

N,N'-Bis[2-(4-pyridyl)ethyl]naphthalene-1,8:4,5-bis(dicarboximide)

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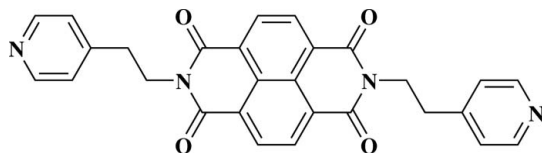
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 Key indicators: single-crystal X-ray study; $T = 93$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.037; wR factor = 0.123; data-to-parameter ratio = 11.6.

The title compound, $\text{C}_{28}\text{H}_{20}\text{N}_4\text{O}_4$, is an organic pigment. The molecule has C_i symmetry. Accordingly, the pyridylethyl groups are arranged in a *trans* fashion across the naphthalene-imide skeleton. The interplanar distance between the two aromatic systems is 12.846 (2) Å and this clearly indicates a lack of π - π interactions, as also shown by similar spectra in solution and in the solid state.

Related literature

Three related structural studies of the peryleneimide system have been reported: the solvent-free compound (Tojo & Mizuguchi, 2002), the phenol-solvated compound (Mizuguchi & Hino, 2005) and the cresol-solvated compound (Hino & Mizuguchi, 2005). For related literature, see: Herbst & Hunger (1993); Mizuguchi *et al.* (2006).



Experimental

Crystal data

 $\text{C}_{28}\text{H}_{20}\text{N}_4\text{O}_4$
 $M_r = 476.48$
 Monoclinic, $P2_1/n$
 $a = 10.0900$ (16) Å
 $b = 8.8239$ (15) Å
 $c = 12.846$ (2) Å
 $\beta = 105.811$ (10)°

 $V = 1100.5$ (3) Å³
 $Z = 2$
 Cu $K\alpha$ radiation
 $\mu = 0.81$ mm⁻¹
 $T = 93.1$ K
 $0.50 \times 0.14 \times 0.13$ mm

Data collection

 Rigaku R-AXIS RAPID
 diffractometer
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.881$, $T_{\max} = 0.900$

 9001 measured reflections
 1909 independent reflections
 1751 reflections with $F^2 > 2\sigma(F^2)$
 $R_{\text{int}} = 0.021$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.123$
 $S = 0.94$
 1909 reflections

 164 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.20$ e Å⁻³
 $\Delta\rho_{\min} = -0.28$ e Å⁻³

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK, 2006); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2003); 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: KP2131).

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supplementary materials

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N,N'-Bis[2-(4-pyridyl)ethyl]naphthalene-1,8:4,5-bis(dicarboximide)

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Comment

The title compound (PyENI) is an organic pigment which belongs to the category of perylene and perinone pigments (Herbst & Hunger, 1993). The perylene and perinone pigments differ in the central skeleton being perylene or naphthalene, respectively. We were previously involved in the study of the crystal and electronic structures of pyridylethynaphthaleneimide (PyEPI) (Mizuguchi *et al.*, 2006). In PyEPI there are two structural isomers in the solid state: the *cis* form (two pyridylethyl groups are on the same side as characterized by vivid red color; Tojo & Mizuguchi, 2002) and the *trans* form (across the perylene skeleton as characterized by black color; Mizuguchi & Hino, 2005; Hino & Mizuguchi, 2005). Surprising to say, the *trans* form (black) is found to be easily transformed into the *cis* one (red) by heating above 373 K for several s. This phase transformation has prompted us to investigate the crystal structure of PyENI in order to study whether the similar phenomenon occurs at the shorter wavelengths.

The title molecule is centrosymmetric (Fig. 1) and an asymmetric unit comprises a half of the molecule. Therefore, pyridylethyl groups are arranged in a *trans* fashion across the naphthaleneimide skeleton. The pyridyl rings and naphthaleneimide skeleton are twisted by 9.45 (5)°. The crystal packing of (I) (Fig. 2) is dominated by van der Waals interactions. The present molecular arrangement of PyENI contrasts remarkably with that of PyEPI where the molecules are involved in $\pi \cdots \pi$ interactions with separation distance of about 3.3 – 3.5 Å.

Experimental

PyENI was synthesized by reaction of naphthalenetetracarboxylic dianhydride with 1,2-(4-pyridyl)diamine in dimethylnaphthalene at 453 K for 7 h according to the method reported (Herbst & Hunger, 1993). Single crystals of PyENI were grown by recrystallization from solution in dimethylsulfoxide. After 36 h platelet crystals suitable for X-ray analysis were obtained.

Refinement

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

Figures

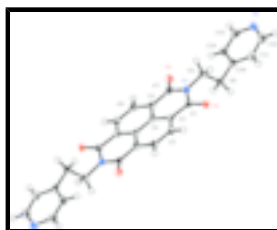


Fig. 1. The molecular structure of (I) with the 50% displacement parameters. Unlabelled atoms are related by the symmetry code (1 - x, 1 - y, 1 - z).

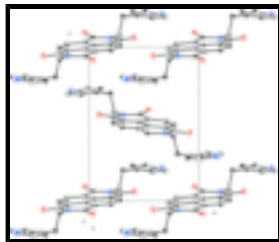


Fig. 2. The crystal packing viewed along the axis *a*. All the H atoms have been omitted for clarity.

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Crystal data

$C_{28}H_{20}N_4O_4$

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Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1n$

$a = 10.0900$ (16) Å

$b = 8.8239$ (15) Å

$c = 12.846$ (2) Å

$\beta = 105.811$ (10)°

$V = 1100.5$ (3) Å³

$Z = 2$

$F_{000} = 496.00$

$D_x = 1.438$ Mg m⁻³

Cu $K\alpha$ radiation

$\lambda = 1.54187$ Å

Cell parameters from 8499 reflections

$\theta = 3.6$ – 68.2 °

$\mu = 0.81$ mm⁻¹

$T = 93.1$ K

Platelet, light brown

$0.50 \times 0.14 \times 0.13$ mm

Data collection

Rigaku R-Axis RAPID
diffractometer

Detector resolution: 10.00 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(ABSCOR; Higashi, 1995)

$T_{\min} = 0.881$, $T_{\max} = 0.900$

9001 measured reflections

1909 independent reflections

1751 reflections with $F^2 > 2\sigma(F^2)$

$R_{\text{int}} = 0.021$

$\theta_{\text{max}} = 68.2$ °

$h = -12 \rightarrow 12$

$k = -9 \rightarrow 9$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.123$

$S = 0.94$

1909 reflections

164 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.2956P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.20$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.28$ e Å⁻³

Extinction correction: none

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 was performed using all reflections. The weighted R -factor (wR) and goodness of fit (S) are based on F^2 . R -factor (gt) are based on F . The threshold expression of $F^2 > 2 \text{ sigma}(F^2)$ is used only for calculating R -factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.63037 (9)	-0.03698 (11)	0.08849 (7)	0.0236 (2)
O2	0.82986 (10)	0.41491 (11)	0.05932 (8)	0.0277 (2)
N1	0.72158 (10)	0.18910 (13)	0.05892 (8)	0.0202 (3)
N2	0.33163 (12)	0.66405 (15)	0.21169 (9)	0.0314 (3)
C1	0.72033 (12)	0.03121 (16)	0.06131 (9)	0.0197 (3)
C2	0.83357 (12)	-0.04762 (16)	0.02935 (9)	0.0192 (3)
C3	0.83190 (13)	-0.20294 (15)	0.01844 (10)	0.0213 (3)
C4	0.94482 (12)	0.03810 (16)	0.01277 (9)	0.0184 (3)
C5	0.94845 (13)	0.19711 (16)	0.02271 (9)	0.0203 (3)
C6	1.05903 (13)	0.27826 (16)	0.00833 (10)	0.0222 (3)
C7	0.83207 (13)	0.27835 (16)	0.04804 (10)	0.0212 (3)
C8	0.60316 (13)	0.27091 (16)	0.07764 (10)	0.0221 (3)
C9	0.62031 (13)	0.30750 (16)	0.19715 (10)	0.0243 (3)
C10	0.51955 (13)	0.43001 (15)	0.20583 (9)	0.0204 (3)
C11	0.39203 (14)	0.39920 (16)	0.22266 (11)	0.0261 (3)
C12	0.30364 (14)	0.51844 (18)	0.22457 (11)	0.0304 (3)
C13	0.45555 (14)	0.69295 (16)	0.19616 (10)	0.0274 (3)
C14	0.55050 (13)	0.58128 (16)	0.19223 (10)	0.0240 (3)
H3	0.7566	-0.2596	0.0291	0.026*
H6	1.0615	0.3853	0.0165	0.027*
H8a	0.5192	0.2088	0.0503	0.027*
H8b	0.5900	0.3667	0.0359	0.027*
H9a	0.6032	0.2154	0.2356	0.029*
H9b	0.7156	0.3421	0.2312	0.029*
H11	0.3659	0.2980	0.2327	0.031*
H12	0.2167	0.4950	0.2359	0.037*
H13	0.4793	0.7954	0.1874	0.033*
H14	0.6364	0.6078	0.1803	0.029*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0208 (4)	0.0240 (5)	0.0273 (5)	-0.0029 (3)	0.0088 (3)	0.0010 (3)
O2	0.0318 (5)	0.0175 (6)	0.0382 (5)	0.0008 (3)	0.0170 (4)	-0.0012 (3)
N1	0.0212 (5)	0.0191 (7)	0.0210 (5)	0.0009 (4)	0.0073 (4)	-0.0010 (4)

supplementary materials

N2	0.0288 (6)	0.0363 (8)	0.0291 (6)	0.0069 (5)	0.0079 (4)	-0.0041 (5)
C1	0.0202 (6)	0.0213 (8)	0.0166 (6)	-0.0007 (4)	0.0032 (4)	0.0001 (4)
C2	0.0219 (6)	0.0184 (7)	0.0174 (6)	-0.0002 (4)	0.0053 (4)	0.0012 (4)
C3	0.0218 (6)	0.0207 (7)	0.0225 (6)	-0.0027 (4)	0.0079 (4)	0.0014 (5)
C4	0.0227 (6)	0.0172 (7)	0.0156 (6)	-0.0009 (4)	0.0055 (4)	0.0010 (4)
C5	0.0237 (6)	0.0190 (8)	0.0187 (6)	0.0003 (4)	0.0067 (5)	0.0007 (4)
C6	0.0267 (6)	0.0158 (7)	0.0249 (6)	-0.0011 (4)	0.0086 (5)	-0.0002 (5)
C7	0.0267 (7)	0.0173 (8)	0.0205 (6)	0.0004 (4)	0.0078 (5)	0.0007 (4)
C8	0.0212 (6)	0.0217 (7)	0.0240 (6)	0.0021 (4)	0.0071 (4)	-0.0008 (5)
C9	0.0250 (6)	0.0249 (8)	0.0232 (6)	0.0026 (5)	0.0070 (5)	-0.0006 (5)
C10	0.0220 (6)	0.0245 (7)	0.0149 (5)	0.0011 (4)	0.0055 (4)	-0.0025 (4)
C11	0.0261 (7)	0.0286 (8)	0.0252 (6)	-0.0043 (5)	0.0097 (5)	-0.0034 (5)
C12	0.0222 (6)	0.0407 (9)	0.0300 (7)	-0.0016 (5)	0.0096 (5)	-0.0053 (6)
C13	0.0337 (7)	0.0253 (8)	0.0230 (6)	0.0001 (5)	0.0074 (5)	-0.0025 (5)
C14	0.0226 (6)	0.0298 (8)	0.0204 (6)	-0.0024 (5)	0.0070 (5)	-0.0026 (5)

Geometric parameters (\AA , $^\circ$)

O1—C1	1.2168 (16)	C6—H6	0.950
O2—C7	1.2146 (17)	C8—H8a	0.990
N1—C1	1.3937 (18)	C8—H8b	0.990
N1—C7	1.4027 (17)	C9—C10	1.5088 (19)
N2—C12	1.335 (2)	C9—H9a	0.990
N2—C13	1.3432 (19)	C9—H9b	0.990
C1—C2	1.4878 (18)	C10—C11	1.388 (2)
C2—C3	1.3773 (19)	C10—C14	1.3926 (19)
C2—C4	1.4170 (18)	C11—C12	1.384 (2)
C3—C6 ⁱ	1.406 (2)	C11—H11	0.950
C3—H3	0.950	C12—H12	0.950
C4—C4 ⁱ	1.4138 (18)	C13—C14	1.385 (2)
C4—C5	1.4085 (19)	C13—H13	0.950
C5—C6	1.3799 (19)	C14—H14	0.950
C5—C7	1.4856 (19)		
O1...O1 ⁱⁱ	3.0425 (11)	C14...C1 ^{viii}	3.4024 (15)
O1...C1 ⁱⁱ	3.5379 (13)	C14...H8a ^v	3.526
O1...C8 ⁱⁱ	3.4099 (14)	C14...H8b ^v	2.923
O1...C9 ⁱⁱⁱ	3.4669 (14)	C14...H9a ^{viii}	3.564
O1...C13 ^{iv}	3.4688 (17)	C14...H9b ^{viii}	3.251
O1...H8a ⁱⁱ	2.507	H3...O2 ^{iv}	2.965
O1...H9b ⁱⁱⁱ	2.637	H3...C8 ⁱⁱ	3.515
O1...H13 ^{iv}	2.680	H3...C9 ⁱⁱⁱ	3.447
O1...H14 ^{iv}	3.344	H3...C11 ⁱⁱ	3.403
O1...H14 ⁱⁱⁱ	3.490	H3...H8a ⁱⁱ	2.727
O2...N2 ^v	3.4884 (14)	H3...H8b ⁱⁱ	3.497
O2...C3 ^{vi}	3.4136 (16)	H3...H9a ⁱⁱⁱ	2.977
O2...C6 ^{vii}	3.1422 (17)	H3...H9b ⁱⁱⁱ	3.146

O2...C12 ^v	3.5753 (16)	H3...H11 ⁱⁱ	3.269
O2...H3 ^{vi}	2.965	H3...H14 ^{iv}	2.810
O2...H6 ^{vii}	2.417	H6...O2 ^{vii}	2.417
O2...H13 ⁱⁱⁱ	3.463	H6...C6 ^{vii}	3.191
N1...C13 ^v	3.4385 (15)	H6...C7 ^{vii}	3.337
N1...C14 ⁱⁱⁱ	3.5223 (14)	H6...C12 ^{xi}	3.307
N1...H13 ^v	3.263	H6...H6 ^{vii}	2.352
N1...H14 ⁱⁱⁱ	3.343	H6...H12 ^{xi}	2.987
N2...O2 ^v	3.4884 (14)	H8a...O1 ⁱⁱ	2.507
N2...C5 ^{viii}	3.5389 (14)	H8a...C1 ⁱⁱ	3.239
N2...C7 ^v	3.3340 (15)	H8a...C3 ⁱⁱ	3.410
N2...C11 ^{ix}	3.339 (2)	H8a...C13 ^v	3.358
N2...C12 ^{ix}	3.595 (2)	H8a...C14 ^v	3.526
N2...H8b ^v	3.490	H8a...H3 ⁱⁱ	2.727
N2...H11 ^{ix}	2.580	H8a...H13 ^v	3.057
N2...H12 ^{ix}	3.066	H8a...H14 ^v	3.365
C1...O1 ⁱⁱ	3.5379 (13)	H8b...N2 ^v	3.490
C1...C10 ⁱⁱⁱ	3.5150 (14)	H8b...C10 ^v	3.495
C1...C14 ⁱⁱⁱ	3.4024 (15)	H8b...C13 ^v	2.937
C1...H8a ⁱⁱ	3.239	H8b...C14 ^v	2.923
C1...H9b ⁱⁱⁱ	3.060	H8b...H3 ⁱⁱ	3.497
C1...H14 ⁱⁱⁱ	3.309	H8b...H8b ^v	2.963
C2...C10 ⁱⁱⁱ	3.3257 (15)	H8b...H13 ^v	3.110
C2...H9a ⁱⁱⁱ	3.585	H8b...H14 ^v	3.087
C2...H9b ⁱⁱⁱ	3.389	H9a...C2 ^{viii}	3.585
C3...O2 ^{iv}	3.4136 (16)	H9a...C3 ^{viii}	3.132
C3...C9 ⁱⁱⁱ	3.5537 (18)	H9a...C14 ⁱⁱⁱ	3.564
C3...H8a ⁱⁱ	3.410	H9a...H3 ^{viii}	2.977
C3...H9a ⁱⁱⁱ	3.132	H9a...H14 ⁱⁱⁱ	2.725
C3...H9b ⁱⁱⁱ	3.401	H9b...O1 ^{viii}	2.637
C3...H11 ⁱⁱ	3.404	H9b...C1 ^{viii}	3.060
C4...C11 ⁱⁱⁱ	3.5657 (17)	H9b...C2 ^{viii}	3.389
C5...N2 ⁱⁱⁱ	3.5389 (14)	H9b...C3 ^{viii}	3.401
C5...C13 ⁱⁱⁱ	3.4749 (16)	H9b...C13 ⁱⁱⁱ	3.453
C5...H11 ^x	3.589	H9b...C14 ⁱⁱⁱ	3.251
C6...O2 ^{vii}	3.1422 (17)	H9b...H3 ^{viii}	3.146
C6...H6 ^{vii}	3.191	H9b...H13 ⁱⁱⁱ	2.997
C6...H12 ^{xi}	3.492	H9b...H14 ⁱⁱⁱ	2.622
C7...N2 ^v	3.3340 (15)	H11...N2 ^{xii}	2.580
C7...C13 ⁱⁱⁱ	3.4814 (16)	H11...C3 ⁱⁱ	3.404
C7...H6 ^{vii}	3.337	H11...C5 ^{xiv}	3.589

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C7...H13 ⁱⁱⁱ	3.416	H11...C12 ^{xii}	3.134
C8...O1 ⁱⁱ	3.4099 (14)	H11...H3 ⁱⁱ	3.269
C8...C13 ^v	3.4187 (18)	H11...H12 ^{xii}	2.862
C8...H3 ⁱⁱ	3.515	H12...N2 ^{xii}	3.066
C8...H13 ^v	3.329	H12...C6 ^{xiii}	3.492
C9...O1 ^{viii}	3.4669 (14)	H12...C13 ^{xii}	3.423
C9...C3 ^{viii}	3.5537 (18)	H12...H6 ^{xiii}	2.987
C9...H3 ^{viii}	3.447	H12...H11 ^{ix}	2.862
C9...H14 ⁱⁱⁱ	3.083	H12...H13 ^{xii}	3.008
C10...C1 ^{viii}	3.5150 (14)	H13...O1 ^{vi}	2.680
C10...C2 ^{viii}	3.3257 (15)	H13...O2 ^{viii}	3.463
C10...H8b ^v	3.495	H13...N1 ^v	3.263
C11...N2 ^{xii}	3.339 (2)	H13...C7 ^{viii}	3.416
C11...C4 ^{viii}	3.5657 (17)	H13...C8 ^v	3.329
C11...H3 ⁱⁱ	3.403	H13...H8a ^v	3.057
C12...O2 ^v	3.5753 (16)	H13...H8b ^v	3.110
C12...N2 ^{xii}	3.595 (2)	H13...H9b ^{viii}	2.997
C12...H6 ^{xiii}	3.307	H13...H12 ^{ix}	3.008
C12...H11 ^{ix}	3.134	H14...O1 ^{vi}	3.344
C13...O1 ^{vi}	3.4688 (17)	H14...O1 ^{viii}	3.490
C13...N1 ^v	3.4385 (15)	H14...N1 ^{viii}	3.343
C13...C5 ^{viii}	3.4749 (16)	H14...C1 ^{viii}	3.309
C13...C7 ^{viii}	3.4814 (16)	H14...C9 ^{viii}	3.083
C13...C8 ^v	3.4187 (18)	H14...H3 ^{vi}	2.810
C13...H8a ^v	3.358	H14...H8a ^v	3.365
C13...H8b ^v	2.937	H14...H8b ^v	3.087
C13...H9b ^{viii}	3.453	H14...H9a ^{viii}	2.725
C13...H12 ^{ix}	3.423	H14...H9b ^{viii}	2.622
C14...N1 ^{viii}	3.5223 (14)		
C1—N1—C7	125.15 (11)	N1—C8—H8a	109.0
C1—N1—C8	118.32 (10)	N1—C8—H8b	109.0
C7—N1—C8	116.35 (11)	C9—C8—H8a	109.0
C12—N2—C13	115.97 (12)	C9—C8—H8b	109.0
O1—C1—N1	120.84 (12)	H8a—C8—H8b	107.8
O1—C1—C2	122.48 (12)	C8—C9—C10	109.31 (9)
N1—C1—C2	116.68 (11)	C8—C9—H9a	109.8
C1—C2—C3	120.28 (12)	C8—C9—H9b	109.8
C1—C2—C4	119.43 (12)	C10—C9—H9a	109.8
C3—C2—C4	120.27 (12)	C10—C9—H9b	109.8
C2—C3—C6 ⁱ	120.43 (12)	H9a—C9—H9b	108.3
C2—C3—H3	119.8	C9—C10—C11	122.88 (12)
C6 ⁱ —C3—H3	119.8	C9—C10—C14	119.92 (12)

C2—C4—C4 ⁱ	119.16 (12)	C11—C10—C14	117.14 (12)
C2—C4—C5	121.35 (12)	C10—C11—C12	118.88 (13)
C4 ⁱ —C4—C5	119.48 (12)	C10—C11—H11	120.6
C4—C5—C6	120.45 (12)	C12—C11—H11	120.6
C4—C5—C7	119.87 (12)	N2—C12—C11	124.77 (14)
C6—C5—C7	119.68 (12)	N2—C12—H12	117.6
C3 ⁱ —C6—C5	120.18 (12)	C11—C12—H12	117.6
C3 ⁱ —C6—H6	119.9	N2—C13—C14	123.48 (13)
C5—C6—H6	119.9	N2—C13—H13	118.3
O2—C7—N1	120.28 (12)	C14—C13—H13	118.3
O2—C7—C5	123.10 (12)	C10—C14—C13	119.76 (12)
N1—C7—C5	116.62 (11)	C10—C14—H14	120.1
N1—C8—C9	113.10 (9)	C13—C14—H14	120.1
C1—N1—C7—O2	-171.45 (10)	C2—C3—C6 ⁱ —C5 ⁱ	0.74 (17)
C1—N1—C7—C5	8.47 (16)	C2—C4—C4 ⁱ —C5 ⁱ	0.88 (15)
C7—N1—C1—O1	167.88 (10)	C2—C4—C5—C6	178.72 (10)
C7—N1—C1—C2	-12.06 (15)	C2—C4—C5—C7	-1.74 (15)
C1—N1—C8—C9	90.12 (12)	C4 ⁱ —C4—C5—C6	-0.38 (15)
C8—N1—C1—O1	-7.03 (15)	C4 ⁱ —C4—C5—C7	179.16 (9)
C8—N1—C1—C2	173.03 (9)	C5—C4—C4 ⁱ —C2 ⁱ	-0.88 (15)
C7—N1—C8—C9	-85.24 (13)	C4—C5—C6—C3 ⁱ	1.20 (16)
C8—N1—C7—O2	3.55 (16)	C4—C5—C7—O2	178.82 (11)
C8—N1—C7—C5	-176.52 (9)	C4—C5—C7—N1	-1.10 (15)
C12—N2—C13—C14	0.61 (17)	C6—C5—C7—O2	-1.63 (17)
C13—N2—C12—C11	-0.15 (19)	C6—C5—C7—N1	178.44 (10)
O1—C1—C2—C3	6.97 (16)	C7—C5—C6—C3 ⁱ	-178.35 (10)
O1—C1—C2—C4	-171.52 (10)	N1—C8—C9—C10	162.48 (11)
N1—C1—C2—C3	-173.10 (9)	C8—C9—C10—C11	95.71 (14)
N1—C1—C2—C4	8.41 (14)	C8—C9—C10—C14	-81.51 (13)
C1—C2—C3—C6 ⁱ	-177.93 (10)	C9—C10—C11—C12	-177.04 (11)
C1—C2—C4—C5	-1.96 (15)	C9—C10—C14—C13	177.55 (10)
C1—C2—C4—C4 ⁱ	177.15 (9)	C11—C10—C14—C13	0.17 (16)
C3—C2—C4—C5	179.55 (10)	C14—C10—C11—C12	0.25 (17)
C3—C2—C4—C4 ⁱ	-1.34 (15)	C10—C11—C12—N2	-0.3 (2)
C4—C2—C3—C6 ⁱ	0.54 (16)	N2—C13—C14—C10	-0.64 (18)

Symmetry codes: (i) $-x+2, -y, -z$; (ii) $-x+1, -y, -z$; (iii) $-x+3/2, y-1/2, -z+1/2$; (iv) $x, y-1, z$; (v) $-x+1, -y+1, -z$; (vi) $x, y+1, z$; (vii) $-x+2, -y+1, -z$; (viii) $-x+3/2, y+1/2, -z+1/2$; (ix) $-x+1/2, y+1/2, -z+1/2$; (x) $x+1/2, -y+1/2, z-1/2$; (xi) $x+1, y, z$; (xii) $-x+1/2, y-1/2, -z+1/2$; (xiii) $x-1, y, z$; (xiv) $x-1/2, -y+1/2, z+1/2$.

Fig. 1

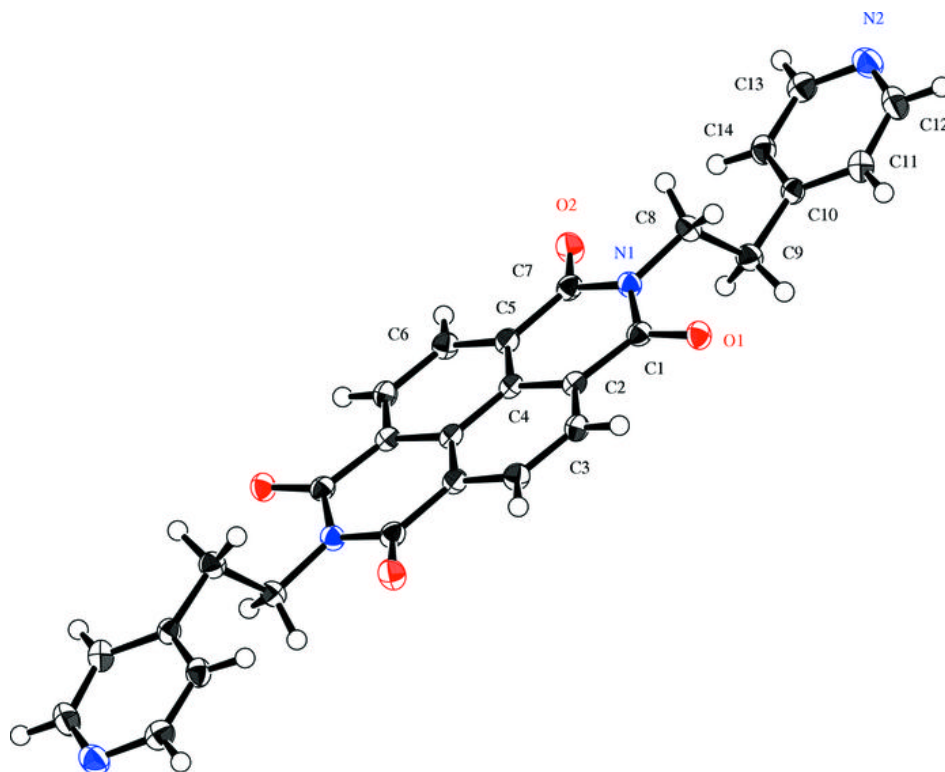


Fig. 2

