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(*E*)-3-[4-(Diphenylamino)phenyl]-1-(pyridin-2-yl)prop-2-en-1-one

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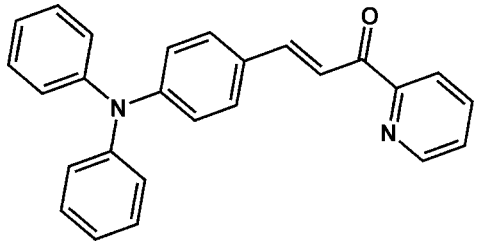
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.055; wR factor = 0.167; data-to-parameter ratio = 13.3.

The title compound, $C_{26}H_{20}N_2O$, belongs to a new family of organic two-photon absorption materials with triphenylamine and pyridine units. In the molecule, the three benzene rings are arranged in a propeller-like fashion; the dihedral angles between the rings are 80.01 (14), 75.68 (13) and 56.93 (14)°. The pyridine ring is oriented at dihedral angles of 56.24 (14), 48.92 (15) and 22.02 (13)° with respect to the three benzene rings. Weak intermolecular C—H···O hydrogen bonding is present in the crystal structure.

Related literature

For applications of two-photon absorption compounds, see: Fan *et al.* (2012); He *et al.* (2008).



Experimental

Crystal data

$C_{26}H_{20}N_2O$ M_r = 376.44
Monoclinic, $P2_1/c$
a = 12.0342 (3) Å
b = 17.4069 (4) Å
c = 9.4392 (2) Å
β = 91.757 (2)°
V = 1976.38 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
15074 measured reflections
3488 independent reflections
2210 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.167
S = 1.03
3488 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1^{i}	0.93	2.55	3.404 (3)	153
C6—H6···O1^{ii}	0.93	2.58	3.505 (3)	179

Symmetry codes: (i) $x+1, y, z$; (ii) $-x, -y, -z+1$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5410).

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supporting information

Acta Cryst. (2012). E**68**, o417 [doi:10.1107/S1600536811055036]

(*E*)-3-[4-(Diphenylamino)phenyl]-1-(pyridin-2-yl)prop-2-en-1-one

Cong-Bin Fan and Xiao-Mei Wang

S1. Comment

Organic materials with two-photon absorption (TPA) properties have attracted increasing attention due to their versatile potential applications in two-photon excited fluorescence (Fan *et al.*, 2012), three-dimensional microfabrication, high-density optical data storage, optical limiting, stabilization and reshaping (He *et al.*, 2008). However, the basic structure-function relationships regarding enhanced TPA properties remain unclear. To further understand this important issue, we synthesized the two-photon absorption material with triphenylamine and pyridine units. This compound when dissolved in tetrahydrofuran shows absorption peak 430 nm. It must be noted that there is no linear absorption for the title chromophores beyond 800 nm. The laser pumped wavelength is 850 nm which is matching with absorption peak 430 nm, the linear absorption can be excluded because two-photon excitation via virtual intermediate state can proceed, consistent with the fact that the nonlinear absorption occurs at a frequency in the region of one-photon transparency. The title chromophore shows two-photon absorption fluorescence spectra at 546 nm when excited with 850 nm femtosecond laser pulses.

S2. Experimental

To a 100 mL methanol solution of 4-(diphenylamino) benzaldehyde (1.37 g, 5.0 mmol) was added 2-acetylpridine (0.61 g, 5.0 mmol) and 2% aqueous NaOH (0.44 g, 22 mL). The mixture was stirred for 2 h at room temperature (Scheme 1). The yellow precipitate formed was collected by filtration, and washed sequentially with water and methanol for three times, respectively.

S3. Refinement

All H atoms were placed in calculated positions with C—H equal 0.93 Å. They were included in the refinement in the riding model approximation with isotropic displacement parameters set equal to $1.2U_{eq}$(C).

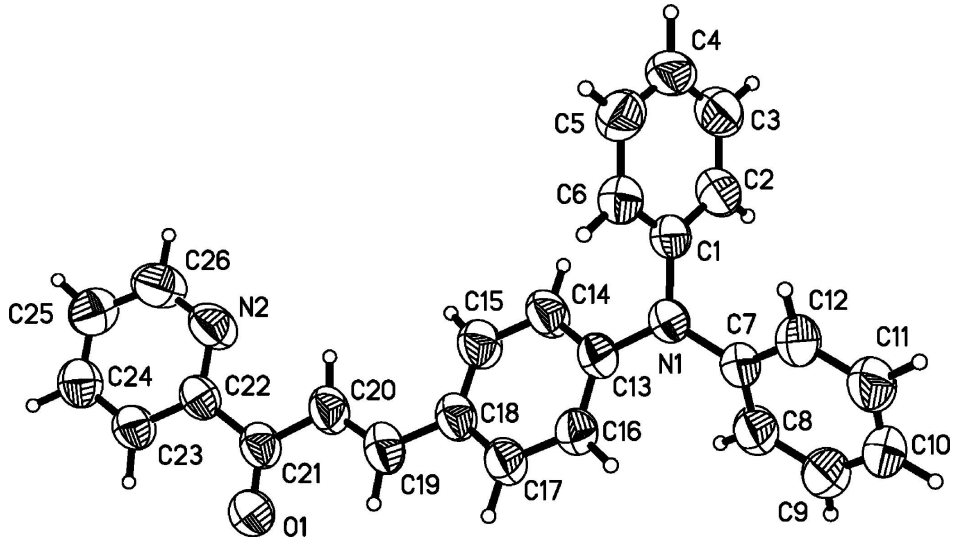

Figure 1

Molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

(*E*)-3-[4-(Diphenylamino)phenyl]-1-(pyridin-2-yl)prop-2-en-1-one

Crystal data

$C_{26}H_{20}N_2O$
$M_r = 376.44$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.0342\ (3)$ Å
$b = 17.4069\ (4)$ Å
$c = 9.4392\ (2)$ Å
$\beta = 91.757\ (2)°$
$V = 1976.38\ (8)$ Å^3
$Z = 4$
$F(000) = 792$
$D_x = 1.265$ Mg m^{-3}
Melting point: 467 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2266 reflections
$\theta = 2.5–21.1°$
$\mu = 0.08$ mm^{-1}
$T = 296$ K
Block, orange
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
15074 measured reflections
3488 independent reflections
2210 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
$h = -14\rightarrow14$
$k = -17\rightarrow20$
$l = -11\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.167$
$S = 1.03$
3488 reflections
263 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0774P)^2 + 0.1969P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0084 (18)

Special details

Experimental. ^{1}H NMR ($CDCl_3$; 400 MHz; TMS): ppm: 7.00-7.03 (m, 2H, Ar-H), 7.09-7.18 (m, 6H, Ar-H), 7.26-7.36 (m, 7H, Ar-H, pyr-H), 7.46-7.49 (m, 1H, Ar-H), 7.57, 7.59 (d, 1H, -CH=), 7.67, 7.69 (d, 1H, -CH=), 7.87-7.92 (m, 1H, pyr-H), 8.13-8.20 (m, 1H, pyr-H), 8.72, 8.74 (d, 1H, pyr-H)

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. 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 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	0.37944 (18)	0.15352 (15)	0.1848 (2)	0.0604 (6)
C2	0.4306 (2)	0.22083 (15)	0.1472 (3)	0.0724 (7)
H2	0.4013	0.2498	0.0721	0.087*
C3	0.5246 (2)	0.24556 (18)	0.2199 (3)	0.0821 (8)
H3	0.5590	0.2911	0.1939	0.099*
C4	0.5675 (2)	0.2031 (2)	0.3304 (3)	0.0829 (9)
H4	0.6305	0.2204	0.3803	0.099*
C5	0.5181 (2)	0.13502 (18)	0.3686 (3)	0.0794 (8)
H5	0.5484	0.1059	0.4428	0.095*
C6	0.4231 (2)	0.11022 (15)	0.2955 (3)	0.0686 (7)
H6	0.3890	0.0646	0.3210	0.082*
C7	0.28491 (19)	0.11150 (14)	−0.0356 (2)	0.0592 (6)
C8	0.1950 (2)	0.12480 (17)	−0.1262 (3)	0.0757 (8)
H8	0.1298	0.1450	−0.0913	0.091*
C9	0.2017 (3)	0.1082 (2)	−0.2684 (3)	0.0987 (11)
H9	0.1402	0.1166	−0.3285	0.118*
C10	0.2972 (3)	0.0796 (2)	−0.3223 (3)	0.1014 (11)
H10	0.3008	0.0683	−0.4183	0.122*
C11	0.3868 (3)	0.06786 (17)	−0.2342 (3)	0.0889 (9)
H11	0.4526	0.0493	−0.2706	0.107*
C12	0.3814 (2)	0.08311 (15)	−0.0914 (3)	0.0728 (7)
H12	0.4432	0.0742	−0.0321	0.087*
C13	0.18324 (18)	0.11941 (14)	0.1885 (2)	0.0615 (6)
C14	0.1670 (2)	0.16653 (16)	0.3048 (3)	0.0728 (7)
H14	0.2185	0.2047	0.3277	0.087*
C15	0.0747 (2)	0.15704 (16)	0.3865 (3)	0.0735 (7)
H15	0.0651	0.1894	0.4636	0.088*
C16	0.10415 (18)	0.06364 (14)	0.1553 (2)	0.0630 (6)

H16	0.1133	0.0319	0.0773	0.076*
C17	0.01208 (19)	0.05508 (15)	0.2374 (3)	0.0662 (7)
H17	−0.0406	0.0180	0.2125	0.079*
C18	−0.00423 (19)	0.10043 (15)	0.3566 (3)	0.0634 (6)
C19	−0.0996 (2)	0.08741 (15)	0.4450 (3)	0.0703 (7)
H19	−0.1560	0.0565	0.4068	0.084*
C20	−0.1147 (2)	0.11495 (15)	0.5740 (3)	0.0700 (7)
H20	−0.0612	0.1476	0.6138	0.084*
C21	−0.2123 (2)	0.09591 (15)	0.6561 (3)	0.0652 (7)
C22	−0.21265 (18)	0.11975 (13)	0.8081 (3)	0.0593 (6)
C23	−0.2974 (2)	0.09692 (16)	0.8930 (3)	0.0709 (7)
H23	−0.3557	0.0674	0.8556	0.085*
C24	−0.2956 (2)	0.11791 (17)	1.0331 (3)	0.0776 (8)
H24	−0.3519	0.1023	1.0920	0.093*
C25	−0.2104 (2)	0.16171 (17)	1.0843 (3)	0.0808 (8)
H25	−0.2081	0.1782	1.1780	0.097*
C26	−0.1279 (2)	0.18110 (19)	0.9946 (4)	0.0951 (10)
H26	−0.0683	0.2096	1.0312	0.114*
N1	0.28066 (15)	0.12811 (12)	0.1108 (2)	0.0678 (6)
N2	−0.12745 (18)	0.16178 (14)	0.8578 (3)	0.0838 (7)
O1	−0.29203 (14)	0.06052 (12)	0.60544 (19)	0.0871 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0511 (12)	0.0775 (17)	0.0531 (13)	−0.0055 (12)	0.0112 (11)	−0.0105 (12)
C2	0.0659 (15)	0.0799 (19)	0.0721 (16)	−0.0092 (14)	0.0117 (13)	0.0002 (14)
C3	0.0770 (18)	0.088 (2)	0.082 (2)	−0.0209 (16)	0.0153 (16)	−0.0128 (16)
C4	0.0626 (16)	0.113 (2)	0.0733 (18)	−0.0179 (17)	0.0095 (14)	−0.0329 (18)
C5	0.0730 (17)	0.105 (2)	0.0602 (16)	0.0035 (17)	0.0014 (14)	−0.0096 (15)
C6	0.0686 (15)	0.0775 (17)	0.0601 (15)	−0.0093 (13)	0.0092 (13)	−0.0035 (13)
C7	0.0565 (13)	0.0688 (16)	0.0528 (13)	−0.0087 (11)	0.0108 (11)	−0.0030 (11)
C8	0.0592 (15)	0.102 (2)	0.0659 (17)	−0.0043 (14)	0.0051 (13)	0.0095 (15)
C9	0.083 (2)	0.149 (3)	0.0627 (18)	−0.030 (2)	−0.0072 (16)	0.0169 (18)
C10	0.104 (2)	0.141 (3)	0.0603 (17)	−0.049 (2)	0.0226 (18)	−0.0211 (18)
C11	0.085 (2)	0.102 (2)	0.082 (2)	−0.0166 (17)	0.0294 (17)	−0.0265 (17)
C12	0.0631 (15)	0.090 (2)	0.0660 (16)	0.0002 (13)	0.0146 (12)	−0.0121 (14)
C13	0.0496 (13)	0.0759 (17)	0.0596 (14)	−0.0029 (12)	0.0119 (11)	0.0001 (12)
C14	0.0644 (15)	0.0803 (19)	0.0751 (17)	−0.0125 (13)	0.0238 (13)	−0.0141 (14)
C15	0.0672 (16)	0.0824 (18)	0.0719 (16)	−0.0018 (14)	0.0205 (13)	−0.0113 (14)
C16	0.0568 (14)	0.0767 (17)	0.0559 (14)	−0.0016 (12)	0.0077 (11)	−0.0004 (12)
C17	0.0561 (13)	0.0777 (17)	0.0651 (15)	−0.0067 (12)	0.0088 (12)	0.0049 (13)
C18	0.0532 (13)	0.0729 (16)	0.0649 (15)	0.0024 (12)	0.0119 (11)	0.0076 (13)
C19	0.0601 (14)	0.0805 (18)	0.0710 (17)	0.0008 (13)	0.0165 (13)	0.0107 (13)
C20	0.0548 (14)	0.0858 (18)	0.0705 (16)	−0.0019 (12)	0.0173 (12)	0.0074 (14)
C21	0.0528 (14)	0.0754 (17)	0.0680 (16)	0.0014 (12)	0.0106 (12)	0.0091 (13)
C22	0.0477 (12)	0.0608 (15)	0.0699 (15)	0.0034 (11)	0.0119 (11)	0.0023 (12)
C23	0.0572 (14)	0.0858 (19)	0.0705 (16)	−0.0067 (13)	0.0139 (12)	−0.0055 (14)

C24	0.0697 (17)	0.090 (2)	0.0737 (18)	0.0008 (15)	0.0190 (14)	−0.0040 (15)
C25	0.0719 (17)	0.097 (2)	0.0740 (18)	0.0114 (16)	0.0064 (14)	−0.0146 (16)
C26	0.0718 (18)	0.113 (2)	0.101 (2)	−0.0186 (17)	0.0135 (17)	−0.0349 (19)
N1	0.0469 (11)	0.1011 (16)	0.0559 (12)	−0.0106 (10)	0.0117 (9)	−0.0101 (11)
N2	0.0690 (14)	0.0918 (17)	0.0919 (17)	−0.0185 (12)	0.0224 (12)	−0.0184 (14)
O1	0.0638 (11)	0.1250 (16)	0.0731 (12)	−0.0188 (11)	0.0105 (9)	−0.0031 (11)

Geometric parameters (Å, º)

C1—C2	1.375 (3)	C13—N1	1.410 (3)
C1—C6	1.379 (3)	C14—C15	1.381 (3)
C1—N1	1.430 (3)	C14—H14	0.9300
C2—C3	1.374 (4)	C15—C18	1.392 (3)
C2—H2	0.9300	C15—H15	0.9300
C3—C4	1.366 (4)	C16—C17	1.380 (3)
C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.379 (4)	C17—C18	1.394 (3)
C4—H4	0.9300	C17—H17	0.9300
C5—C6	1.386 (3)	C18—C19	1.457 (3)
C5—H5	0.9300	C19—C20	1.326 (3)
C6—H6	0.9300	C19—H19	0.9300
C7—C8	1.378 (3)	C20—C21	1.466 (3)
C7—C12	1.382 (3)	C20—H20	0.9300
C7—N1	1.414 (3)	C21—O1	1.225 (3)
C8—C9	1.377 (4)	C21—C22	1.493 (3)
C8—H8	0.9300	C22—N2	1.333 (3)
C9—C10	1.365 (4)	C22—C23	1.375 (3)
C9—H9	0.9300	C23—C24	1.372 (4)
C10—C11	1.357 (4)	C23—H23	0.9300
C10—H10	0.9300	C24—C25	1.355 (4)
C11—C12	1.377 (4)	C24—H24	0.9300
C11—H11	0.9300	C25—C26	1.366 (4)
C12—H12	0.9300	C25—H25	0.9300
C13—C14	1.389 (3)	C26—N2	1.335 (3)
C13—C16	1.389 (3)	C26—H26	0.9300
C2—C1—C6	119.9 (2)	C13—C14—H14	119.8
C2—C1—N1	120.6 (2)	C14—C15—C18	121.8 (2)
C6—C1—N1	119.5 (2)	C14—C15—H15	119.1
C3—C2—C1	120.4 (3)	C18—C15—H15	119.1
C3—C2—H2	119.8	C17—C16—C13	120.4 (2)
C1—C2—H2	119.8	C17—C16—H16	119.8
C4—C3—C2	119.8 (3)	C13—C16—H16	119.8
C4—C3—H3	120.1	C16—C17—C18	121.9 (2)
C2—C3—H3	120.1	C16—C17—H17	119.1
C3—C4—C5	120.6 (3)	C18—C17—H17	119.1
C3—C4—H4	119.7	C15—C18—C17	116.9 (2)
C5—C4—H4	119.7	C15—C18—C19	122.6 (2)

C4—C5—C6	119.5 (3)	C17—C18—C19	120.5 (2)
C4—C5—H5	120.2	C20—C19—C18	127.0 (3)
C6—C5—H5	120.2	C20—C19—H19	116.5
C1—C6—C5	119.8 (3)	C18—C19—H19	116.5
C1—C6—H6	120.1	C19—C20—C21	122.6 (3)
C5—C6—H6	120.1	C19—C20—H20	118.7
C8—C7—C12	118.5 (2)	C21—C20—H20	118.7
C8—C7—N1	121.4 (2)	O1—C21—C20	122.5 (2)
C12—C7—N1	120.1 (2)	O1—C21—C22	119.3 (2)
C9—C8—C7	120.1 (3)	C20—C21—C22	118.1 (2)
C9—C8—H8	119.9	N2—C22—C23	122.0 (2)
C7—C8—H8	119.9	N2—C22—C21	117.8 (2)
C10—C9—C8	120.9 (3)	C23—C22—C21	120.2 (2)
C10—C9—H9	119.5	C24—C23—C22	119.6 (3)
C8—C9—H9	119.5	C24—C23—H23	120.2
C11—C10—C9	119.3 (3)	C22—C23—H23	120.2
C11—C10—H10	120.4	C25—C24—C23	118.9 (3)
C9—C10—H10	120.4	C25—C24—H24	120.6
C10—C11—C12	120.7 (3)	C23—C24—H24	120.6
C10—C11—H11	119.7	C24—C25—C26	118.3 (3)
C12—C11—H11	119.7	C24—C25—H25	120.8
C11—C12—C7	120.5 (3)	C26—C25—H25	120.8
C11—C12—H12	119.8	N2—C26—C25	124.2 (3)
C7—C12—H12	119.8	N2—C26—H26	117.9
C14—C13—C16	118.6 (2)	C25—C26—H26	117.9
C14—C13—N1	119.2 (2)	C13—N1—C7	122.81 (19)
C16—C13—N1	122.2 (2)	C13—N1—C1	118.08 (18)
C15—C14—C13	120.4 (2)	C7—N1—C1	119.09 (18)
C15—C14—H14	119.8	C22—N2—C26	116.9 (2)

C6—C1—C2—C3	−0.5 (4)	C18—C19—C20—C21	−177.7 (2)
N1—C1—C2—C3	179.1 (2)	C19—C20—C21—O1	−8.4 (4)
C1—C2—C3—C4	−0.1 (4)	C19—C20—C21—C22	170.5 (2)
C2—C3—C4—C5	0.9 (4)	O1—C21—C22—N2	−176.4 (2)
C3—C4—C5—C6	−1.1 (4)	C20—C21—C22—N2	4.6 (3)
C2—C1—C6—C5	0.3 (4)	O1—C21—C22—C23	5.1 (4)
N1—C1—C6—C5	−179.3 (2)	C20—C21—C22—C23	−173.8 (2)
C4—C5—C6—C1	0.5 (4)	N2—C22—C23—C24	0.3 (4)
C12—C7—C8—C9	1.5 (4)	C21—C22—C23—C24	178.7 (2)
N1—C7—C8—C9	179.8 (3)	C22—C23—C24—C25	0.8 (4)
C7—C8—C9—C10	−1.0 (5)	C23—C24—C25—C26	−2.0 (4)
C8—C9—C10—C11	−0.4 (5)	C24—C25—C26—N2	2.3 (5)
C9—C10—C11—C12	1.2 (5)	C14—C13—N1—C7	−150.5 (2)
C10—C11—C12—C7	−0.7 (4)	C16—C13—N1—C7	31.4 (4)
C8—C7—C12—C11	−0.6 (4)	C14—C13—N1—C1	30.6 (3)
N1—C7—C12—C11	−179.0 (2)	C16—C13—N1—C1	−147.4 (2)
C16—C13—C14—C15	1.0 (4)	C8—C7—N1—C13	34.6 (4)
N1—C13—C14—C15	−177.2 (2)	C12—C7—N1—C13	−147.1 (2)

C13—C14—C15—C18	0.4 (4)	C8—C7—N1—C1	−146.6 (2)
C14—C13—C16—C17	−0.6 (4)	C12—C7—N1—C1	31.7 (3)
N1—C13—C16—C17	177.5 (2)	C2—C1—N1—C13	−119.3 (3)
C13—C16—C17—C18	−1.1 (4)	C6—C1—N1—C13	60.2 (3)
C14—C15—C18—C17	−2.0 (4)	C2—C1—N1—C7	61.8 (3)
C14—C15—C18—C19	177.4 (2)	C6—C1—N1—C7	−118.6 (2)
C16—C17—C18—C15	2.4 (4)	C23—C22—N2—C26	−0.1 (4)
C16—C17—C18—C19	−177.0 (2)	C21—C22—N2—C26	−178.5 (2)
C15—C18—C19—C20	−13.4 (4)	C25—C26—N2—C22	−1.2 (5)
C17—C18—C19—C20	165.9 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	0.93	2.55	3.404 (3)	153
C6—H6···O1^{ii}	0.93	2.58	3.505 (3)	179

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