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4-(Diphenylmethylene)-3-pentyl-5,6-dihydro-4*H*-pyrrolo[1,2-e][1,2,3]triazole

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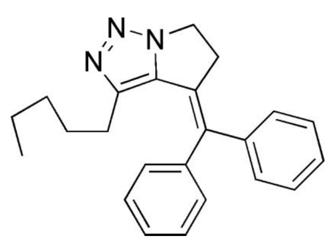
Key indicators: single-crystal X-ray study; *T* = 298 K; mean σ(C–C) = 0.002 Å; *R* factor = 0.044; *wR* factor = 0.132; data-to-parameter ratio = 14.3.

The title compound, $C_{23}H_{25}N_3$, is an important pyrrolotriazole compound. The two phenyl rings are nearly perpendicular, with a dihedral angle between them of 85.88 (8)°. The five-membered pyrrolidine ring adopts an envelope conformation.

Related literature

For related literature, see: Dulcere *et al.* (1990); Pearson *et al.* (1990).



Experimental

Crystal data

$C_{23}H_{25}N_3$
M_r = 343.46
Triclinic, $P\overline{1}$
a = 8.5670 (17) Å
b = 9.4620 (19) Å
c = 12.626 (3) Å
α = 110.15 (3)°
β = 96.53 (3)°
γ = 92.35 (3)°
V = 951.1 (4) Å^3
Z = 2
Mo *K*α radiation
μ = 0.07 mm^{-1}
T = 298 (2) K
0.46 × 0.34 × 0.30 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.968, T_{max} = 0.979
7658 measured reflections
3390 independent reflections
2760 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.132
S = 1.05
3390 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2050).

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supplementary materials

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4-(Diphenylmethylene)-3-pentyl-5,6-dihydro-4*H*-pyrrolo[1,2-*e*][1,2,3]triazole

Y.-H. Zhu, S.-S. Li, Y.-H. Xu and C.-A. Ma

Comment

Pyrrolotriazoles are an important class of heterocycles due to their applications as bioactive compounds and synthetic intermediates in organic synthesis (Dulcere *et al.*, 1990; Pearson *et al.*, 1990). The molecular structure of **I** contains an exocyclic double bondconnecting two benzene rings (Fig. 1). The two benzene rings are near perpendicular with the dihedral angle of 85.88 (8)°. The five-membered pyrrolidine ring adopts an envelope conformation, with atom C4 lying at the flap position. All bond lengths and angles in (I) are normal.

Experimental

1-(3-Iodo-4, 4-diphenylbut-3-enyl)-4-pentyl-1*H*-1,2,3-triazole (0.25 mmol), $Pd(OAc)_2$ (0.025 mmol), tetrabutylammonium chloride (TBAC, 0.25 mmol), $NaHCO_3$ (0.5 mmol), and *N*,*N*-dimethylformamide (DMF, 1 ml) were added into a Schlenk tube at r.t. The reaction mixture was stirred at 100 °C until the reaction was completed, as monitored by TLC. Then the reaction mixture was cooled and H_2O (15 ml) was added. The aqueous layer was extracted with EtOAc (3 × 15 ml). The organic layer was dried over anhyd $MgSO_4$. After evaporation, the residue was subjected to preparative TLC (eluent: PE–EtOAc, 1:4) to afford 4,4-diphenylmethylene-3-pentyl-5,6-dihydro-4*H*-pyrrolo-[1,2-*c*][1,2,3]-triazoles and the single crystals were obtained by evaporation of a petroleum ether–dichloromethane (1:9) mixed solution. m.p. 401–403 K, ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.81 (t, 3H, J = 7.28 Hz), 0.91–0.95 (m, 2H), 1.13–1.18 (m, 2H), 1.25–1.29 (m, 2H), 1.49 (t, 2H, J = 7.49 Hz), 3.52 (t, 2H, J = 6.94 Hz), 4.38 (t, 2H, J = 6.94 Hz), 7.19–7.37 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.98, 141.31, 138.41, 137.64, 129.93, 129.18, 128.73, 128.21, 127.85, 127.69, 123.53, 45.24, 37.51, 31.36, 29.16, 25.60, 22.30, 13.96; IR ν_{max}(cm^{-1}): 2964, 2922, 1440, 764, 702; MS (70 eV, EI) *m/z* (%): 343 (M^+, 10.23); Anal. calcd for $C_{23}H_{25}N_3$: C 80.43, H 7.34, N 12.23; Found: C, 80.20 H 7.41 N 12.33.

Refinement

H atoms were positioned geometrically and treated as riding, with C—H bond lengths constrained to 0.93 (aromatic CH), 0.97 Å (methylene CH2)or 0.96 Å (methyl CH3) and with U_{iso}(H) = 1.2Ueq (carrier aromatic C and methylene C) and U_{iso}(H) = 1.5Ueq (methyl C)

Figures

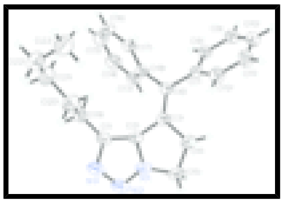

Fig. 1. The molecular structure of (**I**), with displacement ellipsoids drawn at the 40% probability level. H atoms are shown as spheres of arbitrary radius.

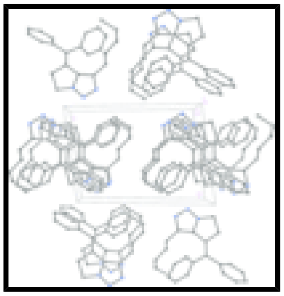

Fig. 2. The molecular packing of (**I**). H atoms have been omitted for clarity.

4-(Diphenylmethylene)-3-pentyl-5,6-dihydro-4*H*-pyrrolo[1,2-e][1,2,3]triazole

Crystal data

$C_{23}H_{25}N_3$	$Z = 2$
$M_r = 343.46$	$F_{000} = 368$
Triclinic, $P\overline{1}$	$D_x = 1.199$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 401-403 K
$a = 8.5670$ (17) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 9.4620$ (19) Å	Cell parameters from 7563 reflections
$c = 12.626$ (3) Å	$\theta = 3.1$–27.5º
$\alpha = 110.15$ (3)º	$\mu = 0.07$ mm^{-1}
$\beta = 96.53$ (3)º	$T = 298$ (2) K
$\gamma = 92.35$ (3)º	Prism, colourless
$V = 951.1$ (4) Å^3	0.46 × 0.34 × 0.30 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer	3390 independent reflections
Radiation source: fine-focus sealed tube	2760 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
$T = 298(2)$ K	$\theta_{max} = 25.2$º
φ and ω scans	$\theta_{min} = 3.2$º
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	$h = -10 \rightarrow 10$
$T_{min} = 0.968$, $T_{max} = 0.979$	$k = -10 \rightarrow 11$
7658 measured reflections	$l = -15 \rightarrow 14$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.044$	$w = 1/[\sigma^2(F_o^2) + (0.079P)^2 + 0.0929P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.132$	$(\Delta/\sigma)_{max} < 0.001$

$S = 1.05$	$\Delta\rho_{max} = 0.28$ e Å^{-3}
3390 reflections	$\Delta\rho_{min} = -0.16$ e Å^{-3}
237 parameters	Extinction correction: SHELXTL (Sheldrick, 2001), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.064 (7)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.33609 (17)	0.27301 (16)	0.25285 (13)	0.0482 (4)
C2	0.35129 (15)	0.24224 (14)	0.13890 (12)	0.0421 (3)
C3	0.45343 (16)	0.23998 (14)	0.05331 (11)	0.0408 (3)
C4	0.35889 (18)	0.14039 (17)	−0.06004 (13)	0.0516 (4)
H4A	0.3933	0.0391	−0.0836	0.062*
H4B	0.3720	0.1823	−0.1189	0.062*
C5	0.18669 (19)	0.13781 (19)	−0.03883 (15)	0.0587 (4)
H5A	0.1298	0.2083	−0.0656	0.070*
H5B	0.1329	0.0374	−0.0747	0.070*
C6	0.59495 (15)	0.31716 (14)	0.06819 (11)	0.0389 (3)
C7	0.68776 (15)	0.30490 (15)	−0.02667 (11)	0.0403 (3)
C8	0.76621 (17)	0.43428 (16)	−0.03088 (13)	0.0476 (4)
H8	0.7613	0.5266	0.0266	0.057*
C9	0.85109 (18)	0.42807 (18)	−0.11863 (14)	0.0542 (4)
H9	0.9008	0.5161	−0.1207	0.065*
C10	0.8624 (2)	0.2925 (2)	−0.20268 (14)	0.0592 (4)
H10	0.9200	0.2884	−0.2616	0.071*
C11	0.7883 (2)	0.16252 (19)	−0.19965 (14)	0.0628 (5)
H11	0.7965	0.0703	−0.2563	0.075*
C12	0.70185 (19)	0.16862 (17)	−0.11269 (13)	0.0530 (4)
H12	0.6521	0.0800	−0.1116	0.064*
C13	0.59302 (19)	0.56081 (17)	0.23027 (14)	0.0533 (4)
H13	0.4989	0.5778	0.1938	0.064*
C14	0.6605 (2)	0.6666 (2)	0.33246 (16)	0.0702 (5)
H14	0.6123	0.7549	0.3643	0.084*

C15	0.7988 (3)	0.6422 (2)	0.38757 (16)	0.0769 (6)
H15	0.8432	0.7130	0.4573	0.092*
C16	0.8709 (2)	0.5131 (2)	0.33934 (15)	0.0697 (5)
H16	0.9648	0.4969	0.3765	0.084*
C17	0.80560 (17)	0.40706 (19)	0.23614 (13)	0.0516 (4)
H17	0.8565	0.3208	0.2035	0.062*
C18	0.66401 (15)	0.42899 (15)	0.18103 (11)	0.0410 (3)
C19	0.45400 (19)	0.32105 (18)	0.35752 (13)	0.0545 (4)
H19A	0.3994	0.3543	0.4240	0.065*
H19B	0.5223	0.4061	0.3588	0.065*
C20	0.5532 (2)	0.1953 (2)	0.36372 (15)	0.0688 (5)
H20A	0.6011	0.1575	0.2944	0.083*
H20B	0.4849	0.1131	0.3671	0.083*
C21	0.6819 (2)	0.2416 (2)	0.46465 (15)	0.0719 (5)
H21A	0.7497	0.3245	0.4617	0.086*
H21B	0.6340	0.2783	0.5340	0.086*
C22	0.7820 (3)	0.1160 (3)	0.46995 (17)	0.0785 (6)
H22A	0.8562	0.1533	0.5395	0.094*
H22B	0.7141	0.0343	0.4745	0.094*
C23	0.8721 (3)	0.0538 (3)	0.37182 (18)	0.0864 (6)
H23A	0.8000	0.0007	0.3042	0.130*
H23B	0.9435	−0.0144	0.3874	0.130*
H23C	0.9307	0.1351	0.3608	0.130*
N1	0.20552 (13)	0.18469 (13)	0.08445 (11)	0.0491 (3)
N2	0.10358 (15)	0.18025 (16)	0.15497 (14)	0.0627 (4)
N3	0.18367 (16)	0.23448 (16)	0.25885 (13)	0.0610 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0419 (8)	0.0454 (8)	0.0559 (9)	−0.0007 (6)	0.0133 (7)	0.0146 (6)
C2	0.0325 (7)	0.0360 (7)	0.0536 (8)	−0.0028 (5)	0.0021 (6)	0.0124 (6)
C3	0.0376 (7)	0.0386 (7)	0.0424 (8)	−0.0015 (6)	−0.0005 (6)	0.0118 (6)
C4	0.0495 (9)	0.0499 (8)	0.0472 (9)	−0.0106 (7)	−0.0051 (7)	0.0121 (6)
C5	0.0463 (9)	0.0558 (9)	0.0654 (10)	−0.0125 (7)	−0.0114 (8)	0.0183 (8)
C6	0.0353 (7)	0.0380 (7)	0.0411 (7)	0.0000 (5)	0.0016 (6)	0.0124 (6)
C7	0.0355 (7)	0.0446 (7)	0.0392 (7)	−0.0003 (6)	−0.0002 (6)	0.0146 (6)
C8	0.0440 (8)	0.0454 (8)	0.0499 (8)	−0.0038 (6)	0.0061 (7)	0.0132 (6)
C9	0.0501 (9)	0.0592 (9)	0.0560 (9)	−0.0069 (7)	0.0064 (7)	0.0252 (7)
C10	0.0561 (9)	0.0760 (11)	0.0456 (9)	−0.0004 (8)	0.0134 (7)	0.0202 (8)
C11	0.0716 (11)	0.0565 (9)	0.0524 (10)	0.0015 (8)	0.0189 (8)	0.0065 (7)
C12	0.0595 (9)	0.0436 (8)	0.0535 (9)	−0.0023 (7)	0.0121 (7)	0.0133 (7)
C13	0.0491 (9)	0.0474 (8)	0.0567 (9)	−0.0047 (7)	0.0079 (7)	0.0107 (7)
C14	0.0756 (12)	0.0530 (10)	0.0646 (11)	−0.0174 (9)	0.0189 (10)	−0.0016 (8)
C15	0.0759 (13)	0.0854 (13)	0.0463 (10)	−0.0385 (11)	0.0045 (9)	0.0001 (9)
C16	0.0459 (9)	0.1048 (15)	0.0518 (10)	−0.0249 (9)	−0.0086 (8)	0.0275 (10)
C17	0.0372 (8)	0.0684 (10)	0.0470 (8)	−0.0052 (7)	0.0031 (6)	0.0197 (7)
C18	0.0347 (7)	0.0446 (7)	0.0407 (7)	−0.0077 (6)	0.0055 (6)	0.0124 (6)

C19	0.0560 (9)	0.0591 (9)	0.0444 (9)	−0.0047 (7)	0.0140 (7)	0.0118 (7)
C20	0.0696 (11)	0.0648 (11)	0.0600 (11)	−0.0012 (9)	−0.0041 (9)	0.0116 (8)
C21	0.0791 (13)	0.0765 (12)	0.0485 (10)	−0.0009 (10)	0.0027 (9)	0.0098 (8)
C22	0.0752 (13)	0.0949 (14)	0.0607 (11)	0.0034 (11)	−0.0047 (10)	0.0263 (10)
C23	0.0782 (14)	0.1045 (16)	0.0700 (13)	0.0172 (12)	0.0027 (11)	0.0236 (11)
N1	0.0332 (6)	0.0461 (7)	0.0633 (8)	−0.0047 (5)	0.0015 (6)	0.0158 (6)
N2	0.0372 (7)	0.0612 (8)	0.0871 (11)	−0.0037 (6)	0.0146 (7)	0.0218 (7)
N3	0.0473 (8)	0.0612 (8)	0.0724 (10)	−0.0024 (6)	0.0200 (7)	0.0179 (7)

Geometric parameters (Å, °)

C1—N3	1.359 (2)	C13—C18	1.388 (2)
C1—C2	1.389 (2)	C13—H13	0.9300
C1—C19	1.489 (2)	C14—C15	1.373 (3)
C2—N1	1.3489 (18)	C14—H14	0.9300
C2—C3	1.461 (2)	C15—C16	1.371 (3)
C3—C6	1.3489 (19)	C15—H15	0.9300
C3—C4	1.529 (2)	C16—C17	1.380 (2)
C4—C5	1.530 (2)	C16—H16	0.9300
C4—H4A	0.9700	C17—C18	1.388 (2)
C4—H4B	0.9700	C17—H17	0.9300
C5—N1	1.452 (2)	C19—C20	1.508 (2)
C5—H5A	0.9700	C19—H19A	0.9700
C5—H5B	0.9700	C19—H19B	0.9700
C6—C7	1.4861 (19)	C20—C21	1.513 (3)
C6—C18	1.489 (2)	C20—H20A	0.9700
C7—C12	1.391 (2)	C20—H20B	0.9700
C7—C8	1.392 (2)	C21—C22	1.508 (3)
C8—C9	1.379 (2)	C21—H21A	0.9700
C8—H8	0.9300	C21—H21B	0.9700
C9—C10	1.370 (2)	C22—C23	1.493 (3)
C9—H9	0.9300	C22—H22A	0.9700
C10—C11	1.375 (2)	C22—H22B	0.9700
C10—H10	0.9300	C23—H23A	0.9600
C11—C12	1.379 (2)	C23—H23B	0.9600
C11—H11	0.9300	C23—H23C	0.9600
C12—H12	0.9300	N1—N2	1.3254 (19)
C13—C14	1.376 (2)	N2—N3	1.326 (2)
N3—C1—C2	107.72 (14)	C16—C15—C14	119.71 (17)
N3—C1—C19	119.73 (14)	C16—C15—H15	120.1
C2—C1—C19	132.18 (13)	C14—C15—H15	120.1
N1—C2—C1	103.58 (13)	C15—C16—C17	120.64 (17)
N1—C2—C3	108.11 (13)	C15—C16—H16	119.7
C1—C2—C3	148.26 (13)	C17—C16—H16	119.7
C6—C3—C2	128.27 (13)	C16—C17—C18	120.09 (17)
C6—C3—C4	126.70 (14)	C16—C17—H17	120.0
C2—C3—C4	104.86 (12)	C18—C17—H17	120.0
C3—C4—C5	105.79 (13)	C13—C18—C17	118.64 (14)
C3—C4—H4A	110.6	C13—C18—C6	120.85 (13)

C5—C4—H4A	110.6	C17—C18—C6	120.42 (13)
C3—C4—H4B	110.6	C1—C19—C20	112.15 (13)
C5—C4—H4B	110.6	C1—C19—H19A	109.2
H4A—C4—H4B	108.7	C20—C19—H19A	109.2
N1—C5—C4	100.99 (12)	C1—C19—H19B	109.2
N1—C5—H5A	111.6	C20—C19—H19B	109.2
C4—C5—H5A	111.6	H19A—C19—H19B	107.9
N1—C5—H5B	111.6	C19—C20—C21	114.11 (15)
C4—C5—H5B	111.6	C19—C20—H20A	108.7
H5A—C5—H5B	109.4	C21—C20—H20A	108.7
C3—C6—C7	123.05 (13)	C19—C20—H20B	108.7
C3—C6—C18	121.56 (13)	C21—C20—H20B	108.7
C7—C6—C18	115.28 (11)	H20A—C20—H20B	107.6
C12—C7—C8	117.43 (13)	C22—C21—C20	113.99 (16)
C12—C7—C6	123.08 (13)	C22—C21—H21A	108.8
C8—C7—C6	119.49 (12)	C20—C21—H21A	108.8
C9—C8—C7	121.25 (14)	C22—C21—H21B	108.8
C9—C8—H8	119.4	C20—C21—H21B	108.8
C7—C8—H8	119.4	H21A—C21—H21B	107.6
C10—C9—C8	120.16 (15)	C23—C22—C21	115.16 (18)
C10—C9—H9	119.9	C23—C22—H22A	108.5
C8—C9—H9	119.9	C21—C22—H22A	108.5
C9—C10—C11	119.84 (15)	C23—C22—H22B	108.5
C9—C10—H10	120.1	C21—C22—H22B	108.5
C11—C10—H10	120.1	H22A—C22—H22B	107.5
C10—C11—C12	120.13 (15)	C22—C23—H23A	109.5
C10—C11—H11	119.9	C22—C23—H23B	109.5
C12—C11—H11	119.9	H23A—C23—H23B	109.5
C11—C12—C7	121.18 (15)	C22—C23—H23C	109.5
C11—C12—H12	119.4	H23A—C23—H23C	109.5
C7—C12—H12	119.4	H23B—C23—H23C	109.5
C14—C13—C18	120.66 (17)	N2—N1—C2	112.88 (13)
C14—C13—H13	119.7	N2—N1—C5	131.20 (13)
C18—C13—H13	119.7	C2—N1—C5	115.92 (13)
C15—C14—C13	120.23 (18)	N1—N2—N3	106.16 (12)
C15—C14—H14	119.9	N2—N3—C1	109.65 (14)
C13—C14—H14	119.9		

N3—C1—C2—N1	−0.93 (15)	C13—C14—C15—C16	1.2 (3)
C19—C1—C2—N1	171.87 (15)	C14—C15—C16—C17	−0.3 (3)
N3—C1—C2—C3	−177.8 (2)	C15—C16—C17—C18	−1.2 (3)
C19—C1—C2—C3	−5.0 (3)	C14—C13—C18—C17	−0.9 (2)
N1—C2—C3—C6	162.70 (13)	C14—C13—C18—C6	−177.46 (14)
C1—C2—C3—C6	−20.5 (3)	C16—C17—C18—C13	1.8 (2)
N1—C2—C3—C4	−12.67 (14)	C16—C17—C18—C6	178.33 (14)
C1—C2—C3—C4	164.2 (2)	C3—C6—C18—C13	−65.61 (18)
C6—C3—C4—C5	−155.29 (14)	C7—C6—C18—C13	110.64 (14)
C2—C3—C4—C5	20.18 (15)	C3—C6—C18—C17	117.91 (15)
C3—C4—C5—N1	−19.41 (15)	C7—C6—C18—C17	−65.84 (17)
C2—C3—C6—C7	−179.97 (12)	N3—C1—C19—C20	100.21 (18)

C4—C3—C6—C7	−5.6 (2)	C2—C1—C19—C20	−71.9 (2)
C2—C3—C6—C18	−4.0 (2)	C1—C19—C20—C21	176.16 (15)
C4—C3—C6—C18	170.40 (13)	C19—C20—C21—C22	−179.40 (17)
C3—C6—C7—C12	−41.1 (2)	C20—C21—C22—C23	62.1 (3)
C18—C6—C7—C12	142.75 (14)	C1—C2—N1—N2	1.04 (15)
C3—C6—C7—C8	139.42 (14)	C3—C2—N1—N2	179.32 (11)
C18—C6—C7—C8	−36.77 (18)	C1—C2—N1—C5	−178.51 (12)
C12—C7—C8—C9	1.7 (2)	C3—C2—N1—C5	−0.23 (16)
C6—C7—C8—C9	−178.76 (13)	C4—C5—N1—N2	−166.64 (14)
C7—C8—C9—C10	−1.4 (2)	C4—C5—N1—C2	12.81 (17)
C8—C9—C10—C11	0.3 (3)	C2—N1—N2—N3	−0.73 (16)
C9—C10—C11—C12	0.5 (3)	C5—N1—N2—N3	178.73 (14)
C10—C11—C12—C7	−0.1 (3)	N1—N2—N3—C1	0.09 (16)
C8—C7—C12—C11	−0.9 (2)	C2—C1—N3—N2	0.55 (17)
C6—C7—C12—C11	179.52 (14)	C19—C1—N3—N2	−173.31 (13)
C18—C13—C14—C15	−0.5 (3)		

Fig. 1

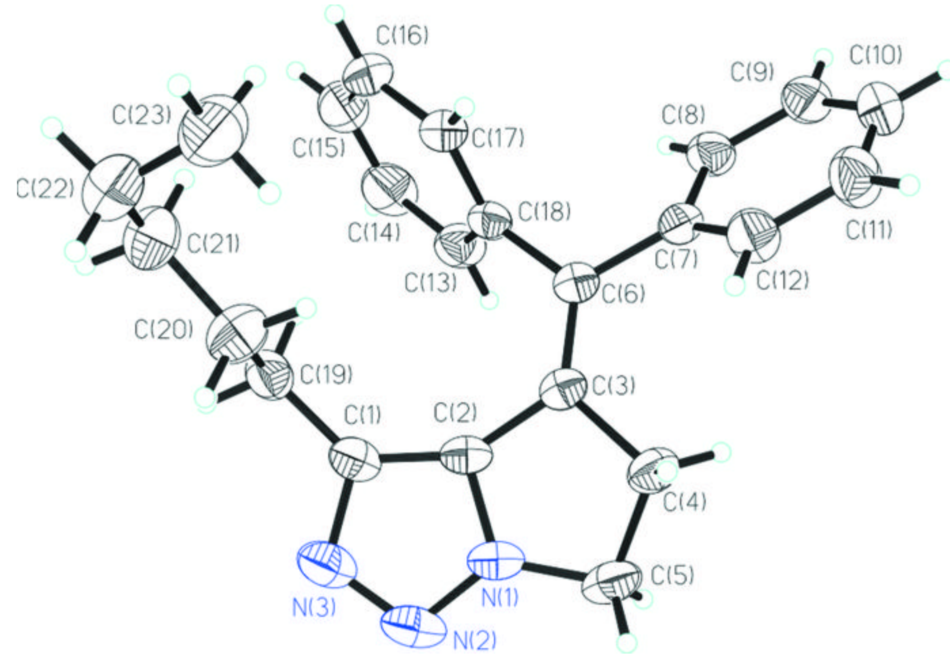
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Fig. 2