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data reports

11,11-Diphenyl-11H-indeno[1,2-b]quinoxaline

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In the title compound, $C_{27}H_{18}N_2$, the mean planes of the pendant benzene rings are approximately perpendicular to one another, making a dihedral angle of 79.3 (5)°; the indeno[1,2-*b*]quinoxaline ring system (r.m.s. deviation = 0.1197 Å) is twisted with respect to the pendant benzene rings by 70.0 (4) and 67.6 (3)°. Weak aromatic π - π stacking [centroid-centroid separation = 3.628 (2) Å] and C-H··· π interactions occur in the crystal.



Structure description

Some quinoxaline-based *N*-heteroacenes show a narrow band-gap, high thermal stability and aligned film morphology, which can be applied as the hole transport layers in quantum dot light-emitting diodes (QLEDs) (Bai *et al.*, 2015). As part of our work in this area, we now report the synthesis and crystal structure of the title indeno[1,2-b]quinoxaline derivative.

The molecular structure of the title compound is shown in Fig. 1. The pendant C1–C6 and C8–C13 benzene rings are nearly perpendicular to one another [dihedral angle = 79.3 (5)°] while the indeno[1,2-*b*]quinoxaline fused ring system (N1–N2/C7,C14–C27) is twisted with respect to the C1–C6 and C8–C13 benzene rings, subtending dihedral angles of 70.0 (4) and 67.6 (3)°, respectively.

In the crystal, weak $Cg6 \cdots Cg6^{i}$ aromatic π - π stacking interactions [centroid-centroid separation = 3.628 (2), slippage = 1.717 Å, symmetry code: (i) = 1 - x, 1 - y, 1 - z; where Cg6 is the centroid of the C22–C27 benzene ring] link the molecules into inversion dimers and weak C–H··· π interactions link the dimers (Table 1, Fig. 2).





Figure 1

The molecular structure of the title molecule with displacement ellipsoids drawn at the 30% probability level.

Synthesis and crystallization

The title compound was prepared in three steps. In the first step, a mixture of 1*H*-indene-1,2,3-trione (3.20 g, 20 mmol) and benzene-1,2-diamine (2.16 g, 20 mmol) in ethanol (100 ml) was heated to reflux under stirring for 5 h. 11*H*-Indeno[1,2-*b*]quinoxalin-11-one (1) was obtained as yellow powder by filtering after cooling. Then, a solution of compound 1 (2.32 g, 10 mmol) in THF (30 ml) was added dropwise into a solution of phenylmagnesium bromide (2.17 g, 12 mmol) in THF (30 ml). The mixture was heated to reflux with stirring for 12 h. This reaction was quenched by a saturated solution of NH₄Cl and the intermediate 11-phenyl-11*H*-





Table 1 Hydrogen bond geometry (

Hydrogen-bond geometry (Å, $^{\circ}$).

Cg2 and Cg3 are the centroids of the N1/N2/C20–C23 and C1–C6 rings, respectively.

$D - H \cdot \cdot \cdot A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - H \cdots A$
C15 $-$ H15 \cdots Cg2 ⁱ	0.93	2.92	3.728 (2)	145
C25 $-$ H25 \cdots Cg3 ⁱⁱ	0.93	2.96	3.830 (3)	156

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

Tal	ble	2	
Ex	peri	mental	details.

$C_{27}H_{18}N_2$
370.43
Monoclinic, $P2_1/n$
296
9.642 (5), 11.407 (5), 17.858 (8)
103.606 (5)
1909.0 (16)
4
Μο Κα
0.08
$0.20 \times 0.20 \times 0.10$
Bruker APEXII CCD
Multi-scan (<i>SADABS</i> ; Bruker, 2004)
0.859, 1.000
11621, 4429, 3277
0.023
0.653
0.043, 0.108, 1.03
4429
262
H-atom parameters constrained
0.15, -0.20

Computer programs: APEX2 (Bruker, 2007), SAINT (Bruker, 2004), SHELXT (Sheldrick, 2015a), SHELXL (Sheldrick, 2015b) and OLEX2 (Dolomanov et al., 2009).

indeno[1,2-*b*]quinoxalin-11-ol (2) was obtained by flash chromatography. In the last step, trifluoroacetic acid (7 ml) was added dropwise to a solution of compound 2 (0.58 g, 2.50 mmol) in benzene (3 ml) and the mixture was heated at 50° C for 12 h. Then, the reaction mixture was transferred to an ice bath and NaOH was used to increase the pH of the solution to 10. After the reaction, DCM was used to extract the product and Na₂SO₄ was used as desiccant. The crude product was purified by flash chromatography to obtain a yellow powder product of the title compound. The total yield was about 15%. Single crystals of the title compound suitable for X-ray data collection were obtained by the slow evaporation of a methanol solution.

Refinement

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

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full crystallographic data

IUCrData (2020). 5, x201213 [https://doi.org/10.1107/S2414314620012134]

11,11-Diphenyl-11*H*-indeno[1,2-b]quinoxaline

Lin Chen, Jin Hu, Li-Li Wu and Hong-Shun Sun

11,11-Diphenyl-11H-indeno[1,2-b]guinoxaline

Crystal data

C27H18N2 $M_r = 370.43$ Monoclinic, $P2_1/n$ a = 9.642 (5) Åb = 11.407 (5) Åc = 17.858 (8) Å $\beta = 103.606 (5)^{\circ}$ $V = 1909.0 (16) \text{ Å}^3$ Z = 4

Data collection

Bruker APEXII CCD
diffractometer
Graphite monochromator
ω scans
Absorption correction: multi-scan
(SADABS; Bruker, 2004)
$T_{\min} = 0.859, T_{\max} = 1.000$
11621 measured reflections

Refinement

Refinement on F^2 Least-squares matrix: full neighbouring sites $R[F^2 > 2\sigma(F^2)] = 0.043$ H-atom parameters constrained $wR(F^2) = 0.108$ S = 1.03where $P = (F_0^2 + 2F_c^2)/3$ 4429 reflections $(\Delta/\sigma)_{\rm max} = 0.001$ 262 parameters $\Delta \rho_{\rm max} = 0.15 \ {\rm e} \ {\rm \AA}^{-3}$ $\Delta \rho_{\rm min} = -0.20 \ {\rm e} \ {\rm \AA}^{-3}$ 0 restraints Primary atom site location: dual

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.

Refinement. H atoms were placed geometrically (C—H = 0.93 Å) and refined as riding atoms with $U_{iso}(H) = 1.2U_{er}(C)$.

F(000) = 776 $D_{\rm x} = 1.289 {\rm Mg m^{-3}}$ Mo *K* α radiation, $\lambda = 0.71073$ Å Cell parameters from 3937 reflections $\theta = 2.4 - 27.4^{\circ}$ $\mu = 0.08 \text{ mm}^{-1}$ T = 296 KBlock, colourless $0.20\times0.20\times0.10~mm$

4429 independent reflections 3277 reflections with $I > 2\sigma(I)$ $R_{\rm int} = 0.023$ $\theta_{\rm max} = 27.6^\circ, \ \theta_{\rm min} = 2.4^\circ$ $h = -12 \rightarrow 12$ $k = -14 \rightarrow 14$ $l = -23 \rightarrow 18$

Hydrogen site location: inferred from $w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 0.3316P]$

	x	11	-	IT */IT
	л О ГІОР ((11)	<i>y</i>	2	
NI	0.51226 (11)	0.55738 (9)	0.65772 (6)	0.0394 (3)
N2	0.23762 (11)	0.47436 (9)	0.57474 (6)	0.0395 (3)
CI	0.5462 (2)	1.01277 (15)	0.63861 (11)	0.0695 (5)
H1	0.5840	1.0786	0.6200	0.083*
C2	0.4016 (2)	0.99914 (15)	0.62609 (11)	0.0716 (5)
H2	0.3410	1.0565	0.5995	0.086*
C3	0.34490 (17)	0.90057 (13)	0.65275 (9)	0.0541 (4)
H3	0.2464	0.8923	0.6439	0.065*
C4	0.43262 (13)	0.81433 (11)	0.69233 (7)	0.0375 (3)
C5	0.57958 (15)	0.83006 (12)	0.70533 (9)	0.0495 (3)
Н5	0.6409	0.7734	0.7322	0.059*
C6	0.63502 (18)	0.92863 (14)	0.67879 (11)	0.0631 (4)
H6	0.7334	0.9382	0.6882	0.076*
C7	0.37522 (12)	0.70131 (11)	0.72101 (7)	0.0350 (3)
C8	0.44723 (13)	0.67853 (11)	0.80551 (7)	0.0382 (3)
C9	0.45826 (15)	0.76998 (14)	0.85801 (8)	0.0495 (3)
Н9	0.4275	0.8445	0.8405	0.059*
C10	0.51424 (17)	0.75184 (17)	0.93576 (9)	0.0620 (4)
H10	0.5191	0.8135	0.9704	0.074*
C11	0.56268 (18)	0.64278 (19)	0.96174 (10)	0.0707 (5)
H11	0.6005	0.6304	1.0140	0.085*
C12	0.55541 (18)	0.55199 (17)	0.91067 (10)	0.0667 (5)
H12	0.5904	0.4786	0.9284	0.080*
C13	0.49617 (15)	0.56892 (13)	0.83284 (9)	0.0504 (4)
H13	0.4893	0.5063	0.7988	0.060*
C14	0.21179 (13)	0.70151 (11)	0.70965 (7)	0.0363 (3)
C15	0.12920 (14)	0.76476 (12)	0.74945 (8)	0.0450 (3)
H15	0.1717	0.8172	0.7879	0.054*
C16	-0.01721 (15)	0.74878 (13)	0.73120 (9)	0.0486 (3)
H16	-0.0727	0.7907	0.7580	0.058*
C17	-0.08276 (14)	0.67165 (13)	0.67389 (9)	0.0486 (3)
H17	-0.1814	0.6630	0.6622	0.058*
C18	-0.00211 (14)	0.60742 (12)	0.63394 (8)	0.0434 (3)
H18	-0.0454	0.5555	0.5953	0.052*
C19	0.14523 (13)	0.62214 (11)	0.65281 (7)	0.0358 (3)
C20	0.25545 (13)	0.55958 (10)	0.62526 (7)	0.0345 (3)
C21	0.39212 (13)	0.60103 (10)	0.66650 (7)	0.0345 (3)
C22	0.49792 (14)	0.46536 (11)	0.60637 (7)	0.0382 (3)
C23	0.36232 (14)	0.42444 (11)	0.56559 (7)	0.0378 (3)
C24	0.35458(17)	0.32749(12)	0.51582 (8)	0.0483 (3)
H24	0 2661	0 2993	0 4894	0.058*
C25	0.47617 (18)	0.27492 (13)	0.50633 (9)	0.0547 (4)
H25	0.4701	0.2115	0.4730	0.066*
C26	0.61001 (17)	0 31559 (13)	0 54628 (9)	0 0547 (4)
H26	0.6921	0.2787	0.5394	0.066*

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\hat{A}^2)

data reports

C27	0.62156 (15)	0.40861 (12)	0.59517 (9)	0.0481 (3)
H27	0.7112	0.4348	0.6213	0.058*

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U ³³	U^{12}	U^{13}	U^{23}
N1	0.0374 (6)	0.0388 (6)	0.0444 (6)	0.0031 (5)	0.0144 (5)	0.0002 (5)
N2	0.0425 (6)	0.0388 (6)	0.0375 (6)	0.0012 (5)	0.0099 (5)	-0.0035 (5)
C1	0.0864 (13)	0.0474 (9)	0.0773 (12)	-0.0137 (9)	0.0241 (10)	0.0124 (9)
C2	0.0785 (12)	0.0502 (9)	0.0802 (13)	0.0038 (9)	0.0069 (10)	0.0227 (9)
C3	0.0501 (8)	0.0495 (8)	0.0577 (9)	0.0020 (7)	0.0027 (7)	0.0076 (7)
C4	0.0425 (7)	0.0346 (6)	0.0354 (7)	0.0000 (5)	0.0093 (5)	-0.0031 (5)
C5	0.0438 (8)	0.0458 (8)	0.0601 (9)	0.0000 (6)	0.0143 (7)	0.0061 (7)
C6	0.0559 (9)	0.0569 (10)	0.0786 (12)	-0.0120 (8)	0.0201 (8)	0.0063 (9)
C7	0.0323 (6)	0.0350 (6)	0.0380 (7)	0.0017 (5)	0.0088 (5)	-0.0035 (5)
C8	0.0323 (6)	0.0451 (7)	0.0379 (7)	-0.0007 (5)	0.0097 (5)	0.0017 (6)
C9	0.0470 (8)	0.0578 (9)	0.0422 (8)	0.0025 (7)	0.0076 (6)	-0.0065 (7)
C10	0.0554 (9)	0.0887 (13)	0.0408 (9)	-0.0076 (9)	0.0087 (7)	-0.0100 (8)
C11	0.0606 (10)	0.1086 (15)	0.0401 (9)	-0.0102 (10)	0.0062 (7)	0.0181 (10)
C12	0.0644 (11)	0.0752 (12)	0.0589 (11)	0.0029 (9)	0.0113 (8)	0.0293 (9)
C13	0.0507 (8)	0.0505 (8)	0.0513 (9)	0.0006 (7)	0.0146 (7)	0.0102 (7)
C14	0.0349 (6)	0.0364 (6)	0.0381 (7)	0.0029 (5)	0.0095 (5)	0.0006 (5)
C15	0.0424 (7)	0.0459 (7)	0.0473 (8)	0.0032 (6)	0.0116 (6)	-0.0110 (6)
C16	0.0426 (7)	0.0523 (8)	0.0544 (9)	0.0082 (6)	0.0183 (6)	-0.0072 (7)
C17	0.0327 (7)	0.0566 (8)	0.0568 (9)	0.0031 (6)	0.0108 (6)	-0.0035 (7)
C18	0.0368 (7)	0.0460 (7)	0.0460 (8)	0.0004 (6)	0.0068 (6)	-0.0057 (6)
C19	0.0350 (6)	0.0361 (6)	0.0365 (7)	0.0025 (5)	0.0088 (5)	0.0001 (5)
C20	0.0363 (6)	0.0336 (6)	0.0341 (7)	0.0010 (5)	0.0093 (5)	0.0012 (5)
C21	0.0368 (6)	0.0324 (6)	0.0357 (6)	0.0013 (5)	0.0114 (5)	0.0015 (5)
C22	0.0446 (7)	0.0339 (6)	0.0398 (7)	0.0043 (5)	0.0174 (6)	0.0052 (5)
C23	0.0465 (7)	0.0356 (6)	0.0335 (7)	0.0049 (5)	0.0137 (5)	0.0031 (5)
C24	0.0601 (9)	0.0433 (7)	0.0426 (8)	0.0030 (6)	0.0143 (6)	-0.0052 (6)
C25	0.0788 (11)	0.0408 (8)	0.0509 (9)	0.0103 (7)	0.0278 (8)	-0.0044 (7)
C26	0.0614 (9)	0.0458 (8)	0.0657 (10)	0.0147 (7)	0.0324 (8)	0.0033 (7)
C27	0.0457 (8)	0.0454 (8)	0.0582 (9)	0.0069 (6)	0.0225 (7)	0.0040 (7)

Geometric parameters (Å, °)

N1—C21	1.3038 (16)	C11—C12	1.371 (3)
N1-C22	1.3791 (17)	C12—H12	0.9300
N2-C20	1.3099 (16)	C12—C13	1.386 (2)
N2-C23	1.3744 (17)	С13—Н13	0.9300
C1—H1	0.9300	C14—C15	1.3878 (18)
C1—C2	1.368 (3)	C14—C19	1.3984 (18)
C1—C6	1.371 (2)	C15—H15	0.9300
С2—Н2	0.9300	C15—C16	1.384 (2)
C2—C3	1.383 (2)	C16—H16	0.9300
С3—Н3	0.9300	C16—C17	1.384 (2)

C3—C4	1.3790 (19)	С17—Н17	0.9300
C4—C5	1.3925 (19)	C17—C18	1.3826 (19)
C4—C7	1.5375 (18)	C18—H18	0.9300
C5—H5	0.9300	C18—C19	1.3909 (19)
C5—C6	1 376 (2)	C19-C20	1 4583 (17)
С6—Н6	0.9300	C20—C21	1 4303 (18)
C7—C8	1 5276 (19)	C^{22} C^{23}	1 4176 (19)
C7-C14	1 5408 (18)	C^{22} C^{27}	1 4116 (18)
C7-C21	1.5353(17)	$C_{22} = C_{24}$	1 4097 (18)
C_{8}	1 390 (2)	C24_H24	0.9300
C8-C13	1.390(2) 1.384(2)	C_{24} C_{25}	1 362 (2)
С9—Н9	0.9300	C25_H25	0.9300
C_{0} C_{10}	1.382(2)	C25 C26	1300(2)
C10 H10	0.0300	C26 H26	0.0300
C_{10} C_{11}	1.371(3)	$C_{20} = 1120$	1.362(2)
	0.0300	$C_{20} = C_{27}$	1.302(2)
Сп—нп	0.9300	C27—H27	0.9300
C21 N1 C22	114 69 (11)	C12 C12 H12	110.9
$C_2 I \longrightarrow C_2 Z$	114.00(11) 114.27(11)	C_{12} C_{13} C_{14} C_{7}	119.0 129.72(12)
$C_{20} = N_2 = C_{23}$	114.37 (11)	C15 - C14 - C7	126.75(12)
$C_2 = C_1 = C_1$	120.2	C10 - C14 - C7	119.19(12)
$C_2 = C_1 = C_0$	119.55 (15)	C14 - C14 - C7	112.05 (10)
	120.2	С14—С15—П15	120.4
C1 = C2 = H2	119.8	C16 - C15 - C14	119.10 (13)
C1 = C2 = C3	120.42 (16)	C16—C15—H15	120.4
C3—C2—H2	119.8	C15—C16—H16	119.3
С2—С3—Н3	119.6	C15—C16—C17	121.38 (12)
C4—C3—C2	120.81 (15)	С17—С16—Н16	119.3
C4—C3—H3	119.6	С16—С17—Н17	119.9
C3—C4—C5	118.09 (13)	C18—C17—C16	120.25 (13)
C3—C4—C7	122.92 (12)	С18—С17—Н17	119.9
C5—C4—C7	118.97 (11)	C17—C18—H18	120.7
C4—C5—H5	119.7	C17—C18—C19	118.52 (13)
C6—C5—C4	120.69 (14)	C19—C18—H18	120.7
С6—С5—Н5	119.7	C14—C19—C20	108.37 (11)
C1—C6—C5	120.45 (16)	C18—C19—C14	121.48 (11)
C1—C6—H6	119.8	C18—C19—C20	130.03 (12)
С5—С6—Н6	119.8	N2—C20—C19	127.41 (11)
C4—C7—C14	113.08 (10)	N2—C20—C21	123.76 (11)
C8—C7—C4	110.86 (10)	C21—C20—C19	108.72 (11)
C8—C7—C14	110.09 (10)	N1—C21—C7	126.20 (11)
C8—C7—C21	114.09 (10)	N1—C21—C20	123.29 (12)
C21—C7—C4	108.26 (10)	C20—C21—C7	110.51 (10)
C21—C7—C14	100.11 (9)	N1—C22—C23	121.89 (11)
C9—C8—C7	118.92 (12)	N1-C22-C27	119.16 (12)
C13—C8—C7	122.69 (12)	C27—C22—C23	118.94 (13)
C13—C8—C9	118.32 (13)	N2-C23-C22	121.97 (12)
С8—С9—Н9	119.5	N2—C23—C24	118.80 (12)
C10—C9—C8	121.01 (15)	C24—C23—C22	119.20 (12)

С10—С9—Н9	119.5	C23—C24—H24	119.9
С9—С10—Н10	120.1	C25—C24—C23	120.28 (14)
C11—C10—C9	119.83 (16)	C25—C24—H24	119.9
C11—C10—H10	120.1	C24—C25—H25	119.7
C10—C11—H11	120.0	C_{24} C_{25} C_{26}	120.55 (14)
C10-C11-C12	120.03 (16)	C26—C25—H25	119.7
C12—C11—H11	120.00 (10)	$C_{25} = C_{26} = H_{26}$	119.6
C11—C12—H12	119.8	C_{27} C_{26} C_{25}	120 79 (14)
$C_{11} - C_{12} - C_{13}$	120.41 (16)	$C_{27} = C_{26} = H_{26}$	119.6
C13 - C12 - H12	119.8	$C_{22} = C_{27} = H_{27}$	119.9
C8-C13-C12	120.35 (15)	$C_{22} = C_{27} = C_{27}$	120 24 (14)
C_{8} C_{13} H_{13}	119.8	$C_{26} = C_{27} = H_{27}$	119.9
0 015 1115	119.0	020-027-1127	11).)
C6—C1—C2—C3	-0.9 (3)	C17—C18—C19—C14	-1.3(2)
C1—C2—C3—C4	0.0 (3)	C17—C18—C19—C20	174.12 (13)
C2—C3—C4—C5	0.7 (2)	C15—C14—C19—C18	1.67 (19)
C2-C3-C4-C7	-178.05(15)	C7-C14-C19-C18	179.30 (11)
$C_{3}-C_{4}-C_{5}-C_{6}$	-0.5(2)	C_{15} C_{14} C_{19} C_{20}	-174.64 (11)
C7-C4-C5-C6	178.31 (14)	C7-C14-C19-C20	2.99 (14)
C_{2} C_{1} C_{6} C_{5}	11(3)	C_{23} N2 C_{20} C_{21}	1.74(17)
C4-C5-C6-C1	-0.4(3)	$C_{23} = N_2 = C_{20} = C_{19}$	-173.95(11)
$C_{3}-C_{4}-C_{7}-C_{8}$	$-131\ 10\ (13)$	C18 - C19 - C20 - N2	07(2)
$C_{5}-C_{4}-C_{7}-C_{8}$	50 19 (15)	C14 - C19 - C20 - N2	176.62(12)
C_{3} C_{4} C_{7} C_{21}	103.05(14)	C18 - C19 - C20 - C21	-17549(13)
$C_{5} - C_{4} - C_{7} - C_{21}$	-75.66(14)	C_{14} C_{19} C_{20} C_{21}	0.40(14)
$C_{3} - C_{4} - C_{7} - C_{14}$	-6.91(17)	$C_{22} = N_1 = C_{21} = C_{20}$	-1.39(17)
$C_{5} - C_{4} - C_{7} - C_{14}$	$174 \ 37 \ (11)$	$C_{22} = N_1 = C_{21} = C_{20}$	1.59(17) 178 39(11)
C_{21} C_{7} C_{8} C_{13}	-13.19(16)	$N_2 = C_2 = C_1 = C_1 = C_1$	-0.19(19)
$C_{1} = C_{1} = C_{1} = C_{1}$	-135.71(13)	12 - 22 - 221 - 111	176 10 (11)
$C_{14} = C_{7} = C_{8} = C_{13}$	133.71(13) 98.41(14)	$N_{2} = C_{20} = C_{21} = N_{1}$	170.19(11) 180.00(11)
$C_{11} = C_{12} = C_{13} = C_{13}$	160.06(11)	12 - 220 - 221 - 27	-3.62(13)
$C_{21} = C_{7} = C_{8} = C_{9}$	109.90(11) 47.44(15)	$C_{1}^{8} = C_{2}^{7} = C_{2}^{1} = C_{1}^{7}$	-57.24(15)
$C_{4} - C_{7} - C_{8} - C_{9}$	-78.44(13)	$C_{0} = C_{1} = C_{21} = N_{1}$	-37.34(10)
$C_{14} = C_{14} = C$	-70.44(14)	$C_{4} - C_{7} - C_{21} - N_{1}$	174.95(12)
$C_{13} = C_{8} = C_{9} = C_{10}$	-1.1(2)	$C_{14} - C_{7} - C_{21} - N_{1}$	-1/4.83(12)
$C^{2} = C^{2} = C^{2$	1/3.64(12)	$C_{0} = C_{1} = C_{21} = C_{20}$	122.40(11)
$C_{0} = C_{10} = C_{11} = C_{12}$	1.4(2)	$C_4 - C_7 - C_{21} - C_{20}$	-115.01(11)
C_{9} C_{10} C_{11} C_{12} C_{12}	-0.1(3)	C14 - C7 - C21 - C20	4.95 (12)
C10-C11-C12-C13	-1.5(3)	$C_2I = NI = C_22 = C_27$	-1//.33(11)
$C_{2} = C_{3} = C_{12} = C_{12}$	-0.4(2)	$C_{21} = N_{1} = C_{22} = C_{23}$	1.35(17)
C/-C8-C13-C12	-1//.30(13)	$C_{20} = N_2 = C_{23} = C_{24}$	1/6.38 (11)
C11 - C12 - C13 - C8	1.8 (2)	$C_{20} = N_2 = C_{23} = C_{22}$	-1.72(17)
	52.10 (17)	N1—C22—C23—N2	0.21 (19)
$C_{21} - C_{1} - C_{14} - C_{15}$	1/2.54 (13)	$C_2 / - C_{22} - C_{23} - N_2$	1/8.89 (11)
C4 - C / - C14 - C15	-/2.51 (1/)	N1 - C22 - C23 - C24	-1//.89(11)
$C_{8} - C_{1} - C_{14} - C_{19}$	-125.24 (12)	$C_2/-C_{22}-C_{23}-C_{24}$	0.79 (18)
$C_2I - C_1 - C_14 - C_19$	-4.80 (13)	$N_2 - C_{23} - C_{24} - C_{25}$	-179.05 (13)
C4—C/—C14—C19	110.15 (12)	C22—C23—C24—C25	-0.9 (2)
C19—C14—C15—C16	-0.8 (2)	C23—C24—C25—C26	0.6 (2)

C7-C14-C15-C16	-177.99 (13)	C24—C25—C26—C27	-0.2 (2)
C14—C15—C16—C17	-0.4 (2)	C25—C26—C27—C22	0.1 (2)
C15—C16—C17—C18	0.7 (2)	N1-C22-C27-C26	178.29 (12)
C16—C17—C18—C19	0.1 (2)	C23—C22—C27—C26	-0.4 (2)

Hydrogen-bond geometry (Å, °)

Cg2 and Cg3 are the centroids of the N1/N2/C20–C23 and C1–C6 rings, respectively.

D—H···A	D—H	Н…А	D····A	<i>D</i> —H··· <i>A</i>
C15—H15…Cg2 ⁱ	0.93	2.92	3.728 (2)	145
C25—H25…Cg3 ⁱⁱ	0.93	2.96	3.830 (3)	156

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