organic compounds

N-Phenyl-N-{4-[5-(2-phenyl-3-pyridyl)-1,3,4-oxadiazol-2-yl]phenyl}aniline

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The title compound, $C_{31}H_{22}N_4O$, is a bipolar ligand which contains triphenylamine and 1,3,4-oxadiazole units. Within the molecule, the 1,3,4-oxadiazole and pyridine rings are nearly coplanar, making a dihedral angle of 4.7 (6)°. The molecules are linked by intermolecular C—H⋯N hydrogen bonding.

Related literature

For general background, see: Tang & Vanslyke (1987); Gong et al. (1998); Kim et al. (2001); He et al. (2006); Tamoto et al. (1997). For the synthesis, see: Tamoto et al. (1997).
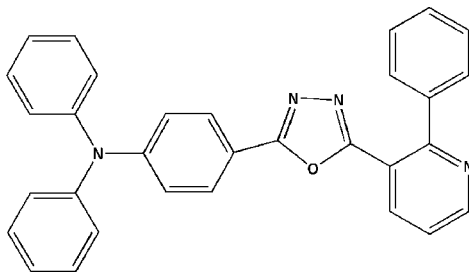
Experimental

Crystal data

$C_{31}H_{22}N_4O$	$\gamma = 92.2210\ (9)°$
$M_r = 466.53$	$V = 1203.34\ (10)$ Å^3
Triclinic, $P\bar{1}$	$Z = 2$
$a = 9.7220\ (5)$ Å	Mo $K\alpha$ radiation
$b = 10.8380\ (5)$ Å	$\mu = 0.08$ mm^{-1}
$c = 12.1740\ (6)$ Å	$T = 293\ (2)$ K
$\alpha = 90.8820\ (9)°$	$0.40 \times 0.30 \times 0.25$ mm
$\beta = 110.0740\ (9)°$	

Data collection

Bruker APEX CCD area-detector diffractometer	5527 independent reflections
Absorption correction: none	3377 reflections with $I > 2\sigma(I)$
7506 measured reflections	$R_{int} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$	325 parameters
$wR(F^2) = 0.133$	H-atom parameters constrained
$S = 1.02$	$\Delta\rho_{max} = 0.15$ e Å^{-3}
5527 reflections	$\Delta\rho_{min} = -0.22$ e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C30—H30⋯N3^i	0.93	2.60	3.444 (3)	151

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2340).

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supplementary materials

N-Phenyl-N-{4-[5-(2-phenyl-3-pyridyl)-1,3,4-oxadiazol-2-yl]phenyl}aniline

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Comment

Recently organic light-emitting diodes (OLEDs) have attracted much attention because of their potential applications in full-color flat panel displays (Tang & Vanslyke, 1987). It is known that a reasonable device configuration should offer balanced charge carriers injection and transportation, which ensure their high recombination chance at the emitting layer. One method to balance the injection/transport rates of hole and electron is incorporate the hole-transporting group and electron transporting group into one molecule as the emitting layer (Gong *et al.*, 1998; Kim *et al.*, 2001; He *et al.*, 2006; Tamoto *et al.*, 1997). In this work, a new ligand, which contains both hole transporting triphenylamine and electron-transporting 1,3,4-oxadiazol moieties, has been synthesized and its structure studied in detail. This compound emits bright blue light under excitation of UV light, implying its potential application in OLEDs.

The molecular skeleton of the title compound is non-planar (Fig. 1), with the benzene ring, the 1,3,4-oxadiazol ring, and the pyridine ring being slightly twisted with respect to each other. The dihedral angle between the 1,3,4-oxadiazol ring and the benzene ring of C13 to C18 is 27.9 (6)°, while the dihedral angle between the 1,3,4-oxadiazol ring and the pyridine ring is 4.7 (6)°. The angle of O1—C19—C16 of 119.34 (14) is slightly smaller than the O1—C20—C21 angle of 122.67 (14)°. The bond distances of C16—C19 and C20—C21 are 1.453 (2) and 1.465 (2) Å, respectively. All other feathers appear to be normal. The molecules are liked together by intermolecular C—H⋯N hydrogen bonding (Table 1).

Experimental

The title compound is synthesized by reaction between 4-tetrazoyltriphenylamine (Tamoto *et al.*, 1997) and 2-phenyl-nicotinoyl chloride in high yield. 3-Methyl-2-phenylpyridine (1 ml) and KMnO4 (3.16 g) were heated at reflux in 150 ml of water for 12 h. Removal of brown precipitate by filtration gave a solution, then addition of concentrated hydrochloric acid precipitated white crystals. The solid was filtered, washed with water, and dried *in vacuo*. The resulting 2-phenylnicotinic acid (0.3 g) was then refluxed with thionyl chloride (15 ml) for 5 h. The solvent was removed by rotary evaporation. The crude product was extracted with benzene to obtained 2-phenylnicotinoyl chloride. A mixture of 2-phenylnicotinoyl chloride (0.20 g), 4-tetrazolytriphenylamine (0.31 g), and dry pyridine (30 ml) was refluxed for one day under nitrogen atmosphere. After cooling, the reaction mixture was poured into water, and then filtered to collect the solid. The crude product was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1/10, *v/v*) as the eluent. Crystals suitable for X-ray diffraction study were obtained by slow evaporation of ethyl acetate/petroleum ether (1/10, *v/v*) solution.

Refinement

H atoms were placed in calculated positions with C—H = 0.93 Å and refined in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$.
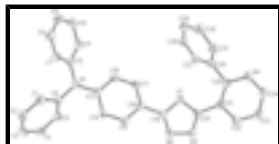
supplementary materials

Figures

Fig. 1. A view of the molecule of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

N-Phenyl-*N*-{4-[5-(2-phenyl-3-pyridyl)-1,3,4-oxadiazol-2-yl]phenyl}aniline

Crystal data

$C_{31}H_{22}N_4O$	$Z = 2$
$M_r = 466.53$	$F_{000} = 488$
Triclinic, $P\bar{1}$	$D_x = 1.288$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å
$a = 9.7220$ (5) Å	Cell parameters from 3377 reflections
$b = 10.8380$ (5) Å	$\theta = 1.8–28.5º$
$c = 12.1740$ (6) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 90.8820$ (9)º	$T = 293$ (2) K
$\beta = 110.0740$ (9)º	Block, colorless
$\gamma = 92.2210$ (9)º	$0.40 \times 0.30 \times 0.25$ mm
$V = 1203.34$ (10) Å^3	

Data collection

Bruker APEX CCD area-detector diffractometer	5527 independent reflections
Radiation source: fine-focus sealed tube	3377 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 28.5º$
$T = 293(2)$ K	$\theta_{min} = 1.8º$
φ and ω scans	$h = -12 \rightarrow 8$
Absorption correction: none	$k = -14 \rightarrow 14$
7506 measured reflections	$l = -15 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	H-atom parameters constrained
$wR(F^2) = 0.133$	$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2 + 0.0144P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
5527 reflections	$\Delta\rho_{max} = 0.15$ e Å^{-3}

325 parameters

$\Delta\rho_{min} = -0.22$ e Å^{-3}

Primary atom site location: structure-invariant direct methods

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 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$^2 > 2$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 (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
C1	0.1710 (2)	0.31142 (18)	1.12588 (17)	0.0546 (5)
H1	0.0890	0.3413	1.1383	0.066*
C2	0.2916 (3)	0.2818 (2)	1.21994 (19)	0.0712 (6)
H2	0.2906	0.2916	1.2957	0.085*
C3	0.4131 (2)	0.2380 (2)	1.2020 (2)	0.0795 (7)
H3	0.4945	0.2189	1.2655	0.095*
C4	0.4140 (2)	0.2223 (2)	1.0903 (2)	0.0717 (7)
H4	0.4962	0.1922	1.0783	0.086*
C5	0.2938 (2)	0.25082 (18)	0.99541 (18)	0.0574 (5)
H5	0.2945	0.2392	0.9198	0.069*
C6	0.17242 (19)	0.29668 (16)	1.01353 (16)	0.0448 (4)
C7	−0.0953 (2)	0.13836 (18)	0.91380 (18)	0.0575 (5)
H7	−0.0108	0.0950	0.9264	0.069*
C8	−0.2251 (3)	0.0759 (2)	0.9030 (2)	0.0742 (7)
H8	−0.2278	−0.0096	0.9085	0.089*
C9	−0.3506 (2)	0.1380 (3)	0.88446 (19)	0.0769 (7)
H9	−0.4387	0.0951	0.8756	0.092*
C10	−0.3450 (2)	0.2646 (2)	0.87899 (19)	0.0701 (7)
H10	−0.4295	0.3076	0.8680	0.084*
C11	−0.2153 (2)	0.32875 (19)	0.88964 (17)	0.0554 (5)
H11	−0.2126	0.4144	0.8859	0.067*
C12	−0.08951 (19)	0.26537 (17)	0.90593 (15)	0.0437 (4)
C13	0.05914 (18)	0.41427 (15)	0.83651 (15)	0.0416 (4)
C14	0.18425 (19)	0.49327 (16)	0.86272 (15)	0.0470 (4)
H14	0.2598	0.4874	0.9340	0.056*
C15	0.19715 (19)	0.57934 (16)	0.78471 (15)	0.0465 (4)
H15	0.2820	0.6299	0.8036	0.056*
C16	0.08545 (18)	0.59220 (16)	0.67801 (15)	0.0419 (4)
C17	−0.03949 (18)	0.51404 (16)	0.65130 (15)	0.0434 (4)
H17	−0.1155	0.5216	0.5806	0.052*

C18	−0.05244 (19)	0.42562 (16)	0.72790 (15)	0.0439 (4)
H18	−0.1358	0.3731	0.7074	0.053*
C19	0.10460 (18)	0.68373 (15)	0.59788 (15)	0.0413 (4)
C20	0.04367 (18)	0.81628 (16)	0.46433 (15)	0.0409 (4)
C21	−0.04570 (19)	0.89590 (15)	0.37367 (15)	0.0413 (4)
C22	0.0314 (2)	0.98177 (18)	0.33002 (17)	0.0536 (5)
H22	0.1333	0.9835	0.3562	0.064*
C23	−0.0430 (2)	1.06349 (18)	0.24852 (18)	0.0601 (5)
H23	0.0069	1.1208	0.2181	0.072*
C24	−0.1932 (2)	1.05845 (19)	0.21310 (18)	0.0596 (5)
H24	−0.2436	1.1145	0.1583	0.072*
C25	−0.19941 (18)	0.89634 (16)	0.33163 (15)	0.0428 (4)
C26	−0.29814 (18)	0.81137 (17)	0.36889 (15)	0.0459 (4)
C27	−0.2998 (2)	0.68467 (18)	0.35371 (17)	0.0532 (5)
H27	−0.2340	0.6500	0.3232	0.064*
C28	−0.3985 (2)	0.6089 (2)	0.3835 (2)	0.0697 (6)
H28	−0.3996	0.5237	0.3724	0.084*
C29	−0.4950 (2)	0.6600 (3)	0.4296 (2)	0.0796 (8)
H29	−0.5610	0.6090	0.4501	0.096*
C30	−0.4945 (2)	0.7848 (3)	0.4455 (2)	0.0796 (7)
H30	−0.5598	0.8185	0.4771	0.096*
C31	−0.3970 (2)	0.8619 (2)	0.41461 (18)	0.0620 (6)
H31	−0.3979	0.9471	0.4245	0.074*
N1	0.04653 (15)	0.32771 (14)	0.91669 (13)	0.0475 (4)
N2	0.22489 (16)	0.72776 (15)	0.58904 (14)	0.0552 (4)
N3	0.18459 (16)	0.81617 (15)	0.50184 (14)	0.0547 (4)
N4	−0.27100 (17)	0.97835 (15)	0.25235 (14)	0.0554 (4)
O1	−0.01557 (12)	0.73448 (10)	0.52130 (10)	0.0426 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0568 (12)	0.0575 (12)	0.0469 (12)	−0.0024 (9)	0.0146 (9)	0.0071 (9)
C2	0.0694 (15)	0.0828 (16)	0.0474 (13)	−0.0075 (12)	0.0030 (11)	0.0116 (11)
C3	0.0535 (14)	0.0858 (17)	0.0736 (17)	−0.0101 (12)	−0.0106 (12)	0.0291 (14)
C4	0.0384 (11)	0.0771 (15)	0.0934 (19)	0.0034 (10)	0.0136 (12)	0.0235 (14)
C5	0.0469 (11)	0.0649 (13)	0.0613 (13)	0.0067 (9)	0.0189 (10)	0.0134 (10)
C6	0.0401 (10)	0.0440 (10)	0.0459 (11)	−0.0032 (8)	0.0095 (8)	0.0108 (8)
C7	0.0551 (12)	0.0544 (12)	0.0593 (13)	−0.0032 (9)	0.0153 (10)	0.0051 (10)
C8	0.0683 (15)	0.0678 (15)	0.0747 (16)	−0.0201 (12)	0.0118 (12)	0.0078 (12)
C9	0.0526 (14)	0.108 (2)	0.0598 (14)	−0.0274 (13)	0.0084 (11)	0.0191 (13)
C10	0.0426 (12)	0.1054 (19)	0.0642 (15)	0.0057 (12)	0.0197 (10)	0.0209 (13)
C11	0.0494 (11)	0.0633 (12)	0.0561 (12)	0.0046 (9)	0.0207 (9)	0.0108 (10)
C12	0.0405 (10)	0.0534 (11)	0.0365 (10)	−0.0012 (8)	0.0125 (8)	0.0075 (8)
C13	0.0413 (10)	0.0436 (10)	0.0395 (10)	0.0024 (8)	0.0130 (8)	0.0044 (8)
C14	0.0414 (10)	0.0513 (11)	0.0404 (10)	−0.0021 (8)	0.0042 (8)	0.0063 (9)
C15	0.0419 (10)	0.0478 (10)	0.0454 (11)	−0.0052 (8)	0.0098 (8)	0.0056 (9)
C16	0.0415 (10)	0.0425 (10)	0.0419 (10)	0.0024 (8)	0.0143 (8)	0.0057 (8)

C17	0.0395 (9)	0.0511 (10)	0.0366 (10)	0.0012 (8)	0.0092 (8)	0.0039 (8)
C18	0.0386 (9)	0.0489 (10)	0.0420 (10)	−0.0038 (8)	0.0116 (8)	0.0029 (8)
C19	0.0370 (9)	0.0437 (10)	0.0408 (10)	0.0027 (7)	0.0101 (8)	0.0037 (8)
C20	0.0385 (9)	0.0451 (10)	0.0419 (10)	−0.0012 (7)	0.0176 (8)	0.0048 (8)
C21	0.0434 (10)	0.0434 (10)	0.0398 (10)	0.0033 (8)	0.0175 (8)	0.0064 (8)
C22	0.0472 (11)	0.0605 (12)	0.0560 (12)	0.0004 (9)	0.0212 (9)	0.0140 (10)
C23	0.0689 (14)	0.0563 (12)	0.0599 (13)	0.0004 (10)	0.0280 (11)	0.0185 (10)
C24	0.0639 (14)	0.0566 (12)	0.0574 (13)	0.0101 (10)	0.0180 (11)	0.0204 (10)
C25	0.0429 (10)	0.0463 (10)	0.0401 (10)	0.0042 (8)	0.0153 (8)	0.0018 (8)
C26	0.0362 (9)	0.0579 (12)	0.0427 (10)	0.0030 (8)	0.0122 (8)	0.0074 (9)
C27	0.0444 (11)	0.0578 (12)	0.0549 (12)	0.0000 (9)	0.0139 (9)	0.0060 (10)
C28	0.0532 (13)	0.0732 (15)	0.0738 (16)	−0.0093 (11)	0.0109 (11)	0.0233 (12)
C29	0.0509 (13)	0.108 (2)	0.0790 (17)	−0.0087 (13)	0.0210 (12)	0.0368 (16)
C30	0.0523 (13)	0.121 (2)	0.0781 (17)	0.0143 (14)	0.0368 (12)	0.0258 (16)
C31	0.0529 (12)	0.0760 (14)	0.0637 (14)	0.0117 (11)	0.0273 (11)	0.0091 (11)
N1	0.0366 (8)	0.0545 (9)	0.0479 (9)	−0.0018 (7)	0.0097 (7)	0.0160 (7)
N2	0.0397 (9)	0.0652 (11)	0.0592 (10)	0.0035 (7)	0.0140 (8)	0.0224 (8)
N3	0.0402 (9)	0.0675 (11)	0.0562 (10)	0.0019 (7)	0.0156 (7)	0.0217 (8)
N4	0.0522 (10)	0.0591 (10)	0.0539 (10)	0.0091 (8)	0.0156 (8)	0.0160 (8)
O1	0.0361 (6)	0.0490 (7)	0.0437 (7)	0.0021 (5)	0.0146 (5)	0.0119 (6)

Geometric parameters (Å, °)

C1—C6	1.379 (2)	C16—C19	1.453 (2)
C1—C2	1.381 (3)	C17—C18	1.379 (2)
C1—H1	0.9300	C17—H17	0.9300
C2—C3	1.372 (3)	C18—H18	0.9300
C2—H2	0.9300	C19—N2	1.285 (2)
C3—C4	1.372 (3)	C19—O1	1.3618 (19)
C3—H3	0.9300	C20—N3	1.287 (2)
C4—C5	1.381 (3)	C20—O1	1.3609 (18)
C4—H4	0.9300	C20—C21	1.465 (2)
C5—C6	1.382 (2)	C21—C22	1.395 (2)
C5—H5	0.9300	C21—C25	1.404 (2)
C6—N1	1.433 (2)	C22—C23	1.370 (2)
C7—C8	1.374 (3)	C22—H22	0.9300
C7—C12	1.382 (3)	C23—C24	1.372 (3)
C7—H7	0.9300	C23—H23	0.9300
C8—C9	1.368 (3)	C24—N4	1.328 (2)
C8—H8	0.9300	C24—H24	0.9300
C9—C10	1.375 (3)	C25—N4	1.349 (2)
C9—H9	0.9300	C25—C26	1.489 (2)
C10—C11	1.381 (3)	C26—C27	1.381 (3)
C10—H10	0.9300	C26—C31	1.391 (2)
C11—C12	1.382 (2)	C27—C28	1.384 (2)
C11—H11	0.9300	C27—H27	0.9300
C12—N1	1.425 (2)	C28—C29	1.377 (3)
C13—N1	1.396 (2)	C28—H28	0.9300
C13—C14	1.400 (2)	C29—C30	1.363 (4)

C13—C18	1.404 (2)	C29—H29	0.9300
C14—C15	1.374 (2)	C30—C31	1.390 (3)
C14—H14	0.9300	C30—H30	0.9300
C15—C16	1.391 (2)	C31—H31	0.9300
C15—H15	0.9300	N2—N3	1.4049 (19)
C16—C17	1.393 (2)		
C6—C1—C2	119.9 (2)	C16—C17—H17	119.4
C6—C1—H1	120.0	C17—C18—C13	120.58 (16)
C2—C1—H1	120.0	C17—C18—H18	119.7
C3—C2—C1	120.2 (2)	C13—C18—H18	119.7
C3—C2—H2	119.9	N2—C19—O1	112.44 (14)
C1—C2—H2	119.9	N2—C19—C16	128.21 (16)
C4—C3—C2	119.9 (2)	O1—C19—C16	119.34 (14)
C4—C3—H3	120.1	N3—C20—O1	111.92 (15)
C2—C3—H3	120.1	N3—C20—C21	125.39 (15)
C3—C4—C5	120.5 (2)	O1—C20—C21	122.67 (14)
C3—C4—H4	119.8	C22—C21—C25	118.15 (16)
C5—C4—H4	119.8	C22—C21—C20	115.90 (16)
C4—C5—C6	119.6 (2)	C25—C21—C20	125.88 (14)
C4—C5—H5	120.2	C23—C22—C21	119.97 (18)
C6—C5—H5	120.2	C23—C22—H22	120.0
C1—C6—C5	119.85 (17)	C21—C22—H22	120.0
C1—C6—N1	119.37 (17)	C22—C23—C24	118.10 (17)
C5—C6—N1	120.78 (17)	C22—C23—H23	121.0
C8—C7—C12	120.3 (2)	C24—C23—H23	121.0
C8—C7—H7	119.8	N4—C24—C23	123.94 (18)
C12—C7—H7	119.8	N4—C24—H24	118.0
C9—C8—C7	120.7 (2)	C23—C24—H24	118.0
C9—C8—H8	119.6	N4—C25—C21	121.16 (15)
C7—C8—H8	119.6	N4—C25—C26	113.76 (15)
C8—C9—C10	119.2 (2)	C21—C25—C26	125.07 (15)
C8—C9—H9	120.4	C27—C26—C31	119.16 (17)
C10—C9—H9	120.4	C27—C26—C25	122.08 (16)
C9—C10—C11	120.7 (2)	C31—C26—C25	118.67 (18)
C9—C10—H10	119.6	C26—C27—C28	120.52 (19)
C11—C10—H10	119.6	C26—C27—H27	119.7
C10—C11—C12	119.9 (2)	C28—C27—H27	119.7
C10—C11—H11	120.1	C29—C28—C27	119.8 (2)
C12—C11—H11	120.1	C29—C28—H28	120.1
C7—C12—C11	119.11 (17)	C27—C28—H28	120.1
C7—C12—N1	119.12 (16)	C30—C29—C28	120.4 (2)
C11—C12—N1	121.76 (16)	C30—C29—H29	119.8
N1—C13—C14	120.61 (15)	C28—C29—H29	119.8
N1—C13—C18	121.53 (15)	C29—C30—C31	120.3 (2)
C14—C13—C18	117.86 (15)	C29—C30—H30	119.8
C15—C14—C13	121.01 (17)	C31—C30—H30	119.8
C15—C14—H14	119.5	C30—C31—C26	119.8 (2)
C13—C14—H14	119.5	C30—C31—H31	120.1
C14—C15—C16	121.15 (16)	C26—C31—H31	120.1

C14—C15—H15	119.4	C13—N1—C12	122.27 (14)
C16—C15—H15	119.4	C13—N1—C6	120.67 (14)
C15—C16—C17	118.20 (15)	C12—N1—C6	117.05 (13)
C15—C16—C19	119.18 (16)	C19—N2—N3	106.02 (14)
C17—C16—C19	122.60 (16)	C20—N3—N2	106.70 (13)
C18—C17—C16	121.17 (16)	C24—N4—C25	118.67 (16)
C18—C17—H17	119.4	C20—O1—C19	102.91 (12)
C6—C1—C2—C3	0.1 (3)	C20—C21—C25—N4	176.26 (17)
C1—C2—C3—C4	−0.7 (3)	C22—C21—C25—C26	−179.94 (17)
C2—C3—C4—C5	0.3 (3)	C20—C21—C25—C26	−2.8 (3)
C3—C4—C5—C6	0.7 (3)	N4—C25—C26—C27	120.63 (19)
C2—C1—C6—C5	0.8 (3)	C21—C25—C26—C27	−60.2 (3)
C2—C1—C6—N1	179.97 (17)	N4—C25—C26—C31	−55.9 (2)
C4—C5—C6—C1	−1.2 (3)	C21—C25—C26—C31	123.3 (2)
C4—C5—C6—N1	179.64 (17)	C31—C26—C27—C28	0.0 (3)
C12—C7—C8—C9	0.0 (3)	C25—C26—C27—C28	−176.47 (17)
C7—C8—C9—C10	−1.3 (4)	C26—C27—C28—C29	−0.6 (3)
C8—C9—C10—C11	1.3 (3)	C27—C28—C29—C30	0.4 (3)
C9—C10—C11—C12	0.0 (3)	C28—C29—C30—C31	0.4 (4)
C8—C7—C12—C11	1.4 (3)	C29—C30—C31—C26	−0.9 (3)
C8—C7—C12—N1	−179.61 (18)	C27—C26—C31—C30	0.7 (3)
C10—C11—C12—C7	−1.4 (3)	C25—C26—C31—C30	177.32 (18)
C10—C11—C12—N1	179.64 (17)	C14—C13—N1—C12	165.61 (16)
N1—C13—C14—C15	−179.51 (16)	C18—C13—N1—C12	−14.1 (3)
C18—C13—C14—C15	0.2 (3)	C14—C13—N1—C6	−15.2 (3)
C13—C14—C15—C16	1.0 (3)	C18—C13—N1—C6	165.11 (17)
C14—C15—C16—C17	−0.9 (3)	C7—C12—N1—C13	130.57 (19)
C14—C15—C16—C19	−179.44 (16)	C11—C12—N1—C13	−50.4 (2)
C15—C16—C17—C18	−0.4 (3)	C7—C12—N1—C6	−48.6 (2)
C19—C16—C17—C18	178.07 (15)	C11—C12—N1—C6	130.35 (19)
C16—C17—C18—C13	1.6 (3)	C1—C6—N1—C13	122.93 (18)
N1—C13—C18—C17	178.21 (16)	C5—C6—N1—C13	−57.9 (2)
C14—C13—C18—C17	−1.5 (3)	C1—C6—N1—C12	−57.9 (2)
C15—C16—C19—N2	26.5 (3)	C5—C6—N1—C12	121.29 (19)
C17—C16—C19—N2	−151.98 (19)	O1—C19—N2—N3	1.0 (2)
C15—C16—C19—O1	−152.41 (16)	C16—C19—N2—N3	−177.91 (18)
C17—C16—C19—O1	29.2 (3)	O1—C20—N3—N2	0.8 (2)
N3—C20—C21—C22	−3.2 (3)	C21—C20—N3—N2	179.18 (17)
O1—C20—C21—C22	175.04 (16)	C19—N2—N3—C20	−1.1 (2)
N3—C20—C21—C25	179.62 (18)	C23—C24—N4—C25	−0.2 (3)
O1—C20—C21—C25	−2.1 (3)	C21—C25—N4—C24	0.9 (3)
C25—C21—C22—C23	0.1 (3)	C26—C25—N4—C24	−179.92 (17)
C20—C21—C22—C23	−177.31 (18)	N3—C20—O1—C19	−0.16 (19)
C21—C22—C23—C24	0.6 (3)	C21—C20—O1—C19	−178.64 (16)
C22—C23—C24—N4	−0.6 (3)	N2—C19—O1—C20	−0.57 (19)
C22—C21—C25—N4	−0.8 (3)	C16—C19—O1—C20	178.46 (15)

Hydrogen-bond geometry (Å, °)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C30—H30⋯N3[i]	0.93	2.60	3.444 (3)	151

Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1