Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,1′-(1,4-Phenylenedimethylene)-dipyridinium bis(tetraphenylborate)

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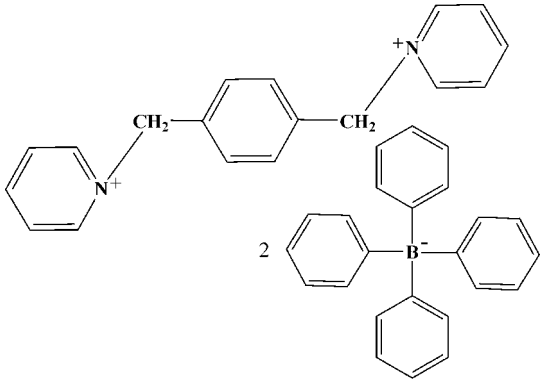
Received 16 June 2007; accepted 4 July 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.058; wR factor = 0.149; data-to-parameter ratio = 15.2.

The title compound, $C_{18}H_{18}N_2^{2+}\cdot 2B(C_6H_5)_4^-$, consists of a 1,1′-(1,4-phenylenedimethylene)dipyridinium cation located on an inversion center and two tetraphenylborate anions. There are C—H$\cdots\pi$ interactions of intermediate strength between the pyridinium group of the cation and the surrounding anions.

Related literature

For related literature, see: Kiviniemi *et al.* (2001); Liu, Liao *et al.* (2007); Liu, Shi *et al.* (2007).



Experimental

Crystal data

$C_{18}H_{18}N_2^{2+}\cdot 2C_{24}H_{20}B^-$
M_r = 900.76
Triclinic, $P\overline{1}$
a = 9.8194 (8) Å
b = 10.3074 (9) Å
c = 13.3980 (12) Å
α = 97.224 (2)°
β = 92.143 (2)°
γ = 111.530 (2)°
V = 1246.28 (19) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 298 (2) K
0.40 × 0.20 × 0.06 mm

Data collection

Bruker APEX II CCD area-detector diffractometer
Absorption correction: none
9445 measured reflections
4794 independent reflections
3179 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.149
S = 1.00
4794 reflections
316 parameters
H-atom parameters not refined
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C16–C21, C22–C27 and C28–C33 phenyl rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C9—H9$\cdots$N1^{i}	0.93	2.57	2.897 (3)	101
C1—H1$\cdots$*Cg*1	0.93	2.44	3.313 (2)	156
C4—H4$\cdots$*Cg*3^{ii}	0.93	2.63	3.280 (2)	127
C5—H5$\cdots$*Cg*2^{ii}	0.93	2.53	3.446 (2)	168

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

Data collection: *APEX2* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

The authors thank the National Natural Science Foundation (No. 20671083), the Henan Province Excellent Youth Foundation (Nos. 0612002800) and Jinan Henghua Science and Technology Co. Ltd for supporting this work. We also thank Luoyang Normal College for the diffraction measurements.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2181).

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 doi:10.1107/S1600536807032588

supplementary materials

Acta Cryst. (2007). E**63**, o3457 [**doi:10.1107/S1600536807032588**]

1,1'-(1,4-Phenylenedimethylene)dipyridinium bis(tetraphenylborate)

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Comment

The tetraphenylborate ion, BPh_4^-, has been widely used as a counterion in cation complex systems. These cations include metal atoms, organic ammonium cations, bipyridinium cations and arenediazonium cations (Kiviniemi *et al.*, 2001). In our previous studies we have investigated the organo-inorganic hybrid compounds containing the 1,ω-alkylidene dipyridine cations (Liu, Liao *et al.*, 2007; Liu, Shi *et al.*, 2007). Herein we report the crystal structure of 1,1'-(1,4-phenylenedimethylene)dipyridinium cation with tetraphenylborate.

The asymmetric unit of the title compound (Fig. 1), $(C_{18}H_{18}N_2)_{0.5}\cdot B(C_6H_5)_4$, contains half a 1,1'-(1,4-phenylenedimethylene)dipyridinium cation and one tetraphenylborate anion; the cation is located on an inversion center. The cation is surrounded by four anions and interacts with three of them *via* C—H···π interactions (Table 1 and Fig. 2).

Experimental

All chemicals used were purchased from Jinan Henghua Sci. & Tec. Co., Ltd. The salt was synthesized from the reaction of 1,1'-(1,4-phenylenedimethylene)dipyridinium dichloride (0.033 g, 0.1 mmol) in methanol (5 ml) and $Na[BPh_4]$ (0.034 g, 0.1 mmol) in DMF (10 ml). The mixture was set aside for the formation of colorless crystals in 54% yield after several days. Anal. Calc. for $C_{33}H_{29}BN$: C 88.00, H 6.44, N 3.11%; Found: C 87.96, H 6.47, N 3.07%.

Refinement

H atoms were generated geometrically (C—H = 0.93 or 0.97 Å) and refined as riding, with $U_{iso}(H)= 1.2U_{eq}(C)$.

Figures

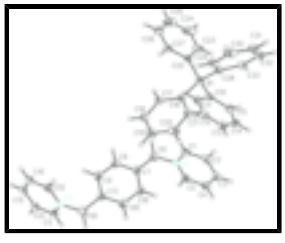


Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids. Atoms labeled with I are at the symmetry position (−*x* + 2, −*y* + 2, −*z* + 1).

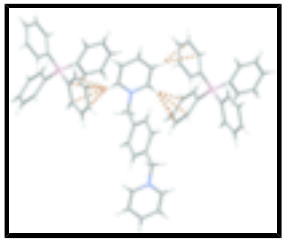


Fig. 2. A partial packing diagram of the title compound, showing C—H···π interactions (dashed lines).

1,1'-(1,4-Phenylenedimethylene)dipyridinium bis(tetraphenylborate)

Crystal data

$C_{18}H_{18}N_2^{2+}\cdot 2C_{24}H_{20}B^-$	$Z = 1$
$M_r = 900.76$	$F_{000} = 478$
Triclinic, $P\overline{1}$	$D_x = 1.200$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.8194$ (8) Å	Cell parameters from 1607 reflections
$b = 10.3074$ (9) Å	$\theta = 1.5$–26.0º
$c = 13.3980$ (12) Å	$\mu = 0.07$ mm^{-1}
$\alpha = 97.224$ (2)º	$T = 298$ (2) K
$\beta = 92.143$ (2)º	Plate, colorless
$\gamma = 111.530$ (2)º	0.40 × 0.20 × 0.06 mm
$V = 1246.28$ (19) Å^3	

Data collection

Bruker APEX II CCD area-detector diffractometer	3179 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.038$
Monochromator: graphite	$\theta_{max} = 26.0$º
$T = 298(2)$ K	$\theta_{min} = 1.5$º
φ and ω scans	$h = -12\rightarrow 8$
Absorption correction: none	$k = -12\rightarrow 12$
9445 measured reflections	$l = -16\rightarrow 16$
4794 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
$R[F^2 > 2\sigma(F^2)] = 0.058$	H-atom parameters not refined
$wR(F^2) = 0.149$	$w = 1/[\sigma^2(F_o^2) + (0.0666P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.008$
4794 reflections	$\Delta\rho_{max} = 0.22$ e Å^{-3}
316 parameters	$\Delta\rho_{min} = -0.18$ 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}
B1	0.2031 (2)	0.5217 (2)	0.23828 (15)	0.0340 (5)
C1	0.6064 (2)	0.9191 (2)	0.28743 (14)	0.0455 (6)
H1	0.5622	0.8386	0.3171	0.055*
C2	0.5276 (2)	0.9974 (2)	0.26334 (15)	0.0499 (6)
H2	0.4295	0.9705	0.2767	0.060*
C3	0.5923 (3)	1.1152 (2)	0.21966 (16)	0.0551 (6)
H3	0.5396	1.1701	0.2046	0.066*
C4	0.7366 (3)	1.1521 (2)	0.19802 (16)	0.0552 (6)
H4	0.7814	1.2308	0.1667	0.066*
C5	0.8125 (2)	1.0725 (2)	0.22287 (16)	0.0505 (6)
H5	0.9099	1.0967	0.2085	0.061*
C6	0.8356 (3)	0.8804 (2)	0.30283 (16)	0.0551 (6)
H6A	0.9058	0.8784	0.2542	0.066*
H6B	0.7710	0.7838	0.3052	0.066*
C7	0.9178 (2)	0.9449 (2)	0.40600 (15)	0.0422 (5)
C8	0.9777 (2)	0.8658 (2)	0.45543 (16)	0.0507 (6)
H8	0.9631	0.7745	0.4260	0.061*
C9	1.0587 (3)	0.9201 (2)	0.54765 (17)	0.0539 (6)
H9	1.0984	0.8650	0.5793	0.065*
C10	0.2930 (2)	0.61470 (19)	0.15340 (13)	0.0339 (5)
C11	0.4208 (2)	0.5992 (2)	0.12074 (14)	0.0415 (5)
H11	0.4465	0.5281	0.1420	0.050*
C12	0.5106 (2)	0.6841 (2)	0.05859 (16)	0.0500 (6)
H12	0.5949	0.6701	0.0396	0.060*
C13	0.4750 (3)	0.7892 (2)	0.02493 (15)	0.0529 (6)
H13	0.5346	0.8467	−0.0171	0.064*
C14	0.3507 (3)	0.8083 (2)	0.05401 (16)	0.0509 (6)
H14	0.3252	0.8786	0.0311	0.061*
C15	0.2626 (2)	0.7235 (2)	0.11752 (14)	0.0420 (5)
H15	0.1797	0.7399	0.1370	0.050*
C16	0.3055 (2)	0.60729 (18)	0.34397 (13)	0.0335 (5)
C17	0.4272 (2)	0.5815 (2)	0.38034 (14)	0.0395 (5)
H17	0.4453	0.5050	0.3478	0.047*

C18	0.5221 (2)	0.6652 (2)	0.46290 (16)	0.0507 (6)
H18	0.6019	0.6443	0.4844	0.061*
C19	0.4984 (3)	0.7787 (2)	0.51278 (16)	0.0578 (7)
H19	0.5613	0.8347	0.5683	0.069*
C20	0.3803 (3)	0.8085 (2)	0.47958 (16)	0.0552 (6)
H20	0.3636	0.8856	0.5125	0.066*
C21	0.2863 (2)	0.7241 (2)	0.39730 (14)	0.0425 (5)
H21	0.2069	0.7461	0.3766	0.051*
C22	0.1924 (2)	0.35750 (19)	0.21150 (14)	0.0371 (5)
C23	0.1626 (2)	0.2894 (2)	0.11149 (17)	0.0548 (6)
H23	0.1498	0.3392	0.0610	0.066*
C24	0.1514 (3)	0.1520 (3)	0.0841 (2)	0.0778 (9)
H24	0.1314	0.1112	0.0165	0.093*
C25	0.1699 (3)	0.0756 (3)	0.1571 (3)	0.0847 (10)
H25	0.1644	−0.0165	0.1391	0.102*
C26	0.1965 (3)	0.1365 (3)	0.2568 (3)	0.0727 (8)
H26	0.2087	0.0857	0.3068	0.087*
C27	0.2053 (2)	0.2746 (2)	0.28269 (18)	0.0525 (6)
H27	0.2205	0.3131	0.3507	0.063*
C28	0.0339 (2)	0.51288 (19)	0.24453 (14)	0.0367 (5)
C29	−0.0361 (2)	0.4910 (2)	0.33345 (16)	0.0471 (6)
H29	0.0169	0.4856	0.3907	0.056*
C30	−0.1818 (3)	0.4770 (2)	0.3396 (2)	0.0636 (7)
H30	−0.2243	0.4625	0.4001	0.076*
C31	−0.2631 (3)	0.4847 (3)	0.2560 (2)	0.0695 (8)
H31	−0.3598	0.4778	0.2602	0.083*
C32	−0.2002 (3)	0.5025 (2)	0.1667 (2)	0.0633 (7)
H32	−0.2547	0.5061	0.1095	0.076*
C33	−0.0560 (2)	0.5152 (2)	0.16148 (17)	0.0478 (6)
H33	−0.0163	0.5259	0.0997	0.057*
N1	0.74748 (19)	0.95834 (17)	0.26829 (12)	0.0426 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
B1	0.0316 (12)	0.0335 (11)	0.0338 (12)	0.0088 (9)	0.0024 (9)	0.0047 (9)
C1	0.0451 (13)	0.0409 (12)	0.0370 (11)	0.0012 (10)	0.0015 (10)	0.0042 (9)
C2	0.0422 (13)	0.0529 (14)	0.0466 (13)	0.0113 (11)	−0.0045 (10)	0.0013 (10)
C3	0.0562 (16)	0.0518 (14)	0.0544 (14)	0.0204 (12)	−0.0155 (12)	0.0031 (11)
C4	0.0580 (16)	0.0441 (13)	0.0564 (14)	0.0088 (11)	−0.0043 (12)	0.0169 (10)
C5	0.0403 (13)	0.0487 (13)	0.0534 (13)	0.0047 (10)	0.0035 (10)	0.0120 (11)
C6	0.0610 (16)	0.0481 (13)	0.0570 (14)	0.0246 (12)	−0.0064 (12)	0.0007 (11)
C7	0.0412 (12)	0.0399 (11)	0.0472 (12)	0.0165 (9)	0.0046 (9)	0.0087 (9)
C8	0.0609 (15)	0.0400 (12)	0.0554 (14)	0.0260 (11)	−0.0008 (11)	0.0018 (10)
C9	0.0638 (16)	0.0484 (13)	0.0573 (14)	0.0314 (12)	−0.0077 (11)	0.0073 (11)
C10	0.0326 (11)	0.0337 (10)	0.0307 (10)	0.0084 (8)	0.0005 (8)	0.0010 (8)
C11	0.0394 (12)	0.0414 (11)	0.0428 (11)	0.0134 (9)	0.0051 (9)	0.0081 (9)
C12	0.0419 (13)	0.0538 (14)	0.0482 (13)	0.0103 (11)	0.0135 (10)	0.0066 (11)

C13	0.0594 (16)	0.0486 (13)	0.0386 (12)	0.0035 (12)	0.0122 (11)	0.0126 (10)
C14	0.0611 (15)	0.0407 (12)	0.0473 (13)	0.0126 (11)	0.0037 (11)	0.0132 (10)
C15	0.0453 (12)	0.0374 (11)	0.0411 (11)	0.0129 (10)	0.0037 (9)	0.0061 (9)
C16	0.0304 (11)	0.0321 (10)	0.0350 (10)	0.0063 (8)	0.0059 (8)	0.0105 (8)
C17	0.0361 (12)	0.0359 (10)	0.0423 (11)	0.0082 (9)	0.0001 (9)	0.0087 (9)
C18	0.0421 (13)	0.0533 (14)	0.0511 (13)	0.0093 (10)	−0.0074 (10)	0.0174 (11)
C19	0.0550 (15)	0.0604 (15)	0.0401 (12)	0.0045 (12)	−0.0103 (11)	0.0009 (11)
C20	0.0576 (15)	0.0479 (13)	0.0471 (13)	0.0092 (11)	0.0058 (11)	−0.0072 (10)
C21	0.0387 (12)	0.0423 (12)	0.0432 (11)	0.0132 (9)	0.0040 (9)	0.0007 (9)
C22	0.0265 (10)	0.0347 (10)	0.0469 (12)	0.0075 (8)	0.0056 (9)	0.0057 (9)
C23	0.0566 (15)	0.0389 (12)	0.0555 (14)	0.0050 (10)	0.0167 (11)	−0.0040 (10)
C24	0.0744 (19)	0.0477 (15)	0.088 (2)	0.0017 (14)	0.0370 (16)	−0.0168 (15)
C25	0.0541 (17)	0.0379 (14)	0.159 (3)	0.0157 (13)	0.0357 (19)	−0.0005 (19)
C26	0.0406 (14)	0.0446 (14)	0.134 (3)	0.0135 (11)	−0.0015 (15)	0.0274 (16)
C27	0.0370 (12)	0.0394 (12)	0.0757 (16)	0.0078 (10)	−0.0050 (11)	0.0118 (11)
C28	0.0326 (11)	0.0292 (10)	0.0435 (11)	0.0074 (8)	0.0024 (9)	0.0015 (8)
C29	0.0352 (12)	0.0446 (12)	0.0528 (13)	0.0065 (9)	0.0080 (10)	0.0012 (10)
C30	0.0471 (15)	0.0517 (14)	0.0799 (18)	0.0079 (11)	0.0253 (13)	−0.0061 (12)
C31	0.0325 (13)	0.0546 (15)	0.118 (2)	0.0180 (11)	0.0076 (15)	−0.0039 (15)
C32	0.0392 (14)	0.0535 (15)	0.095 (2)	0.0164 (11)	−0.0103 (14)	0.0091 (13)
C33	0.0361 (12)	0.0430 (12)	0.0600 (14)	0.0099 (9)	−0.0022 (10)	0.0092 (10)
N1	0.0456 (11)	0.0380 (9)	0.0397 (10)	0.0108 (8)	−0.0036 (8)	0.0062 (7)

Geometric parameters (Å, °)

B1—C28	1.637 (3)	C15—H15	0.9300
B1—C10	1.649 (3)	C16—C21	1.399 (3)
B1—C22	1.649 (3)	C16—C17	1.399 (3)
B1—C16	1.650 (3)	C17—C18	1.389 (3)
C1—N1	1.338 (3)	C17—H17	0.9300
C1—C2	1.364 (3)	C18—C19	1.373 (3)
C1—H1	0.9300	C18—H18	0.9300
C2—C3	1.364 (3)	C19—C20	1.376 (3)
C2—H2	0.9300	C19—H19	0.9300
C3—C4	1.378 (3)	C20—C21	1.385 (3)
C3—H3	0.9300	C20—H20	0.9300
C4—C5	1.356 (3)	C21—H21	0.9300
C4—H4	0.9300	C22—C27	1.390 (3)
C5—N1	1.349 (3)	C22—C23	1.399 (3)
C5—H5	0.9300	C23—C24	1.380 (3)
C6—N1	1.477 (3)	C23—H23	0.9300
C6—C7	1.515 (3)	C24—C25	1.377 (4)
C6—H6A	0.9700	C24—H24	0.9300
C6—H6B	0.9700	C25—C26	1.375 (4)
C7—C8	1.381 (3)	C25—H25	0.9300
C7—C9^{i}	1.383 (3)	C26—C27	1.392 (3)
C8—C9	1.378 (3)	C26—H26	0.9300
C8—H8	0.9300	C27—H27	0.9300
C9—C7^{i}	1.383 (3)	C28—C29	1.399 (3)

C9—H9	0.9300	C28—C33	1.402 (3)
C10—C15	1.396 (3)	C29—C30	1.391 (3)
C10—C11	1.401 (3)	C29—H29	0.9300
C11—C12	1.381 (3)	C30—C31	1.379 (4)
C11—H11	0.9300	C30—H30	0.9300
C12—C13	1.375 (3)	C31—C32	1.369 (4)
C12—H12	0.9300	C31—H31	0.9300
C13—C14	1.368 (3)	C32—C33	1.378 (3)
C13—H13	0.9300	C32—H32	0.9300
C14—C15	1.387 (3)	C33—H33	0.9300
C14—H14	0.9300		
C28—B1—C10	114.81 (16)	C17—C16—B1	123.67 (16)
C28—B1—C22	106.03 (15)	C18—C17—C16	122.81 (19)
C10—B1—C22	109.62 (16)	C18—C17—H17	118.6
C28—B1—C16	111.05 (15)	C16—C17—H17	118.6
C10—B1—C16	101.99 (14)	C19—C18—C17	120.1 (2)
C22—B1—C16	113.55 (16)	C19—C18—H18	120.0
N1—C1—C2	119.8 (2)	C17—C18—H18	120.0
N1—C1—H1	120.1	C18—C19—C20	119.19 (19)
C2—C1—H1	120.1	C18—C19—H19	120.4
C1—C2—C3	120.1 (2)	C20—C19—H19	120.4
C1—C2—H2	120.0	C19—C20—C21	120.2 (2)
C3—C2—H2	120.0	C19—C20—H20	119.9
C2—C3—C4	119.4 (2)	C21—C20—H20	119.9
C2—C3—H3	120.3	C20—C21—C16	122.9 (2)
C4—C3—H3	120.3	C20—C21—H21	118.6
C5—C4—C3	119.3 (2)	C16—C21—H21	118.6
C5—C4—H4	120.4	C27—C22—C23	114.86 (19)
C3—C4—H4	120.4	C27—C22—B1	124.77 (17)
N1—C5—C4	120.4 (2)	C23—C22—B1	120.32 (18)
N1—C5—H5	119.8	C24—C23—C22	123.2 (2)
C4—C5—H5	119.8	C24—C23—H23	118.4
N1—C6—C7	112.98 (16)	C22—C23—H23	118.4
N1—C6—H6A	109.0	C25—C24—C23	119.8 (3)
C7—C6—H6A	109.0	C25—C24—H24	120.1
N1—C6—H6B	109.0	C23—C24—H24	120.1
C7—C6—H6B	109.0	C26—C25—C24	119.4 (2)
H6A—C6—H6B	107.8	C26—C25—H25	120.3
C8—C7—C9^{i}	117.79 (19)	C24—C25—H25	120.3
C8—C7—C6	118.02 (18)	C25—C26—C27	119.7 (3)
C9^{i}—C7—C6	124.15 (19)	C25—C26—H26	120.1
C9—C8—C7	121.02 (19)	C27—C26—H26	120.1
C9—C8—H8	119.5	C22—C27—C26	122.9 (2)
C7—C8—H8	119.5	C22—C27—H27	118.5
C8—C9—C7^{i}	121.2 (2)	C26—C27—H27	118.5
C8—C9—H9	119.4	C29—C28—C33	114.58 (19)
C7^{i}—C9—H9	119.4	C29—C28—B1	121.42 (17)
C15—C10—C11	114.40 (18)	C33—C28—B1	123.82 (18)

C15—C10—B1	125.01 (18)	C30—C29—C28	122.6 (2)
C11—C10—B1	120.16 (17)	C30—C29—H29	118.7
C12—C11—C10	123.4 (2)	C28—C29—H29	118.7
C12—C11—H11	118.3	C31—C30—C29	120.0 (2)
C10—C11—H11	118.3	C31—C30—H30	120.0
C13—C12—C11	119.8 (2)	C29—C30—H30	120.0
C13—C12—H12	120.1	C32—C31—C30	119.3 (2)
C11—C12—H12	120.1	C32—C31—H31	120.3
C14—C13—C12	119.2 (2)	C30—C31—H31	120.3
C14—C13—H13	120.4	C31—C32—C33	120.0 (2)
C12—C13—H13	120.4	C31—C32—H32	120.0
C13—C14—C15	120.4 (2)	C33—C32—H32	120.0
C13—C14—H14	119.8	C32—C33—C28	123.4 (2)
C15—C14—H14	119.8	C32—C33—H33	118.3
C14—C15—C10	122.8 (2)	C28—C33—H33	118.3
C14—C15—H15	118.6	C1—N1—C5	121.03 (19)
C10—C15—H15	118.6	C1—N1—C6	119.39 (18)
C21—C16—C17	114.86 (16)	C5—N1—C6	119.48 (19)
C21—C16—B1	121.03 (17)		
N1—C1—C2—C3	0.1 (3)	B1—C16—C21—C20	−172.40 (19)
C1—C2—C3—C4	1.6 (3)	C28—B1—C22—C27	−94.2 (2)
C2—C3—C4—C5	−1.6 (3)	C10—B1—C22—C27	141.32 (19)
C3—C4—C5—N1	0.0 (3)	C16—B1—C22—C27	28.0 (3)
N1—C6—C7—C8	166.3 (2)	C28—B1—C22—C23	83.1 (2)
N1—C6—C7—C9^{i}	−16.1 (3)	C10—B1—C22—C23	−41.4 (2)
C9^{i}—C7—C8—C9	−0.3 (4)	C16—B1—C22—C23	−154.74 (18)
C6—C7—C8—C9	177.4 (2)	C27—C22—C23—C24	−2.1 (3)
C7—C8—C9—C7^{i}	0.3 (4)	B1—C22—C23—C24	−179.6 (2)
C28—B1—C10—C15	25.6 (2)	C22—C23—C24—C25	0.0 (4)
C22—B1—C10—C15	144.80 (17)	C23—C24—C25—C26	1.3 (4)
C16—B1—C10—C15	−94.6 (2)	C24—C25—C26—C27	−0.4 (4)
C28—B1—C10—C11	−162.31 (15)	C23—C22—C27—C26	3.0 (3)
C22—B1—C10—C11	−43.1 (2)	B1—C22—C27—C26	−179.58 (19)
C16—B1—C10—C11	77.51 (19)	C25—C26—C27—C22	−1.9 (4)
C15—C10—C11—C12	0.3 (3)	C10—B1—C28—C29	−153.73 (17)
B1—C10—C11—C12	−172.63 (17)	C22—B1—C28—C29	85.1 (2)
C10—C11—C12—C13	−0.7 (3)	C16—B1—C28—C29	−38.7 (2)
C11—C12—C13—C14	0.2 (3)	C10—B1—C28—C33	31.4 (2)
C12—C13—C14—C15	0.7 (3)	C22—B1—C28—C33	−89.8 (2)
C13—C14—C15—C10	−1.1 (3)	C16—B1—C28—C33	146.43 (18)
C11—C10—C15—C14	0.6 (3)	C33—C28—C29—C30	−1.8 (3)
B1—C10—C15—C14	173.11 (17)	B1—C28—C29—C30	−177.17 (18)
C28—B1—C16—C21	−37.3 (2)	C28—C29—C30—C31	−0.1 (3)
C10—B1—C16—C21	85.5 (2)	C29—C30—C31—C32	1.6 (4)
C22—B1—C16—C21	−156.69 (17)	C30—C31—C32—C33	−1.2 (4)
C28—B1—C16—C17	150.74 (18)	C31—C32—C33—C28	−0.9 (3)
C10—B1—C16—C17	−86.5 (2)	C29—C28—C33—C32	2.4 (3)
C22—B1—C16—C17	31.4 (3)	B1—C28—C33—C32	177.55 (19)

C21—C16—C17—C18	−0.1 (3)	C2—C1—N1—C5	−1.8 (3)
B1—C16—C17—C18	172.29 (19)	C2—C1—N1—C6	174.56 (17)
C16—C17—C18—C19	0.2 (3)	C4—C5—N1—C1	1.7 (3)
C17—C18—C19—C20	−0.4 (3)	C4—C5—N1—C6	−174.63 (18)
C18—C19—C20—C21	0.5 (3)	C7—C6—N1—C1	−92.6 (2)
C19—C20—C21—C16	−0.4 (3)	C7—C6—N1—C5	83.8 (2)
C17—C16—C21—C20	0.2 (3)		

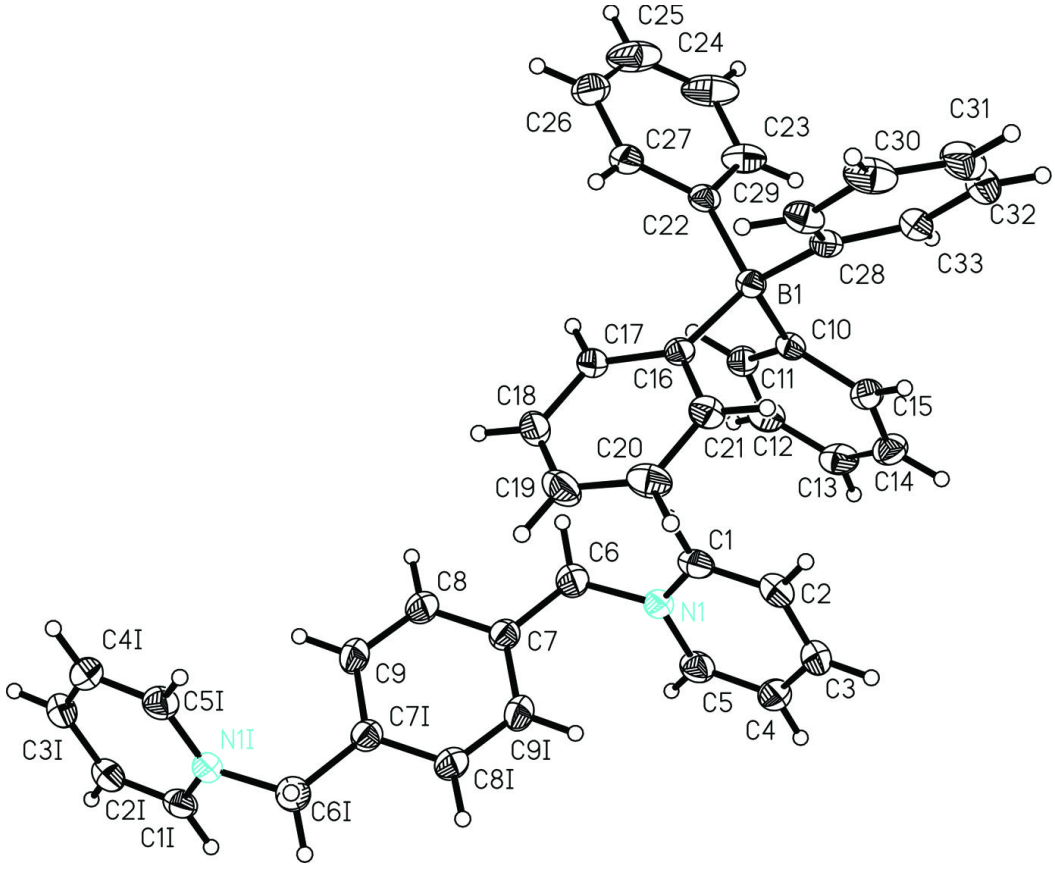
Symmetry codes: (i) −*x*+2, −*y*+2, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···N1^{i}	0.93	2.57	2.897 (3)	101
C1—H1···Cg1	0.93	2.44	3.313 (2)	156
C4—H4···Cg3^{ii}	0.93	2.63	3.280 (2)	127
C5—H5···Cg2^{ii}	0.93	2.53	3.446 (2)	168

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

Fig. 1


C25
C24
C26
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B1
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C11
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C9
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C5I
C7I
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N1I
C3I
C9I
C8I
C2I
C6I
C1I

Fig. 2