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5-(4′-Methylbiphenyl-2-yl)-2-triphenylmethyl-2*H*-tetrazole

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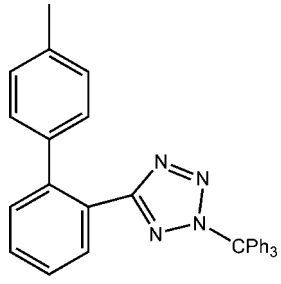
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.060; wR factor = 0.148; data-to-parameter ratio = 17.7.

The title compound, $C_{33}H_{26}N_4$, was synthesized in two steps from 2-phenylbenzonitrile. Geometric parameters are in the usual ranges. The tetrazole ring encloses dihedral angles of 45.76 (9), 71.44 (8) and 72.38 (6)° with the three phenyl rings of the triphenylmethyl group. The dihedral angle between the tetrazole ring and the benzene ring directly attached to it is 49.13 (8)° and the dihedral angle between the aromatic rings of the biphenyl group is 54.29 (8)°.

Related literature

For the chemistry of tetrazole, see: Arp *et al.* (2000); Dunica *et al.* (1991); Wang *et al.* (2005); Wittenberger & Donner (1993).

For related literature, see: Hu *et al.* (2007).



Experimental

Crystal data

$C_{33}H_{26}N_4$
M_r = 478.58
Monoclinic, $P2_1/c$
a = 12.529 (3) Å
b = 12.710 (3) Å
c = 17.707 (7) Å
β = 113.58 (2)°
V = 2584.3 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 (2) K
0.2 × 0.08 × 0.08 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.816, T_{max} = 1.000
(expected range = 0.812–0.994)
26288 measured reflections
5925 independent reflections
3802 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.148
S = 1.03
5925 reflections
335 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL/PC*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2551).

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supplementary materials

Acta Cryst. (2007). E**63**, o4410 [**doi:10.1107/S1600536807051537**]

5-(4'-Methylbiphenyl-2-yl)-2-triphenylmethyl-2*H*-tetrazole

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Comment

Studies on compounds containing a tetrazole ring were in recent years highly stimulated by its a wide range of applications in coordination chemistry as ligands, in medicinal chemistry as a metabolically stable surrogate for a carboxylic acid group, and in materials science as high density energy materials (Hu, *et al.*, 2007, Wang, *et al.*, 2005; Dunica, *et al.*, 1991; Wittenberger *et al.*, 1993). We report here the crystal structure of 2-triphenylmethyl-5-(2-(4-methyl-phenyl)-benzyl)-tetrazole.

The tetrazole moiety is substituted by a triphenyl-methyl group in the position of N2 and a 2-(4-methyl-phenyl)-benzyl group in the position of C1. The bond distances and bond angles of tetrazole functional group are similar to those found in other tetrazole-containing compounds (Wang, *et al.*, 2005; Arp *et al.*, 2000; Hu, *et al.*, 2007). Geometric parameters are in the usual ranges. The tetrazole rings encloses dihedral angles of 45.76 (9)°, 71.44 (8)° and 72.38 (6)° with the three phenyl rings of the triphenylmethyl residue. The dihedral angle between the phenyl ring directly attached to the tetrazole ring is 49.13 (8)° and the dihedral angle between the aromatic rings of the biphenyl moiety is 54.29 (8)°.

Experimental

5-(2-(4-methyl-phenyl)-benzyl)-tetrazole was synthesized by reaction of 2-(4-methyl-phenyl)-benzonitrile and sodium azide in the presence of zinc(II) choride according to the procedure described in the literature method (Dunica, *et al.*, 1991). To a toluene solution (50 ml) containing 5-(2-phenyl-benzyl)-tetrazole (112 mg, 0.5 mmol) and chlorotriphenylmethane (161 mg, 0.5 mmol) was added 5 ml of an aqueous solution of NaOH (22 mg, 0.55 mol). The mixture was stirred for 8 h until a precipitation was observed. After filtration and washing with 2 ml e thanol, the crude product was collected and re-crystallized by slowly evaporating its ethyl acetate solution to obtain colorless block shaped crystals.

Refinement

Positional parameters of all the H atoms were calculated geometrically and were allowed to ride on their parent atoms with U_{iso}(H) = 1.2Ueq(C) or U_{iso}(H) = 1.5Ueq(C_{methyl}).

Figures

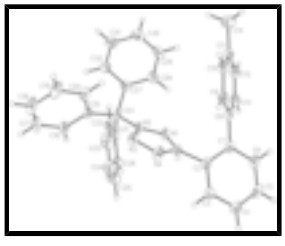

Fig. 1. A view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level.

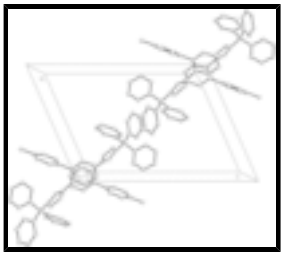

Fig. 2. Fig. i2. The crystal packing of the title compound viewed along the *b* axis.

5-(4'-Methylbiphenyl-2-yl)-2-triphenylmethyl-2*H*-tetrazole

Crystal data

$C_{33}H_{26}N_4$	F_{000} = 1008
M_r = 478.58	D_x = 1.230 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 20885 reflections
a = 12.529 (3) Å	θ = 3.0–27.5º
b = 12.710 (3) Å	μ = 0.07 mm^{-1}
c = 17.707 (7) Å	T = 293 (2) K
β = 113.58 (2)º	Blocck, colorless
V = 2584.3 (13) Å^3	0.2 × 0.08 × 0.08 mm
Z = 4	

Data collection

Rigaku Mercury2 (2x2 bin mode) diffractometer	3802 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.061
Monochromator: graphite	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 3.0º
ω scans	h = −16→16
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	k = −16→16
T_{min} = 0.816, T_{max} = 1.000	l = −22→22
26288 measured reflections	Standard reflections: ?
5925 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.060	H-atom parameters constrained
$wR(F^2)$ = 0.148	$w = 1/[\sigma^2(F_o^2) + (0.0631P)^2 + 0.3939P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max} < 0.001$

5925 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
335 parameters	$\Delta\rho_{min} = -0.24$ 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 $F^2 > 2\text{sigma}(F^2)$ 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}
N1	−0.14908 (13)	−0.37059 (12)	−0.19321 (9)	0.0394 (4)
N2	−0.23004 (12)	−0.32303 (11)	−0.25762 (8)	0.0329 (3)
N3	−0.24932 (14)	−0.22479 (12)	−0.24201 (10)	0.0449 (4)
N4	−0.17693 (15)	−0.20571 (13)	−0.16526 (9)	0.0483 (4)
C1	−0.11690 (15)	−0.29541 (14)	−0.13699 (10)	0.0345 (4)
C2	−0.03109 (15)	−0.31302 (14)	−0.05191 (11)	0.0377 (4)
C3	−0.06098 (18)	−0.28582 (17)	0.01298 (12)	0.0481 (5)
H3	−0.1294	−0.2487	0.0027	0.058*
C4	0.0102 (2)	−0.31350 (18)	0.09289 (12)	0.0574 (6)
H4	−0.0094	−0.2940	0.1364	0.069*
C5	0.1101 (2)	−0.37015 (18)	0.10759 (12)	0.0591 (6)
H5	0.1558	−0.3928	0.1607	0.071*
C6	0.14280 (18)	−0.39344 (16)	0.04398 (12)	0.0503 (5)
H6	0.2117	−0.4301	0.0551	0.060*
C7	0.07479 (16)	−0.36322 (14)	−0.03679 (11)	0.0387 (4)
C8	0.11918 (15)	−0.37666 (14)	−0.10199 (11)	0.0369 (4)
C9	0.12820 (16)	−0.28925 (15)	−0.14663 (11)	0.0418 (5)
H9	0.1028	−0.2240	−0.1367	0.050*
C10	0.17390 (17)	−0.29793 (17)	−0.20499 (12)	0.0470 (5)
H10	0.1801	−0.2381	−0.2332	0.056*
C11	0.21097 (16)	−0.39364 (18)	−0.22289 (12)	0.0472 (5)
C12	0.20315 (18)	−0.48008 (17)	−0.17856 (13)	0.0509 (5)
H12	0.2282	−0.5452	−0.1891	0.061*
C13	0.15893 (17)	−0.47219 (15)	−0.11889 (13)	0.0466 (5)
H13	0.1557	−0.5318	−0.0895	0.056*
C14	0.2569 (2)	−0.4027 (2)	−0.28951 (15)	0.0754 (7)
H14A	0.1971	−0.3826	−0.3415	0.113*
H14B	0.2799	−0.4741	−0.2926	0.113*

H14C	0.3229	−0.3571	−0.2768	0.113*
C15	−0.39586 (15)	−0.30452 (14)	−0.39002 (10)	0.0368 (4)
C16	−0.51412 (17)	−0.31788 (16)	−0.41246 (12)	0.0476 (5)
H16	−0.5408	−0.3732	−0.3903	0.057*
C17	−0.5932 (2)	−0.2493 (2)	−0.46775 (15)	0.0654 (7)
H17	−0.6726	−0.2594	−0.4827	0.078*
C18	−0.5559 (2)	−0.1677 (2)	−0.50024 (15)	0.0719 (8)
H18	−0.6095	−0.1219	−0.5371	0.086*
C19	−0.4384 (2)	−0.15294 (17)	−0.47857 (14)	0.0660 (7)
H19	−0.4127	−0.0969	−0.5007	0.079*
C20	−0.35856 (18)	−0.22107 (15)	−0.42406 (12)	0.0496 (5)
H20	−0.2794	−0.2110	−0.4101	0.060*
C21	−0.36339 (14)	−0.47084 (14)	−0.30304 (11)	0.0365 (4)
C22	−0.38884 (18)	−0.56707 (16)	−0.34185 (13)	0.0516 (5)
H22	−0.3672	−0.5810	−0.3853	0.062*
C23	−0.4464 (2)	−0.6433 (2)	−0.31673 (18)	0.0745 (7)
H23	−0.4638	−0.7076	−0.3440	0.089*
C24	−0.4779 (2)	−0.6253 (2)	−0.25255 (18)	0.0770 (8)
H24	−0.5163	−0.6771	−0.2359	0.092*
C25	−0.4523 (2)	−0.5303 (2)	−0.21283 (16)	0.0698 (7)
H25	−0.4730	−0.5177	−0.1687	0.084*
C26	−0.39603 (18)	−0.45281 (18)	−0.23792 (13)	0.0528 (5)
H26	−0.3800	−0.3882	−0.2110	0.063*
C27	−0.23312 (15)	−0.42746 (13)	−0.37810 (11)	0.0350 (4)
C28	−0.11894 (16)	−0.46003 (16)	−0.33885 (13)	0.0476 (5)
H28	−0.0799	−0.4502	−0.2823	0.057*
C29	−0.06194 (18)	−0.50713 (17)	−0.38280 (16)	0.0586 (6)
H29	0.0153	−0.5278	−0.3554	0.070*
C30	−0.1168 (2)	−0.52379 (18)	−0.46542 (16)	0.0600 (6)
H30	−0.0782	−0.5564	−0.4943	0.072*
C31	−0.2307 (2)	−0.4914 (2)	−0.50548 (15)	0.0653 (7)
H31	−0.2691	−0.5017	−0.5620	0.078*
C32	−0.28783 (19)	−0.44413 (18)	−0.46285 (12)	0.0528 (5)
H32	−0.3647	−0.4228	−0.4910	0.063*
C33	−0.30591 (14)	−0.38266 (13)	−0.33318 (10)	0.0323 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0336 (8)	0.0400 (9)	0.0327 (8)	0.0066 (7)	0.0009 (7)	0.0007 (7)
N2	0.0294 (7)	0.0319 (8)	0.0302 (7)	0.0043 (6)	0.0046 (6)	0.0003 (6)
N3	0.0479 (10)	0.0372 (9)	0.0380 (9)	0.0071 (7)	0.0049 (8)	−0.0028 (7)
N4	0.0521 (10)	0.0411 (9)	0.0363 (9)	0.0055 (8)	0.0015 (8)	−0.0055 (7)
C1	0.0291 (9)	0.0390 (10)	0.0319 (9)	0.0004 (8)	0.0085 (8)	−0.0021 (8)
C2	0.0352 (10)	0.0416 (10)	0.0302 (9)	−0.0024 (8)	0.0067 (8)	−0.0009 (8)
C3	0.0425 (11)	0.0597 (13)	0.0394 (11)	−0.0014 (10)	0.0136 (9)	−0.0063 (9)
C4	0.0618 (14)	0.0740 (15)	0.0333 (11)	−0.0070 (12)	0.0158 (10)	−0.0070 (10)
C5	0.0642 (15)	0.0697 (15)	0.0292 (11)	−0.0002 (12)	0.0039 (10)	0.0040 (10)

C6	0.0480 (12)	0.0539 (13)	0.0365 (11)	0.0048 (10)	0.0037 (9)	0.0019 (9)
C7	0.0374 (10)	0.0380 (10)	0.0319 (9)	−0.0035 (8)	0.0048 (8)	−0.0013 (8)
C8	0.0284 (9)	0.0396 (10)	0.0329 (9)	0.0014 (8)	0.0020 (8)	−0.0018 (8)
C9	0.0408 (11)	0.0400 (10)	0.0389 (10)	0.0068 (8)	0.0101 (9)	−0.0006 (8)
C10	0.0464 (12)	0.0515 (12)	0.0398 (11)	0.0008 (9)	0.0140 (9)	0.0052 (9)
C11	0.0346 (10)	0.0639 (14)	0.0371 (11)	0.0026 (9)	0.0080 (9)	−0.0078 (10)
C12	0.0457 (12)	0.0464 (12)	0.0550 (13)	0.0079 (9)	0.0143 (10)	−0.0102 (10)
C13	0.0439 (11)	0.0388 (11)	0.0500 (12)	0.0028 (9)	0.0114 (10)	0.0006 (9)
C14	0.0712 (17)	0.100 (2)	0.0639 (16)	0.0099 (15)	0.0367 (14)	−0.0083 (14)
C15	0.0346 (10)	0.0393 (10)	0.0274 (9)	0.0052 (8)	0.0028 (8)	−0.0024 (8)
C16	0.0373 (11)	0.0539 (12)	0.0399 (11)	0.0039 (9)	0.0032 (9)	−0.0009 (9)
C17	0.0441 (12)	0.0670 (16)	0.0613 (15)	0.0172 (11)	−0.0038 (11)	0.0008 (12)
C18	0.0707 (17)	0.0571 (15)	0.0525 (14)	0.0210 (13)	−0.0124 (12)	0.0052 (11)
C19	0.0801 (18)	0.0462 (13)	0.0487 (13)	0.0027 (12)	0.0015 (12)	0.0124 (10)
C20	0.0472 (12)	0.0462 (11)	0.0419 (11)	−0.0002 (9)	0.0037 (9)	0.0076 (9)
C21	0.0267 (9)	0.0406 (10)	0.0361 (10)	0.0030 (8)	0.0061 (8)	0.0058 (8)
C22	0.0507 (12)	0.0470 (12)	0.0547 (13)	−0.0096 (10)	0.0187 (11)	0.0001 (10)
C23	0.0743 (17)	0.0569 (15)	0.0890 (19)	−0.0236 (13)	0.0292 (16)	0.0033 (14)
C24	0.0580 (16)	0.0808 (19)	0.0872 (19)	−0.0175 (14)	0.0237 (15)	0.0308 (16)
C25	0.0540 (14)	0.100 (2)	0.0607 (15)	−0.0031 (14)	0.0281 (13)	0.0201 (14)
C26	0.0462 (12)	0.0638 (14)	0.0501 (12)	−0.0015 (10)	0.0210 (11)	0.0032 (10)
C27	0.0341 (9)	0.0327 (9)	0.0372 (10)	−0.0033 (7)	0.0134 (8)	−0.0038 (7)
C28	0.0360 (10)	0.0501 (12)	0.0517 (12)	0.0012 (9)	0.0121 (9)	−0.0096 (9)
C29	0.0392 (12)	0.0577 (14)	0.0823 (17)	−0.0015 (10)	0.0278 (12)	−0.0174 (12)
C30	0.0631 (15)	0.0585 (14)	0.0770 (17)	−0.0154 (12)	0.0475 (14)	−0.0203 (12)
C31	0.0685 (16)	0.0843 (18)	0.0489 (13)	−0.0081 (13)	0.0294 (12)	−0.0165 (12)
C32	0.0494 (12)	0.0671 (14)	0.0413 (12)	0.0015 (10)	0.0177 (10)	−0.0070 (10)
C33	0.0263 (8)	0.0355 (9)	0.0286 (9)	0.0010 (7)	0.0043 (7)	0.0002 (7)

Geometric parameters (Å, °)

N1—C1	1.321 (2)	C15—C33	1.537 (2)
N1—N2	1.3301 (19)	C16—C17	1.387 (3)
N2—N3	1.322 (2)	C16—H16	0.9300
N2—C33	1.500 (2)	C17—C18	1.357 (4)
N3—N4	1.320 (2)	C17—H17	0.9300
N4—C1	1.347 (2)	C18—C19	1.378 (4)
C1—C2	1.476 (2)	C18—H18	0.9300
C2—C3	1.387 (3)	C19—C20	1.382 (3)
C2—C7	1.398 (3)	C19—H19	0.9300
C3—C4	1.383 (3)	C20—H20	0.9300
C3—H3	0.9300	C21—C22	1.376 (3)
C4—C5	1.376 (3)	C21—C26	1.388 (3)
C4—H4	0.9300	C21—C33	1.538 (2)
C5—C6	1.376 (3)	C22—C23	1.383 (3)
C5—H5	0.9300	C22—H22	0.9300
C6—C7	1.394 (3)	C23—C24	1.363 (4)
C6—H6	0.9300	C23—H23	0.9300
C7—C8	1.478 (3)	C24—C25	1.370 (4)

C8—C13	1.390 (3)	C24—H24	0.9300
C8—C9	1.394 (3)	C25—C26	1.384 (3)
C9—C10	1.372 (3)	C25—H25	0.9300
C9—H9	0.9300	C26—H26	0.9300
C10—C11	1.383 (3)	C27—C28	1.380 (3)
C10—H10	0.9300	C27—C32	1.394 (3)
C11—C12	1.376 (3)	C27—C33	1.539 (2)
C11—C14	1.509 (3)	C28—C29	1.385 (3)
C12—C13	1.379 (3)	C28—H28	0.9300
C12—H12	0.9300	C29—C30	1.361 (3)
C13—H13	0.9300	C29—H29	0.9300
C14—H14A	0.9600	C30—C31	1.378 (3)
C14—H14B	0.9600	C30—H30	0.9300
C14—H14C	0.9600	C31—C32	1.370 (3)
C15—C16	1.382 (3)	C31—H31	0.9300
C15—C20	1.390 (3)	C32—H32	0.9300
C1—N1—N2	102.45 (14)	C17—C16—H16	119.8
N3—N2—N1	112.98 (14)	C18—C17—C16	120.6 (2)
N3—N2—C33	124.06 (13)	C18—C17—H17	119.7
N1—N2—C33	121.93 (14)	C16—C17—H17	119.7
N4—N3—N2	106.32 (14)	C17—C18—C19	119.8 (2)
N3—N4—C1	106.18 (15)	C17—C18—H18	120.1
N1—C1—N4	112.04 (15)	C19—C18—H18	120.1
N1—C1—C2	122.50 (16)	C18—C19—C20	120.2 (2)
N4—C1—C2	125.31 (16)	C18—C19—H19	119.9
C3—C2—C7	120.34 (17)	C20—C19—H19	119.9
C3—C2—C1	118.66 (17)	C19—C20—C15	120.4 (2)
C7—C2—C1	120.83 (16)	C19—C20—H20	119.8
C4—C3—C2	120.5 (2)	C15—C20—H20	119.8
C4—C3—H3	119.8	C22—C21—C26	118.36 (18)
C2—C3—H3	119.8	C22—C21—C33	121.42 (17)
C5—C4—C3	119.5 (2)	C26—C21—C33	120.15 (17)
C5—C4—H4	120.3	C21—C22—C23	120.6 (2)
C3—C4—H4	120.3	C21—C22—H22	119.7
C4—C5—C6	120.27 (19)	C23—C22—H22	119.7
C4—C5—H5	119.9	C24—C23—C22	120.9 (2)
C6—C5—H5	119.9	C24—C23—H23	119.6
C5—C6—C7	121.4 (2)	C22—C23—H23	119.6
C5—C6—H6	119.3	C23—C24—C25	119.3 (2)
C7—C6—H6	119.3	C23—C24—H24	120.4
C6—C7—C2	117.77 (18)	C25—C24—H24	120.4
C6—C7—C8	120.18 (17)	C24—C25—C26	120.5 (2)
C2—C7—C8	121.86 (15)	C24—C25—H25	119.8
C13—C8—C9	117.19 (18)	C26—C25—H25	119.8
C13—C8—C7	123.25 (17)	C25—C26—C21	120.4 (2)
C9—C8—C7	119.47 (16)	C25—C26—H26	119.8
C10—C9—C8	121.07 (18)	C21—C26—H26	119.8
C10—C9—H9	119.5	C28—C27—C32	117.43 (18)
C8—C9—H9	119.5	C28—C27—C33	124.04 (16)

C9—C10—C11	121.53 (19)	C32—C27—C33	118.34 (16)
C9—C10—H10	119.2	C27—C28—C29	120.7 (2)
C11—C10—H10	119.2	C27—C28—H28	119.7
C12—C11—C10	117.66 (19)	C29—C28—H28	119.7
C12—C11—C14	121.4 (2)	C30—C29—C28	121.2 (2)
C10—C11—C14	120.9 (2)	C30—C29—H29	119.4
C11—C12—C13	121.40 (19)	C28—C29—H29	119.4
C11—C12—H12	119.3	C29—C30—C31	118.7 (2)
C13—C12—H12	119.3	C29—C30—H30	120.6
C12—C13—C8	121.12 (19)	C31—C30—H30	120.6
C12—C13—H13	119.4	C32—C31—C30	120.6 (2)
C8—C13—H13	119.4	C32—C31—H31	119.7
C11—C14—H14A	109.5	C30—C31—H31	119.7
C11—C14—H14B	109.5	C31—C32—C27	121.3 (2)
H14A—C14—H14B	109.5	C31—C32—H32	119.3
C11—C14—H14C	109.5	C27—C32—H32	119.3
H14A—C14—H14C	109.5	N2—C33—C21	106.03 (14)
H14B—C14—H14C	109.5	N2—C33—C15	107.14 (13)
C16—C15—C20	118.47 (17)	C21—C33—C15	112.06 (14)
C16—C15—C33	121.99 (17)	N2—C33—C27	110.65 (13)
C20—C15—C33	119.43 (16)	C21—C33—C27	111.47 (14)
C15—C16—C17	120.4 (2)	C15—C33—C27	109.37 (14)
C15—C16—H16	119.8		

Fig. 1

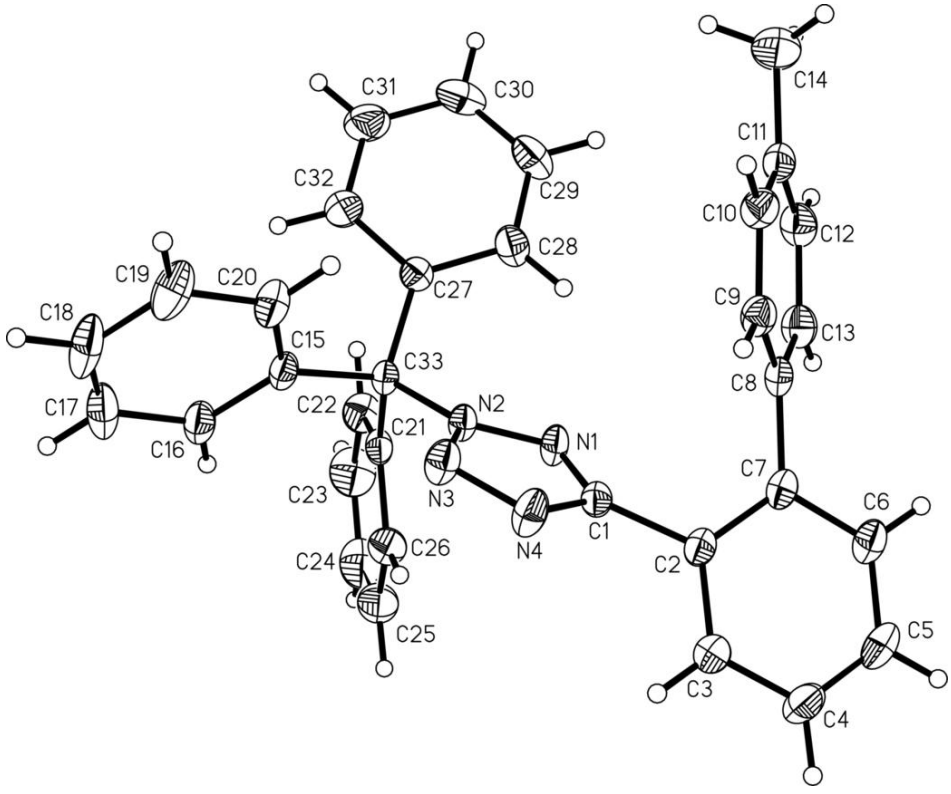
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Fig. 2