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N,*N*-Bis(2-bromobenzyl)-2,6-diisopropylaniline

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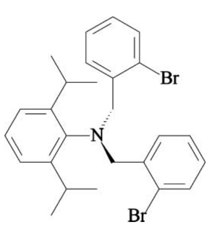
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.006 Å; R factor = 0.053; wR factor = 0.118; data-to-parameter ratio = 18.0.

The crystal structure of the title compound, $C_{26}H_{29}Br_2N$, contains two independent molecules in the asymmetric unit. In molecule *A*, one benzyl group is involved in an intramolecular C—H···benzene contact. Molecules *A* are linked by intermolecular C—H···benzene contacts involving the aniline ring into a one-dimensional association along the *c* axis. Molecules *B* form a different array along the *a* axis, *viz.* dimeric units based on intermolecular C—H···benzene contacts involving one benzyl aromatic ring; they are further linked through C—H···benzene contacts involving the second benzyl aromatic ring. In the crystal structure, supramolecular arrays of the same type are arranged in layers stacked alternately along the *b* axis, with no interactions between the layers.

Related literature

For related literature, see: Balazs *et al.* (2003, 2004, 2006); Opris *et al.* (2004); Fernández *et al.* (2007); Soran *et al.* (2007); Kulcsar *et al.* (2007); Rotar *et al.* (2007).



Experimental

Crystal data

$C_{26}H_{29}Br_2N$
M_r = 515.32
Monoclinic, $P2_1/c$
a = 8.708 (2) Å
b = 35.97 (1) Å
c = 15.032 (4) Å
β = 95.952 (6)°
V = 4683 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 3.47 mm^{-1}
T = 297 (2) K
0.26 × 0.22 × 0.19 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*: Bruker, 2001)
T_{min} = 0.433, T_{max} = 0.519
37601 measured reflections
9570 independent reflections
5782 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.118
S = 1.01
9570 reflections
531 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
C—H···π-ring interactions (Å, °).

C—H···*Cg*	C—H	H···*Cg*	C···*Cg*	C—H···*Cg*
C26—H26*C*···*Cg*1	0.96	2.96	3.67 (1)	131
C11—H11···*Cg*2^{i}	0.93	3.12	3.68 (2)	121
C33—H33*A*···*Cg*3^{ii}	0.97	3.06	3.55 (1)	113
C43—H43···*Cg*4^{iii}	0.93	3.10	3.88 (1)	143

Symmetry code: (i) $x, \frac{1}{2}-y, -\frac{1}{2}+z$, (ii) $2-x, -y, 1-z$, (iii) $-1+x, y, z$. *Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of rings C8–C13, C15–C20, C27–C32 and C34–C39, respectively.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2263).

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supplementary materials

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N,*N*-Bis(2-bromobenzyl)-2,6-diisopropylaniline

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Comment

Aryl groups with pendant arms containing nitrogen atoms with potential for coordination to a metal centre, *e.g.* 2-(Me_2NCH_2)C_6H_4, 2-[O(CH_2CH_2)$_2NCH_2$]C_6H_4 or 2-[MeN(CH_2CH_2)$_2NCH_2$]C_6H_4, are currently used to stabilize unusual organometallic species (Balazs *et al.*, 2003, 2004, 2006; Opris *et al.*, 2004; Fernández *et al.*, 2007; Soran *et al.*, 2007; Kulcsar *et al.*, 2007; Rotar *et al.*, 2007). During attempts to prepare new organic compounds with potential to be used for the synthesis of hypervalent organometallic compounds compound (**I**) was isolated.

The crystal of the title compound contains two independent molecules in the unit cell, *i.e.* molecule A (containing N1) and B (containing N2) (Fig. 1), which differ slightly in the relative orientation of the aromatic rings (dihedral angles: C_6H_3/C_6H_4—Br1 52.8 (1)°, C_6H_3/C_6H_4—Br2 53.8 (1)° and C_6H_4—Br1/C_6H_4—Br2 14.7 (2)° for molecule A; C_6H_3/C_6H_4—Br4 59.5 (1)°, C_6H_3/C_6H_4—Br3 52.1 (1)° and C_6H_4—Br3/C_6H_4—Br4 20.4 (2)° for molecule B). In addition, for molecule A one benzylic arm is involved in an intramolecular *C*—*H*···phenyl contact (H26C···*Cg*1 = 2.96 Å).

Molecules of the same type establish different supramolecular arrays through intermolecular *C*—*H*···phenyl contacts (Fig. 2, Extra Table). Molecules A are associated into a single chain arrangement along *c* axis. Molecules B (containing N2) form a different supramolecular array, *i.e.* dimer units, which are further associated along the *a* axis (Fig. 3). In the crystal the supramoleculat motifs of the same type are arranged in layers stacked alternatively along the *b* axis, with no interactions between layers (Fig. 4).

Experimental

The compound was obtained by reaction between 2-bromo-benzyl bromide and 2,6-diisopropyl-aniline, in 2:1 molar ratio. The reaction was performed in acetonitrile, in the presence of sodium carbonate. Colorless, single-crystals of the title compound were obtained from ethanol. Spectroscopic analysis: ^{1}H NMR ($CDCl_3$, 300 MHz): δ 1.04 [d, 12 H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz], 3.47 [sept, 2H, C*H*(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz], 4.48 (s, 2H, CH_2), 7.05 (m, 4H, C_6H_4, *H-3,5*), 7.16 (m, 5H, C_6H_4, *H-4* + C_6H_3), 7.59 (dd, 2H, C_6H_4, *H-6*, $^3J_{HH}$ = 7.9, $^4J_{HH}$ = 1.1 Hz); ^{13}C NMR ($CDCl_3$, 75.5 MHz): 24.44 [s, CH(*C*H_3)$_2$], 28.16 [s, *C*H(CH_3)$_2$], 59.17 (s, *C*H_2), 124.27 (s, *C*-4), 124.91 (s, *C*$_6H_3$-*ipso*), 126.71 (s, *C*$_6H_3$-*para*), 126.99 (s, *C*$_6H_3$-*meta*), 128.49 (s, *C*-5), 132.03 (s, *C*-3), 132.73 (s, *C*-6), 138.86 (s, *C*-1), 144.05 (s, *C*-2), 148.95 (s, *C*$_6H_3$-*ortho*); ^{13}C NMR ($CDCl_3$, 75.5 MHz): 24.26 [s, CH(*C*H_3)$_2$], 27.69 [s, *C*H(CH_3)$_2$], 55.72 (s, *C*H_2), 123.57 (s, *C*$_6H_3$-*meta*), 123.82 (s, *C*$_6H_3$-*ipso*), 124.11 (s, *C*$_6H_3$-*para*), 127.58 (s, *C*-4), 128.79 (s, *C*-5), 129.97 (s, *C*-3), 132.75 (s, *C*-6), 139.22 (s, *C*-1), 142.38 (s, *C*-2), 142.89 (s, *C*$_6H_3$-*ortho*).

Refinement

All hydrogen atoms were placed in calculated positions using a riding model, with C—H = 0.93–0.97 Å and with U_{iso}= 1.5U_{eq} (C) for methyl H and U_{iso}= 1.2U_{eq} (C) for aryl H. The methyl groups were allowed to rotate but not to tip.

Figures

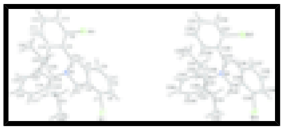
Fig. 1. : A view of the title compound showing the atom-numbering scheme at 30% probability thermal ellipsoids.

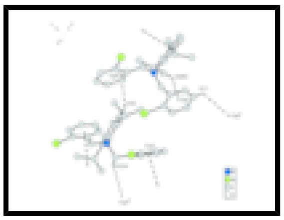
Fig. 2. : H···π interactions in the title compound (indicated as dotted lines). Symmetry codes as in Extra Table.

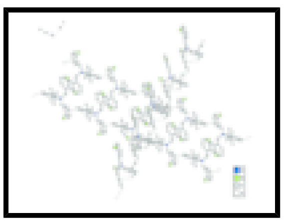
Fig. 3. : Supramolecular association in the crystal of the title compound showing the two different type of arrangements.

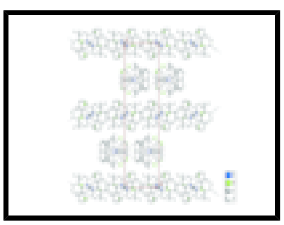
Fig. 4. : The crystal packing of the title compound, view along the *c* axis.

N,*N*-Bis(2-bromobenzyl)-2,6-diisopropylaniline

Crystal data

$C_{26}H_{29}Br_2N$	F_{000} = 2096
M_r = 515.32	D_x = 1.462 Mg m^{-3}
Monoclinic, *P*2(1)/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4464 reflections
a = 8.708 (2) Å	θ = 2.3–19.8º
b = 35.970 (10) Å	μ = 3.47 mm^{-1}
c = 15.032 (4) Å	*T* = 297 (2) K
β = 95.952 (6)º	Block, colourless
V = 4683 (2) Å^3	0.26 × 0.22 × 0.19 mm
Z = 8	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	9570 independent reflections
Radiation source: fine-focus sealed tube	5782 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.065$
$T = 297(2)$ K	$\theta_{max} = 26.4°$
phi and ω scans	$\theta_{min} = 1.1°$
Absorption correction: multi-scan (SADABS: Bruker, 2001)	$h = -10 \rightarrow 10$
$T_{min} = 0.433$, $T_{max} = 0.519$	$k = -44 \rightarrow 44$
37601 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2 + 2.9193P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.053$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.118$	$\Delta\rho_{max} = 0.80$ e Å^{-3}
$S = 1.01$	$\Delta\rho_{min} = -0.56$ e Å^{-3}
9570 reflections	Extinction correction: none
531 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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	0.7282 (3)	0.25118 (8)	0.7287 (2)	0.0362 (8)
Br1	1.07276 (6)	0.306566 (15)	0.93831 (4)	0.07059 (17)
Br2	0.88017 (6)	0.156292 (15)	0.65004 (4)	0.07438 (18)

Br3	1.14239 (6)	0.080170 (14)	0.58227 (3)	0.06397 (16)
Br4	1.26022 (6)	−0.013378 (17)	0.99092 (3)	0.07917 (19)
C1	1.0304 (5)	0.25477 (13)	0.9290 (3)	0.0502 (11)
C2	0.9181 (4)	0.24209 (12)	0.8641 (3)	0.0421 (10)
C3	0.8900 (5)	0.20413 (13)	0.8632 (3)	0.0544 (12)
H3	0.8155	0.1944	0.8207	0.065*
C4	0.9699 (6)	0.18044 (14)	0.9240 (3)	0.0671 (14)
H4	0.9484	0.1551	0.9225	0.081*
C5	1.0812 (6)	0.19451 (17)	0.9864 (3)	0.0755 (16)
H5	1.1366	0.1786	1.0265	0.091*
C6	1.1110 (6)	0.23166 (17)	0.9899 (3)	0.0669 (14)
H6	1.1850	0.2413	1.0328	0.080*
C7	0.8314 (5)	0.26820 (11)	0.8001 (3)	0.0476 (11)
H7A	0.7707	0.2846	0.8339	0.057*
H7B	0.9056	0.2835	0.7729	0.057*
C8	0.7275 (5)	0.18172 (12)	0.5743 (3)	0.0483 (11)
C9	0.7090 (5)	0.21975 (12)	0.5802 (3)	0.0422 (10)
C10	0.5964 (5)	0.23566 (13)	0.5198 (3)	0.0532 (12)
H10	0.5824	0.2613	0.5208	0.064*
C11	0.5054 (6)	0.21489 (16)	0.4588 (3)	0.0644 (13)
H11	0.4298	0.2263	0.4197	0.077*
C12	0.5264 (6)	0.17756 (16)	0.4558 (3)	0.0669 (14)
H12	0.4656	0.1634	0.4141	0.080*
C13	0.6359 (6)	0.16055 (13)	0.5134 (3)	0.0615 (13)
H13	0.6486	0.1349	0.5117	0.074*
C14	0.8026 (5)	0.24417 (12)	0.6468 (3)	0.0478 (11)
H14A	0.9021	0.2325	0.6630	0.057*
H14B	0.8210	0.2678	0.6186	0.057*
C15	0.5762 (4)	0.26793 (11)	0.7168 (2)	0.0349 (9)
C16	0.5543 (5)	0.30594 (12)	0.6987 (3)	0.0431 (10)
C17	0.4070 (5)	0.32031 (12)	0.6976 (3)	0.0510 (11)
H17	0.3910	0.3455	0.6862	0.061*
C18	0.2842 (5)	0.29847 (14)	0.7128 (3)	0.0550 (12)
H18	0.1867	0.3089	0.7136	0.066*
C19	0.3050 (5)	0.26120 (13)	0.7270 (3)	0.0487 (11)
H19	0.2202	0.2465	0.7360	0.058*
C20	0.4499 (4)	0.24477 (11)	0.7284 (2)	0.0381 (9)
C21	0.6832 (5)	0.33256 (11)	0.6799 (3)	0.0481 (11)
H21	0.7783	0.3180	0.6789	0.058*
C22	0.6486 (6)	0.35131 (14)	0.5881 (3)	0.0755 (16)
H22A	0.6457	0.3328	0.5419	0.113*
H22B	0.7280	0.3691	0.5797	0.113*
H22C	0.5506	0.3637	0.5853	0.113*
C23	0.7110 (6)	0.36190 (13)	0.7539 (3)	0.0658 (14)
H23A	0.6168	0.3751	0.7595	0.099*
H23B	0.7889	0.3790	0.7389	0.099*
H23C	0.7448	0.3499	0.8095	0.099*
C24	0.4663 (5)	0.20337 (11)	0.7432 (3)	0.0417 (10)
H24	0.5680	0.1960	0.7268	0.050*

C25	0.4597 (6)	0.19317 (13)	0.8408 (3)	0.0695 (14)
H25A	0.5372	0.2069	0.8773	0.104*
H25B	0.4782	0.1670	0.8486	0.104*
H25C	0.3596	0.1992	0.8581	0.104*
C26	0.3447 (5)	0.18141 (13)	0.6835 (3)	0.0662 (14)
H26A	0.2438	0.1871	0.7002	0.099*
H26B	0.3642	0.1553	0.6909	0.099*
H26C	0.3499	0.1882	0.6221	0.099*
C27	0.9489 (5)	0.05820 (11)	0.5411 (3)	0.0444 (10)
C28	0.9016 (5)	0.02539 (12)	0.5783 (3)	0.0420 (10)
C29	0.7648 (5)	0.01009 (13)	0.5374 (3)	0.0540 (12)
H29	0.7302	−0.0124	0.5583	0.065*
C30	0.6800 (6)	0.02738 (15)	0.4670 (3)	0.0634 (13)
H30	0.5883	0.0167	0.4420	0.076*
C31	0.7297 (6)	0.06035 (15)	0.4333 (3)	0.0635 (13)
H31	0.6725	0.0719	0.3853	0.076*
C32	0.8638 (6)	0.07586 (12)	0.4710 (3)	0.0543 (12)
H32	0.8978	0.0983	0.4495	0.065*
C33	0.9877 (5)	0.00540 (12)	0.6553 (3)	0.0442 (10)
H33A	0.9854	−0.0211	0.6426	0.053*
H33B	1.0948	0.0133	0.6604	0.053*
C34	1.2353 (5)	0.03313 (13)	0.9319 (3)	0.0517 (12)
C35	1.1298 (4)	0.03668 (12)	0.8563 (3)	0.0406 (10)
C36	1.1152 (5)	0.07180 (12)	0.8187 (3)	0.0481 (11)
H36	1.0456	0.0756	0.7683	0.058*
C37	1.2025 (5)	0.10145 (14)	0.8546 (3)	0.0592 (13)
H37	1.1901	0.1248	0.8283	0.071*
C38	1.3039 (7)	0.09686 (17)	0.9265 (4)	0.0768 (16)
H38	1.3621	0.1170	0.9497	0.092*
C39	1.3227 (5)	0.06297 (18)	0.9661 (3)	0.0694 (15)
H39	1.3941	0.0598	1.0160	0.083*
C40	1.0367 (5)	0.00394 (12)	0.8199 (3)	0.0468 (11)
H40A	1.1072	−0.0152	0.8041	0.056*
H40B	0.9803	−0.0059	0.8671	0.056*
C41	0.7727 (4)	−0.00230 (11)	0.7494 (2)	0.0357 (9)
C42	0.6540 (4)	0.02400 (11)	0.7500 (2)	0.0393 (10)
C43	0.5077 (5)	0.01119 (14)	0.7647 (3)	0.0530 (12)
H43	0.4274	0.0282	0.7662	0.064*
C44	0.4798 (5)	−0.02558 (16)	0.7769 (3)	0.0617 (13)
H44	0.3813	−0.0334	0.7871	0.074*
C45	0.5960 (5)	−0.05111 (13)	0.7741 (3)	0.0538 (12)
H45	0.5749	−0.0762	0.7818	0.065*
C46	0.7445 (5)	−0.04030 (11)	0.7602 (3)	0.0414 (10)
C47	0.6815 (5)	0.06504 (12)	0.7389 (3)	0.0473 (11)
H47	0.7770	0.0678	0.7103	0.057*
C48	0.7056 (6)	0.08458 (13)	0.8303 (3)	0.0710 (15)
H48A	0.6164	0.0808	0.8617	0.106*
H48B	0.7207	0.1107	0.8215	0.106*
H48C	0.7949	0.0744	0.8646	0.106*

C49	0.5527 (6)	0.08428 (15)	0.6792 (4)	0.0817 (17)
H49A	0.5339	0.0710	0.6237	0.122*
H49B	0.5831	0.1093	0.6675	0.122*
H49C	0.4602	0.0846	0.7088	0.122*
C50	0.8656 (5)	−0.07080 (11)	0.7580 (3)	0.0535 (12)
H50	0.9622	−0.0590	0.7449	0.064*
C51	0.8198 (7)	−0.09898 (13)	0.6837 (3)	0.0746 (16)
H51A	0.7244	−0.1107	0.6944	0.112*
H51B	0.8991	−0.1175	0.6831	0.112*
H51C	0.8073	−0.0865	0.6270	0.112*
C52	0.8964 (6)	−0.09067 (14)	0.8486 (3)	0.0730 (15)
H52A	0.9336	−0.0730	0.8937	0.109*
H52B	0.9725	−0.1097	0.8445	0.109*
H52C	0.8024	−0.1017	0.8643	0.109*
N2	0.9262 (3)	0.01165 (8)	0.7416 (2)	0.0357 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0271 (17)	0.0425 (19)	0.0379 (19)	0.0037 (14)	−0.0027 (14)	−0.0033 (15)
Br1	0.0590 (3)	0.0781 (4)	0.0704 (4)	−0.0097 (3)	−0.0136 (3)	−0.0161 (3)
Br2	0.0704 (4)	0.0638 (3)	0.0864 (4)	0.0232 (3)	−0.0037 (3)	−0.0034 (3)
Br3	0.0567 (3)	0.0719 (4)	0.0643 (3)	−0.0170 (3)	0.0110 (2)	−0.0002 (3)
Br4	0.0718 (4)	0.1068 (5)	0.0569 (3)	0.0140 (3)	−0.0027 (3)	0.0281 (3)
C1	0.040 (2)	0.068 (3)	0.042 (3)	0.005 (2)	0.002 (2)	−0.004 (2)
C2	0.032 (2)	0.054 (3)	0.039 (2)	0.0031 (19)	−0.0002 (18)	−0.004 (2)
C3	0.055 (3)	0.061 (3)	0.045 (3)	0.002 (2)	−0.008 (2)	0.002 (2)
C4	0.071 (4)	0.060 (3)	0.067 (3)	0.009 (3)	−0.006 (3)	0.012 (3)
C5	0.066 (4)	0.097 (5)	0.058 (3)	0.019 (3)	−0.015 (3)	0.018 (3)
C6	0.059 (3)	0.090 (4)	0.048 (3)	0.004 (3)	−0.013 (2)	0.001 (3)
C7	0.040 (2)	0.050 (3)	0.050 (3)	−0.001 (2)	−0.008 (2)	−0.004 (2)
C8	0.046 (3)	0.054 (3)	0.045 (3)	0.011 (2)	0.009 (2)	−0.004 (2)
C9	0.040 (2)	0.050 (3)	0.039 (2)	0.002 (2)	0.0098 (19)	0.000 (2)
C10	0.064 (3)	0.050 (3)	0.046 (3)	0.002 (2)	0.009 (2)	0.003 (2)
C11	0.067 (3)	0.085 (4)	0.039 (3)	−0.001 (3)	−0.002 (2)	0.005 (3)
C12	0.073 (4)	0.085 (4)	0.041 (3)	−0.008 (3)	0.000 (3)	−0.015 (3)
C13	0.072 (3)	0.055 (3)	0.059 (3)	−0.001 (3)	0.013 (3)	−0.014 (3)
C14	0.039 (2)	0.052 (3)	0.053 (3)	0.005 (2)	0.009 (2)	0.001 (2)
C15	0.037 (2)	0.041 (2)	0.025 (2)	0.0049 (19)	−0.0030 (16)	−0.0020 (17)
C16	0.041 (2)	0.050 (3)	0.037 (2)	0.006 (2)	−0.0044 (19)	−0.005 (2)
C17	0.051 (3)	0.046 (3)	0.054 (3)	0.014 (2)	−0.003 (2)	−0.002 (2)
C18	0.038 (3)	0.069 (3)	0.056 (3)	0.020 (2)	−0.005 (2)	−0.010 (2)
C19	0.035 (2)	0.062 (3)	0.049 (3)	−0.006 (2)	0.006 (2)	−0.006 (2)
C20	0.036 (2)	0.048 (2)	0.030 (2)	0.0014 (19)	−0.0009 (17)	−0.0038 (18)
C21	0.053 (3)	0.044 (3)	0.046 (3)	0.003 (2)	0.001 (2)	0.006 (2)
C22	0.092 (4)	0.066 (3)	0.067 (4)	−0.006 (3)	−0.001 (3)	0.018 (3)
C23	0.067 (3)	0.052 (3)	0.078 (4)	−0.002 (2)	0.002 (3)	−0.009 (3)
C24	0.034 (2)	0.049 (3)	0.041 (2)	−0.0034 (19)	0.0044 (18)	−0.0019 (19)

C25	0.097 (4)	0.056 (3)	0.057 (3)	−0.003 (3)	0.014 (3)	0.008 (2)
C26	0.058 (3)	0.059 (3)	0.080 (4)	−0.009 (2)	−0.003 (3)	−0.011 (3)
C27	0.047 (3)	0.044 (3)	0.044 (3)	0.000 (2)	0.014 (2)	−0.007 (2)
C28	0.040 (2)	0.050 (3)	0.039 (2)	0.008 (2)	0.0162 (19)	−0.003 (2)
C29	0.056 (3)	0.058 (3)	0.049 (3)	−0.006 (2)	0.015 (2)	−0.006 (2)
C30	0.050 (3)	0.090 (4)	0.050 (3)	0.002 (3)	0.002 (2)	−0.015 (3)
C31	0.062 (3)	0.072 (4)	0.054 (3)	0.010 (3)	−0.005 (3)	0.011 (3)
C32	0.068 (3)	0.049 (3)	0.047 (3)	0.009 (2)	0.017 (2)	0.008 (2)
C33	0.038 (2)	0.048 (3)	0.048 (3)	0.007 (2)	0.015 (2)	0.007 (2)
C34	0.040 (2)	0.077 (3)	0.039 (3)	−0.001 (2)	0.007 (2)	0.003 (2)
C35	0.028 (2)	0.058 (3)	0.037 (2)	−0.0005 (19)	0.0084 (18)	−0.003 (2)
C36	0.041 (2)	0.061 (3)	0.042 (3)	−0.001 (2)	0.006 (2)	0.001 (2)
C37	0.056 (3)	0.058 (3)	0.065 (3)	−0.015 (2)	0.010 (3)	−0.006 (3)
C38	0.082 (4)	0.084 (4)	0.066 (4)	−0.031 (3)	0.016 (3)	−0.017 (3)
C39	0.050 (3)	0.116 (5)	0.041 (3)	−0.017 (3)	−0.005 (2)	−0.016 (3)
C40	0.039 (2)	0.050 (3)	0.051 (3)	0.003 (2)	0.006 (2)	0.007 (2)
C41	0.028 (2)	0.046 (2)	0.034 (2)	−0.0034 (18)	0.0053 (17)	−0.0032 (18)
C42	0.030 (2)	0.053 (3)	0.035 (2)	0.0040 (19)	0.0060 (17)	0.0015 (19)
C43	0.032 (2)	0.074 (3)	0.054 (3)	0.009 (2)	0.008 (2)	−0.001 (2)
C44	0.034 (3)	0.090 (4)	0.063 (3)	−0.016 (3)	0.009 (2)	−0.003 (3)
C45	0.049 (3)	0.056 (3)	0.056 (3)	−0.018 (2)	0.008 (2)	−0.004 (2)
C46	0.039 (2)	0.048 (3)	0.038 (2)	−0.007 (2)	0.0065 (18)	−0.0048 (19)
C47	0.039 (2)	0.053 (3)	0.050 (3)	0.013 (2)	0.005 (2)	0.004 (2)
C48	0.082 (4)	0.059 (3)	0.074 (4)	0.000 (3)	0.019 (3)	−0.005 (3)
C49	0.062 (3)	0.080 (4)	0.101 (4)	0.022 (3)	0.000 (3)	0.025 (3)
C50	0.058 (3)	0.040 (3)	0.065 (3)	−0.004 (2)	0.016 (2)	0.000 (2)
C51	0.102 (4)	0.054 (3)	0.073 (4)	−0.008 (3)	0.034 (3)	−0.013 (3)
C52	0.084 (4)	0.060 (3)	0.077 (4)	0.007 (3)	0.017 (3)	0.011 (3)
N2	0.0274 (17)	0.0407 (19)	0.0393 (19)	0.0019 (14)	0.0046 (14)	0.0037 (15)

Geometric parameters (Å, °)

N1—C15	1.448 (4)	C26—H26B	0.9600
N1—C7	1.461 (5)	C26—H26C	0.9600
N1—C14	1.472 (5)	C27—C32	1.378 (6)
Br1—C1	1.902 (5)	C27—C28	1.387 (5)
Br2—C8	1.893 (4)	C28—C29	1.396 (6)
Br3—C27	1.906 (4)	C28—C33	1.497 (5)
Br4—C34	1.896 (5)	C29—C30	1.375 (6)
C1—C6	1.374 (6)	C29—H29	0.9300
C1—C2	1.385 (5)	C30—C31	1.377 (7)
C2—C3	1.387 (6)	C30—H30	0.9300
C2—C7	1.492 (5)	C31—C32	1.364 (6)
C3—C4	1.383 (6)	C31—H31	0.9300
C3—H3	0.9300	C32—H32	0.9300
C4—C5	1.375 (7)	C33—N2	1.471 (5)
C4—H4	0.9300	C33—H33A	0.9700
C5—C6	1.361 (7)	C33—H33B	0.9700
C5—H5	0.9300	C34—C39	1.384 (7)

C6—H6	0.9300	C34—C35	1.391 (5)
C7—H7A	0.9700	C35—C36	1.385 (6)
C7—H7B	0.9700	C35—C40	1.500 (6)
C8—C13	1.380 (6)	C36—C37	1.386 (6)
C8—C9	1.382 (6)	C36—H36	0.9300
C9—C10	1.389 (6)	C37—C38	1.333 (7)
C9—C14	1.506 (6)	C37—H37	0.9300
C10—C11	1.371 (6)	C38—C39	1.359 (7)
C10—H10	0.9300	C38—H38	0.9300
C11—C12	1.357 (7)	C39—H39	0.9300
C11—H11	0.9300	C40—N2	1.468 (5)
C12—C13	1.364 (6)	C40—H40A	0.9700
C12—H12	0.9300	C40—H40B	0.9700
C13—H13	0.9300	C41—C46	1.401 (5)
C14—H14A	0.9700	C41—C42	1.402 (5)
C14—H14B	0.9700	C41—N2	1.444 (4)
C15—C16	1.403 (5)	C42—C43	1.394 (5)
C15—C20	1.405 (5)	C42—C47	1.507 (6)
C16—C17	1.381 (5)	C43—C44	1.361 (6)
C16—C21	1.525 (6)	C43—H43	0.9300
C17—C18	1.365 (6)	C44—C45	1.371 (6)
C17—H17	0.9300	C44—H44	0.9300
C18—C19	1.366 (6)	C45—C46	1.387 (5)
C18—H18	0.9300	C45—H45	0.9300
C19—C20	1.392 (5)	C46—C50	1.524 (6)
C19—H19	0.9300	C47—C49	1.527 (6)
C20—C24	1.510 (5)	C47—C48	1.538 (6)
C21—C23	1.534 (6)	C47—H47	0.9800
C21—C22	1.538 (6)	C48—H48A	0.9600
C21—H21	0.9800	C48—H48B	0.9600
C22—H22A	0.9600	C48—H48C	0.9600
C22—H22B	0.9600	C49—H49A	0.9600
C22—H22C	0.9600	C49—H49B	0.9600
C23—H23A	0.9600	C49—H49C	0.9600
C23—H23B	0.9600	C50—C51	1.530 (6)
C23—H23C	0.9600	C50—C52	1.538 (6)
C24—C25	1.519 (6)	C50—H50	0.9800
C24—C26	1.534 (6)	C51—H51A	0.9600
C24—H24	0.9800	C51—H51B	0.9600
C25—H25A	0.9600	C51—H51C	0.9600
C25—H25B	0.9600	C52—H52A	0.9600
C25—H25C	0.9600	C52—H52B	0.9600
C26—H26A	0.9600	C52—H52C	0.9600

C15—N1—C7	113.7 (3)	C32—C27—C28	122.8 (4)
C15—N1—C14	116.3 (3)	C32—C27—Br3	116.4 (3)
C7—N1—C14	113.3 (3)	C28—C27—Br3	120.7 (3)
C6—C1—C2	123.0 (5)	C27—C28—C29	115.7 (4)
C6—C1—Br1	117.5 (4)	C27—C28—C33	125.1 (4)
C2—C1—Br1	119.4 (3)	C29—C28—C33	119.2 (4)

C1—C2—C3	116.2 (4)	C30—C29—C28	121.8 (4)
C1—C2—C7	121.3 (4)	C30—C29—H29	119.1
C3—C2—C7	122.4 (4)	C28—C29—H29	119.1
C4—C3—C2	121.6 (4)	C29—C30—C31	120.6 (5)
C4—C3—H3	119.2	C29—C30—H30	119.7
C2—C3—H3	119.2	C31—C30—H30	119.7
C5—C4—C3	119.7 (5)	C32—C31—C30	119.2 (4)
C5—C4—H4	120.2	C32—C31—H31	120.4
C3—C4—H4	120.2	C30—C31—H31	120.4
C6—C5—C4	120.4 (5)	C31—C32—C27	119.9 (4)
C6—C5—H5	119.8	C31—C32—H32	120.0
C4—C5—H5	119.8	C27—C32—H32	120.0
C5—C6—C1	119.1 (5)	N2—C33—C28	114.2 (3)
C5—C6—H6	120.4	N2—C33—H33A	108.7
C1—C6—H6	120.4	C28—C33—H33A	108.7
N1—C7—C2	116.2 (3)	N2—C33—H33B	108.7
N1—C7—H7A	108.2	C28—C33—H33B	108.7
C2—C7—H7A	108.2	H33A—C33—H33B	107.6
N1—C7—H7B	108.2	C39—C34—C35	121.6 (5)
C2—C7—H7B	108.2	C39—C34—Br4	118.6 (4)
H7A—C7—H7B	107.4	C35—C34—Br4	119.8 (3)
C13—C8—C9	121.7 (4)	C36—C35—C34	116.2 (4)
C13—C8—Br2	117.0 (3)	C36—C35—C40	123.0 (4)
C9—C8—Br2	121.3 (3)	C34—C35—C40	120.8 (4)
C8—C9—C10	116.4 (4)	C35—C36—C37	121.3 (4)
C8—C9—C14	124.2 (4)	C35—C36—H36	119.4
C10—C9—C14	119.4 (4)	C37—C36—H36	119.4
C11—C10—C9	122.2 (4)	C38—C37—C36	120.8 (5)
C11—C10—H10	118.9	C38—C37—H37	119.6
C9—C10—H10	118.9	C36—C37—H37	119.6
C12—C11—C10	119.4 (5)	C37—C38—C39	120.4 (5)
C12—C11—H11	120.3	C37—C38—H38	119.8
C10—C11—H11	120.3	C39—C38—H38	119.8
C11—C12—C13	120.7 (5)	C38—C39—C34	119.7 (5)
C11—C12—H12	119.6	C38—C39—H39	120.1
C13—C12—H12	119.6	C34—C39—H39	120.1
C12—C13—C8	119.4 (5)	N2—C40—C35	115.4 (3)
C12—C13—H13	120.3	N2—C40—H40A	108.4
C8—C13—H13	120.3	C35—C40—H40A	108.4
N1—C14—C9	113.6 (3)	N2—C40—H40B	108.4
N1—C14—H14A	108.8	C35—C40—H40B	108.4
C9—C14—H14A	108.8	H40A—C40—H40B	107.5
N1—C14—H14B	108.8	C46—C41—C42	121.3 (3)
C9—C14—H14B	108.8	C46—C41—N2	121.5 (3)
H14A—C14—H14B	107.7	C42—C41—N2	117.1 (3)
C16—C15—C20	120.6 (4)	C43—C42—C41	117.7 (4)
C16—C15—N1	122.3 (3)	C43—C42—C47	120.0 (4)
C20—C15—N1	117.1 (3)	C41—C42—C47	122.3 (3)
C17—C16—C15	118.4 (4)	C44—C43—C42	121.4 (4)

C17—C16—C21	117.6 (4)	C44—C43—H43	119.3
C15—C16—C21	124.0 (4)	C42—C43—H43	119.3
C18—C17—C16	121.7 (4)	C43—C44—C45	120.3 (4)
C18—C17—H17	119.2	C43—C44—H44	119.8
C16—C17—H17	119.2	C45—C44—H44	119.8
C17—C18—C19	119.8 (4)	C44—C45—C46	121.3 (4)
C17—C18—H18	120.1	C44—C45—H45	119.3
C19—C18—H18	120.1	C46—C45—H45	119.3
C18—C19—C20	121.6 (4)	C45—C46—C41	117.9 (4)
C18—C19—H19	119.2	C45—C46—C50	117.4 (4)
C20—C19—H19	119.2	C41—C46—C50	124.7 (3)
C19—C20—C15	117.8 (4)	C42—C47—C49	113.2 (4)
C19—C20—C24	119.5 (4)	C42—C47—C48	110.9 (4)
C15—C20—C24	122.7 (3)	C49—C47—C48	110.0 (4)
C16—C21—C23	111.2 (4)	C42—C47—H47	107.5
C16—C21—C22	111.3 (4)	C49—C47—H47	107.5
C23—C21—C22	110.5 (4)	C48—C47—H47	107.5
C16—C21—H21	107.9	C47—C48—H48A	109.5
C23—C21—H21	107.9	C47—C48—H48B	109.5
C22—C21—H21	107.9	H48A—C48—H48B	109.5
C21—C22—H22A	109.5	C47—C48—H48C	109.5
C21—C22—H22B	109.5	H48A—C48—H48C	109.5
H22A—C22—H22B	109.5	H48B—C48—H48C	109.5
C21—C22—H22C	109.5	C47—C49—H49A	109.5
H22A—C22—H22C	109.5	C47—C49—H49B	109.5
H22B—C22—H22C	109.5	H49A—C49—H49B	109.5
C21—C23—H23A	109.5	C47—C49—H49C	109.5
C21—C23—H23B	109.5	H49A—C49—H49C	109.5
H23A—C23—H23B	109.5	H49B—C49—H49C	109.5
C21—C23—H23C	109.5	C46—C50—C51	111.4 (4)
H23A—C23—H23C	109.5	C46—C50—C52	111.9 (4)
H23B—C23—H23C	109.5	C51—C50—C52	110.3 (4)
C20—C24—C25	111.6 (3)	C46—C50—H50	107.7
C20—C24—C26	111.9 (3)	C51—C50—H50	107.7
C25—C24—C26	110.3 (4)	C52—C50—H50	107.7
C20—C24—H24	107.6	C50—C51—H51A	109.5
C25—C24—H24	107.6	C50—C51—H51B	109.5
C26—C24—H24	107.6	H51A—C51—H51B	109.5
C24—C25—H25A	109.5	C50—C51—H51C	109.5
C24—C25—H25B	109.5	H51A—C51—H51C	109.5
H25A—C25—H25B	109.5	H51B—C51—H51C	109.5
C24—C25—H25C	109.5	C50—C52—H52A	109.5
H25A—C25—H25C	109.5	C50—C52—H52B	109.5
H25B—C25—H25C	109.5	H52A—C52—H52B	109.5
C24—C26—H26A	109.5	C50—C52—H52C	109.5
C24—C26—H26B	109.5	H52A—C52—H52C	109.5
H26A—C26—H26B	109.5	H52B—C52—H52C	109.5
C24—C26—H26C	109.5	C41—N2—C40	113.8 (3)
H26A—C26—H26C	109.5	C41—N2—C33	116.4 (3)

H26B—C26—H26C	109.5	C40—N2—C33	114.2 (3)
C6—C1—C2—C3	0.0 (6)	C32—C27—C28—C29	3.0 (6)
Br1—C1—C2—C3	−177.9 (3)	Br3—C27—C28—C29	−174.3 (3)
C6—C1—C2—C7	179.0 (4)	C32—C27—C28—C33	−178.9 (4)
Br1—C1—C2—C7	1.1 (6)	Br3—C27—C28—C33	3.8 (5)
C1—C2—C3—C4	0.0 (7)	C27—C28—C29—C30	−2.4 (6)
C7—C2—C3—C4	−179.0 (4)	C33—C28—C29—C30	179.3 (4)
C2—C3—C4—C5	−0.7 (8)	C28—C29—C30—C31	1.3 (7)
C3—C4—C5—C6	1.3 (8)	C29—C30—C31—C32	−0.5 (7)
C4—C5—C6—C1	−1.2 (8)	C30—C31—C32—C27	1.0 (7)
C2—C1—C6—C5	0.6 (7)	C28—C27—C32—C31	−2.4 (6)
Br1—C1—C6—C5	178.6 (4)	Br3—C27—C32—C31	175.0 (3)
C15—N1—C7—C2	132.9 (4)	C27—C28—C33—N2	100.8 (4)
C14—N1—C7—C2	−91.3 (4)	C29—C28—C33—N2	−81.1 (5)
C1—C2—C7—N1	173.5 (4)	C39—C34—C35—C36	−1.2 (6)
C3—C2—C7—N1	−7.5 (6)	Br4—C34—C35—C36	178.2 (3)
C13—C8—C9—C10	−1.9 (6)	C39—C34—C35—C40	179.7 (4)
Br2—C8—C9—C10	178.3 (3)	Br4—C34—C35—C40	−0.9 (5)
C13—C8—C9—C14	178.4 (4)	C34—C35—C36—C37	0.4 (6)
Br2—C8—C9—C14	−1.5 (6)	C40—C35—C36—C37	179.5 (4)
C8—C9—C10—C11	1.5 (6)	C35—C36—C37—C38	0.4 (7)
C14—C9—C10—C11	−178.7 (4)	C36—C37—C38—C39	−0.4 (8)
C9—C10—C11—C12	−1.0 (7)	C37—C38—C39—C34	−0.4 (8)
C10—C11—C12—C13	0.7 (8)	C35—C34—C39—C38	1.3 (7)
C11—C12—C13—C8	−1.0 (7)	Br4—C34—C39—C38	−178.1 (4)
C9—C8—C13—C12	1.7 (7)	C36—C35—C40—N2	−0.8 (6)
Br2—C8—C13—C12	−178.5 (4)	C34—C35—C40—N2	178.2 (3)
C15—N1—C14—C9	−57.4 (5)	C46—C41—C42—C43	2.1 (6)
C7—N1—C14—C9	168.1 (3)	N2—C41—C42—C43	−175.0 (3)
C8—C9—C14—N1	−94.8 (5)	C46—C41—C42—C47	179.8 (4)
C10—C9—C14—N1	85.5 (5)	N2—C41—C42—C47	2.7 (5)
C7—N1—C15—C16	57.2 (5)	C41—C42—C43—C44	−0.9 (6)
C14—N1—C15—C16	−77.2 (4)	C47—C42—C43—C44	−178.6 (4)
C7—N1—C15—C20	−119.7 (4)	C42—C43—C44—C45	−0.5 (7)
C14—N1—C15—C20	105.9 (4)	C43—C44—C45—C46	0.8 (7)
C20—C15—C16—C17	3.5 (6)	C44—C45—C46—C41	0.4 (6)
N1—C15—C16—C17	−173.3 (3)	C44—C45—C46—C50	−179.8 (4)
C20—C15—C16—C21	−176.3 (3)	C42—C41—C46—C45	−1.9 (6)
N1—C15—C16—C21	6.9 (6)	N2—C41—C46—C45	175.1 (3)
C15—C16—C17—C18	−0.5 (6)	C42—C41—C46—C50	178.3 (4)
C21—C16—C17—C18	179.3 (4)	N2—C41—C46—C50	−4.7 (6)
C16—C17—C18—C19	−2.0 (7)	C43—C42—C47—C49	−43.2 (6)
C17—C18—C19—C20	1.5 (7)	C41—C42—C47—C49	139.2 (4)
C18—C19—C20—C15	1.5 (6)	C43—C42—C47—C48	81.0 (5)
C18—C19—C20—C24	−179.2 (4)	C41—C42—C47—C48	−96.6 (5)
C16—C15—C20—C19	−3.9 (5)	C45—C46—C50—C51	59.5 (5)
N1—C15—C20—C19	173.0 (3)	C41—C46—C50—C51	−120.6 (4)
C16—C15—C20—C24	176.8 (3)	C45—C46—C50—C52	−64.4 (5)
N1—C15—C20—C24	−6.3 (5)	C41—C46—C50—C52	115.4 (5)

C17—C16—C21—C23	65.7 (5)	C46—C41—N2—C40	−60.8 (5)
C15—C16—C21—C23	−114.5 (4)	C42—C41—N2—C40	116.3 (4)
C17—C16—C21—C22	−57.9 (5)	C46—C41—N2—C33	75.2 (4)
C15—C16—C21—C22	121.9 (4)	C42—C41—N2—C33	−107.7 (4)
C19—C20—C24—C25	−76.5 (5)	C35—C40—N2—C41	−130.8 (4)
C15—C20—C24—C25	102.8 (4)	C35—C40—N2—C33	92.3 (4)
C19—C20—C24—C26	47.7 (5)	C28—C33—N2—C41	65.0 (5)
C15—C20—C24—C26	−133.1 (4)	C28—C33—N2—C40	−159.2 (3)

C—H···π-ring interactions (Å, °)

C-H···*Cg*	C-H	H···*Cg*	C···*Cg*	C-H···*Cg*
C26—H26C···*Cg*1	0.96	2.96	3.67 (1)	131
C11—H11···*Cg*2^{i}	0.93	3.12	3.68 (2)	121
C33—H33A···*Cg*3^{ii}	0.97	3.06	3.55 (1)	113
C43—H43···*Cg*4^{iii}	0.93	3.10	3.88 (1)	143

Symmetry code: (i) x, $1/2 - y$, $-1/2 + z$, (ii) $2 - x$, $-y$, $1 - z$, (iii) $-1 + x$, y, z. *Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of rings C8–C13, C15–C20, C27–C32 and C34–C39, respectively.

Fig. 1

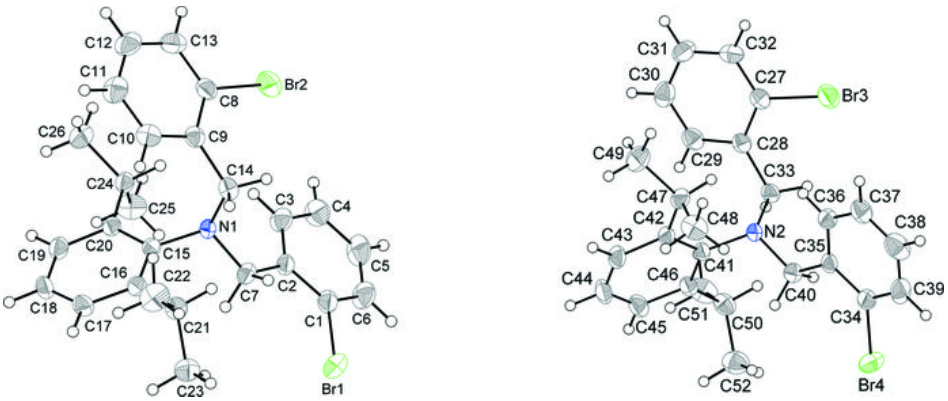
C12
C13
C11
C8
Br2
C26
C10
C9
C14
C24
C25
C3
C4
N1
C19
C20
C15
C5
C16
C22
C18
C17
C7
C2
C21
C1
C6
C23
Br1
C31
C32
C30
C27
Br3
C49
C29
C28
C33
C47
C48
C36
C37
C42
N2
C38
C43
C35
C41
C44
C46
C39
C40
C45
C51
C50
C34
C52
Br4

Fig. 2

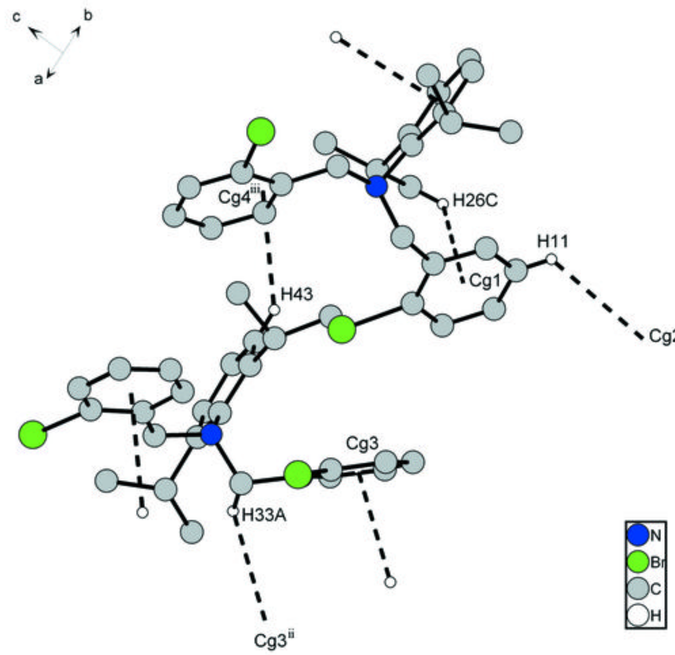

Fig. 3

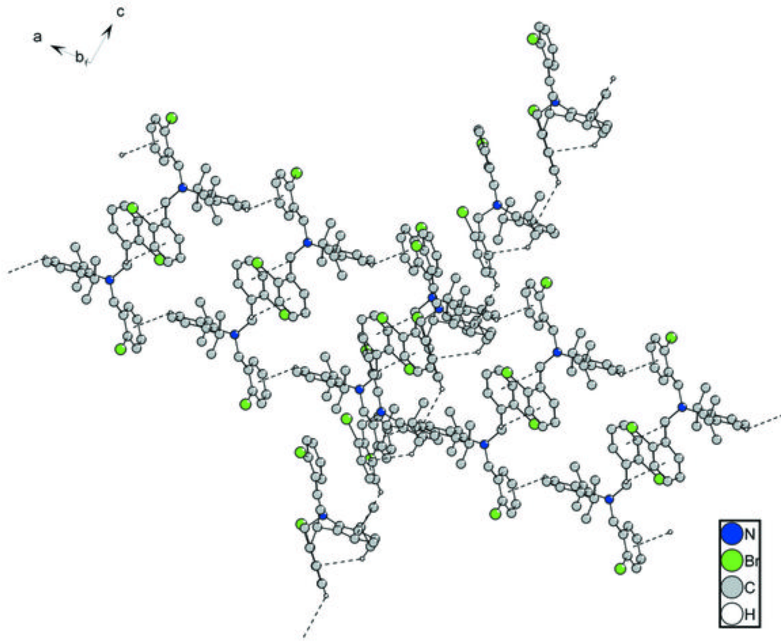

Fig. 4