120.3
H8b—C8—H8a	107.7	C14—C13—H13	120.3

C1—N1—C7—O1	179.62 (14)	C5—C4—C2—C3	−179.92 (15)
C1—N1—C7—C5	−1.5 (2)	C4$^{\mathrm{i}}$—C4—C2—C1	179.44 (14)
C7—N1—C1—O2	−177.03 (14)	C4$^{\mathrm{i}}$—C4—C2—C3	0.2 (2)
C7—N1—C1—C2	3.7 (2)	C2—C4—C4$^{\mathrm{i}}$—C5$^{\mathrm{i}}$	−0.1 (2)
C1—N1—C8—C9	−90.00 (16)	O2—C1—C2—C4	178.20 (14)
C8—N1—C1—O2	2.6 (2)	O2—C1—C2—C3	−2.5 (2)
C8—N1—C1—C2	−176.64 (13)	N1—C1—C2—C4	−2.5 (2)
C7—N1—C8—C9	89.70 (17)	N1—C1—C2—C3	176.75 (14)
C8—N1—C7—O1	−0.05 (19)	C4—C2—C3—C6$^{\mathrm{i}}$	−0.1 (2)
C8—N1—C7—C5	178.80 (13)	C1—C2—C3—C6$^{\mathrm{i}}$	−179.37 (14)
C4—C5—C7—O1	176.99 (15)	C5—C6—C3$^{\mathrm{i}}$—C2$^{\mathrm{i}}$	0.1 (2)
C4—C5—C7—N1	−1.8 (2)	N1—C8—C9—C10	166.24 (13)
C7—C5—C4—C2	2.9 (2)	C11—C10—C15—C14	−0.5 (2)
C7—C5—C4—C4$^{\mathrm{i}}$	−177.23 (14)	C15—C10—C11—C12	0.2 (2)
C4—C5—C6—C3$^{\mathrm{i}}$	−0.1 (2)	C11—C10—C9—C8	97.43 (17)
C6—C5—C4—C2	−179.84 (15)	C9—C10—C11—C12	−176.13 (16)
C6—C5—C4—C4$^{\mathrm{i}}$	0.1 (2)	C15—C10—C9—C8	−78.79 (19)
C7—C5—C6—C3$^{\mathrm{i}}$	177.15 (14)	C9—C10—C15—C14	175.83 (16)
C6—C5—C7—O1	−0.3 (2)	C10—C11—C12—C13	0.3 (2)
C6—C5—C7—N1	−179.15 (14)	C11—C12—C13—C14	−0.4 (2)
C5—C4—C4$^{\mathrm{i}}$—C2$^{\mathrm{i}}$	0.1 (2)	C10—C15—C14—C13	0.4 (2)
C5—C4—C2—C1	−0.6 (2)	C15—C14—C13—C12	0.1 (2)

Symmetry codes: (i) −*x*+2, −*y*, −*z*+1; (ii) *x*, *y*+1, *z*; (iii) *x*, *y*−1, *z*; (iv) −*x*+1, −*y*, −*z*+1; (v) −*x*+1, −*y*−1, −*z*+1; (vi) −*x*+2, −*y*+1, −*z*+1.