organic compounds

N-(2-Benzylidenepropylidene)-4-bromo-aniline

Aliakbar Dehno Khalaji,[a] Alexandra M. Z. Slawin[b] and J. Derek Woollins[b]*

[a]Department of Science, Golestan University, Gorgan, Iran, and [b]Department of Chemistry, University of St Andrews, St Andrews KY16 9ST, Scotland

Correspondence e-mail: jdw3@st-and.ac.uk

The title compound, $C_{16}H_{14}BrN$, at 93 (2) K crystallizes with two independent molecules in the asymmetric unit. The molecules are slightly non-planar with the substituents adopting an *E* configuration with respect to the imine C=N bond.

Related literature

Chemistry and background: Amirnasr *et al.* (2006); Khalaji *et al.* (2007); Khalaji & Welter (2006); Li *et al.* (2006). Similar structure: Yang *et al.* (2006).
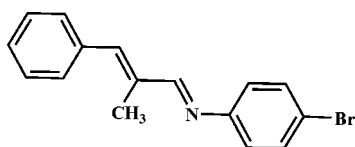
Experimental

Crystal data

$C_{16}H_{14}BrN$

$M_r = 300.19$

Orthorhombic, $P2_12_12_1$
$a = 7.3388 (11)$ Å
$b = 11.798 (2)$ Å
$c = 31.001 (5)$ Å
$V = 2684.2 (7)$ Å^3

$Z = 8$
Mo $K\alpha$ radiation
$\mu = 3.04$ mm^{-1}
$T = 93 (2)$ K
$0.10 \times 0.10 \times 0.01$ mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2004)
$T_{min} = 0.743$, $T_{max} = 0.972$

15150 measured reflections
4632 independent reflections
4105 reflections with $I > 2\sigma(I)$
$R_{int} = 0.060$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.108$
$S = 1.08$
4632 reflections
328 parameters
H-atom parameters constrained

$\Delta\rho_{max} = 0.77$ e Å^{-3}
$\Delta\rho_{min} = -0.63$ e Å^{-3}
Absolute structure: Flack (1983), 1818 Friedel pairs
Flack parameter: 0.066 (13)

Data collection: *CrystalClear* (Rigaku, 2004); 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* (Sheldrick, 2003); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2165).

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supplementary materials

N-(2-Benzylidenepropylidene)-4-bromoaniline

A. D. Khalaji, A. M. Z. Slawin and J. D. Woollins

Comment

Schiff base compounds have been of great interest for many years, because they play an important role in the development of coordination chemistry (Khalaji *et al.*, 2007.; Khalaji & Welter, 2006.; Amirnasr *et al.*, 2006) and new organic nonlinear optical (NLO) materials (Li *et al.*, 2006) due to their ease of preparation. We report here the crystal structure of Meca-Bran (I)·The asymmetric unit of (I) contains two independent molecules (Fig. 1), having the same bond lengths and angles within experimental error (Table 1). The average C=N bond length of 1.290 Å is slightly longer and average N—C bond length of 1.409 Å is slightly shorter than the corresponding bonds in 2-methoxy-*N*-[3-(2-nitrophenyl)allylidene]aniline (Yang *et al.*, 2006). THe two independent molecules are both slightly non-planar (which accounts for the crystallographic chirality) and interact with each other *via* Br(7)·H(34) and Br(27).·H(14) contacts of 2.94 (1) and 3.04 (1) Å respectively and there are no other significant packing interactions.

Experimental

To a solution of α-methylcinnamaldehyde (290 mg, 0.2 mmol) in ethanol (5 ml), cooled in an ice bath, a solution of 4-bromoaniline (344 mg, 0.2 mmol) in ethanol (5 ml) was slowly added dropwise with constant stirring (1 h) at 298 k in the presence of molecular sieves. The mixture was filtered and the yellow solution cooled to 273 K to give the compound in about 85% yield. Yellow crystals were grown from hot ethanol.

Refinement

All H atoms were included in calculated positions (C—H distances are 0.98 Å for methyl H atoms, 0.99 Å for methylene H atoms and 0.95 Å for aryl H atoms) and were refined as riding atoms with $U_{iso}(H) = 1.2\ U_{eq}$ (parent atom, methylene and aryl H atoms) or $U_{iso}(H) = 1.5\ U_{eq}$ (parent atom, methyl H atoms).
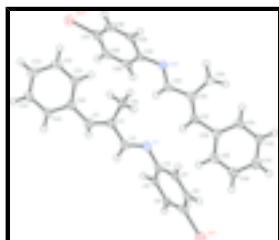
Figures

Fig. 1. The structure of (**1**) with displacement ellipsoids drawn at the 50% probability level.

N-(2-Benzylidenepropylidene)-4-bromoaniline

Crystal data

$C_{16}H_{14}BrN$	$F_{000} = 1216$
$M_r = 300.19$	$D_x = 1.486$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 8299 reflections
$a = 7.3388$ (11) Å	$\theta = 1.9–28.6°$
$b = 11.798$ (2) Å	$\mu = 3.04$ mm^{-1}
$c = 31.001$ (5) Å	$T = 93$ (2) K
$V = 2684.2$ (7) Å^3	Platelet, yellow
$Z = 8$	$0.10 \times 0.10 \times 0.01$ mm

Data collection

Rigaku CCD diffractometer	4632 independent reflections
Radiation source: rotating anode	4105 reflections with $I > 2\sigma(I)$
Monochromator: confocal	$R_{int} = 0.060$
$T = 93(2)$ K	$\theta_{max} = 25.3°$
ω and φ scans	$\theta_{min} = 1.9°$
Absorption correction: multi-scan (CrystalClear; Rigaku, 2004)	$h = -8 \rightarrow 7$
$T_{min} = 0.743$, $T_{max} = 0.972$	$k = -14 \rightarrow 13$
15150 measured reflections	$l = -33 \rightarrow 37$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.048$	$w = 1/[\sigma^2(F_o^2) + (0.0416P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.108$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.08$	$\Delta\rho_{max} = 0.77$ e Å^{-3}
4632 reflections	$\Delta\rho_{min} = -0.62$ e Å^{-3}
328 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983)
Secondary atom site location: difference Fourier map	Flack parameter: 0.066 (13)

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 $F^2 > 2sigma(F^2)$ 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	0.4450 (7)	0.7764 (4)	0.69418 (17)	0.0230 (12)
H1A	0.4559	0.7013	0.7049	0.028*
C2	0.4635 (8)	0.8589 (4)	0.72413 (18)	0.0264 (13)
C3	0.4991 (7)	0.8199 (4)	0.76795 (17)	0.0239 (12)
H3A	0.4975	0.7407	0.7735	0.029*
N3	0.5326 (6)	0.8879 (4)	0.79962 (14)	0.0245 (11)
C4	0.5748 (7)	0.8396 (4)	0.83991 (18)	0.0233 (13)
C5	0.5141 (7)	0.8948 (4)	0.87704 (17)	0.0236 (13)
H5A	0.4452	0.9625	0.8743	0.028*
C6	0.5521 (7)	0.8529 (4)	0.91768 (18)	0.0248 (13)
H6A	0.5104	0.8917	0.9427	0.030*
C7	0.6529 (7)	0.7526 (4)	0.92161 (17)	0.0238 (12)
Br7	0.71050 (8)	0.69448 (4)	0.976917 (18)	0.03333 (17)
C8	0.7155 (7)	0.6963 (4)	0.88542 (17)	0.0238 (12)
H8A	0.7844	0.6286	0.8884	0.029*
C9	0.6771 (7)	0.7392 (4)	0.84467 (17)	0.0249 (12)
H9A	0.7201	0.7006	0.8198	0.030*
C10	0.4109 (7)	0.7850 (4)	0.64776 (17)	0.0249 (13)
C11	0.4592 (8)	0.8791 (4)	0.62138 (18)	0.0269 (13)
H11A	0.5195	0.9422	0.6340	0.032*
C12	0.4197 (7)	0.8804 (5)	0.57758 (19)	0.0280 (13)
H12A	0.4488	0.9453	0.5608	0.034*
C13	0.3373 (7)	0.7866 (4)	0.55793 (18)	0.0297 (13)
H13A	0.3126	0.7866	0.5278	0.036*
C14	0.2929 (7)	0.6947 (4)	0.58296 (16)	0.0255 (12)
H14A	0.2354	0.6311	0.5699	0.031*
C15	0.3299 (7)	0.6925 (4)	0.62678 (17)	0.0258 (12)
H15A	0.2998	0.6268	0.6430	0.031*
C16	0.4448 (8)	0.9841 (4)	0.71717 (18)	0.0270 (13)
H16A	0.5646	1.0166	0.7106	0.041*
H16B	0.3959	1.0195	0.7433	0.041*
H16C	0.3618	0.9982	0.6930	0.041*
C21	1.0160 (7)	1.0188 (4)	0.80943 (17)	0.0251 (12)
H21A	0.9915	0.9430	0.8008	0.030*
C22	0.9956 (7)	1.0981 (4)	0.77804 (17)	0.0229 (12)
C23	0.9445 (7)	1.0577 (4)	0.73543 (17)	0.0257 (12)
H23A	0.9217	0.9792	0.7315	0.031*
N23	0.9290 (6)	1.1249 (4)	0.70288 (14)	0.0243 (11)

C24	0.9004 (7)	1.0788 (4)	0.66142 (18)	0.0230 (13)
C25	0.8120 (7)	1.1454 (4)	0.63070 (17)	0.0243 (12)
H25A	0.7641	1.2171	0.6388	0.029*
C26	0.7930 (8)	1.1084 (4)	0.58845 (17)	0.0303 (13)
H26A	0.7302	1.1536	0.5679	0.036*
C27	0.8674 (8)	1.0035 (4)	0.57635 (17)	0.0270 (13)
Br27	0.85102 (8)	0.95525 (5)	0.518338 (19)	0.03735 (18)
C28	0.9575 (7)	0.9375 (5)	0.60617 (19)	0.0289 (13)
H28A	1.0085	0.8668	0.5978	0.035*
C29	0.9733 (7)	0.9744 (4)	0.64820 (17)	0.0238 (12)
H29A	1.0348	0.9283	0.6686	0.029*
C30	1.0703 (7)	1.0325 (4)	0.85489 (17)	0.0228 (12)
C31	1.1701 (7)	1.1240 (4)	0.87145 (18)	0.0274 (13)
H31A	1.2101	1.1825	0.8526	0.033*
C32	1.2110 (8)	1.1300 (4)	0.91529 (17)	0.0276 (13)
H32A	1.2787	1.1925	0.9261	0.033*
C33	1.1538 (7)	1.0452 (5)	0.94333 (18)	0.0327 (14)
H33A	1.1802	1.0505	0.9733	0.039*
C34	1.0587 (7)	0.9533 (5)	0.92762 (18)	0.0311 (13)
H34A	1.0213	0.8946	0.9466	0.037*
C35	1.0175 (7)	0.9466 (5)	0.88413 (17)	0.0252 (12)
H35A	0.9522	0.8828	0.8737	0.030*
C36	1.0207 (8)	1.2241 (4)	0.78343 (18)	0.0255 (13)
H36A	0.9836	1.2464	0.8126	0.038*
H36B	0.9456	1.2642	0.7622	0.038*
H36C	1.1491	1.2436	0.7790	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.020 (3)	0.022 (3)	0.027 (3)	0.005 (2)	−0.003 (2)	−0.001 (2)
C2	0.027 (3)	0.022 (3)	0.030 (4)	0.001 (2)	−0.001 (2)	0.004 (2)
C3	0.016 (3)	0.020 (3)	0.035 (3)	0.001 (2)	0.001 (2)	0.003 (3)
N3	0.024 (3)	0.022 (2)	0.028 (3)	0.002 (2)	0.001 (2)	−0.003 (2)
C4	0.023 (3)	0.016 (3)	0.031 (3)	−0.004 (2)	−0.003 (2)	0.001 (2)
C5	0.022 (3)	0.016 (3)	0.032 (3)	0.002 (2)	−0.003 (2)	−0.003 (2)
C6	0.016 (3)	0.018 (3)	0.040 (4)	0.001 (2)	0.005 (2)	−0.007 (2)
C7	0.015 (3)	0.023 (3)	0.033 (3)	0.000 (2)	0.002 (2)	0.004 (2)
Br7	0.0409 (4)	0.0301 (3)	0.0290 (3)	0.0020 (2)	0.0003 (3)	0.0039 (3)
C8	0.026 (3)	0.008 (2)	0.037 (3)	0.001 (2)	−0.002 (2)	−0.001 (2)
C9	0.032 (4)	0.016 (3)	0.026 (3)	−0.003 (2)	−0.005 (2)	−0.002 (2)
C10	0.026 (3)	0.021 (3)	0.028 (3)	0.004 (2)	0.003 (2)	0.004 (2)
C11	0.024 (3)	0.024 (3)	0.032 (4)	−0.003 (2)	0.005 (2)	0.002 (2)
C12	0.024 (3)	0.023 (3)	0.037 (4)	0.002 (2)	0.006 (3)	0.008 (3)
C13	0.023 (3)	0.034 (3)	0.032 (3)	0.005 (2)	−0.001 (2)	0.004 (3)
C14	0.023 (3)	0.023 (3)	0.031 (3)	0.006 (2)	0.002 (2)	−0.008 (2)
C15	0.025 (3)	0.017 (3)	0.036 (3)	0.000 (2)	0.006 (2)	−0.003 (2)
C16	0.033 (3)	0.018 (3)	0.029 (3)	0.002 (2)	−0.003 (3)	0.000 (2)

C21	0.031 (3)	0.013 (3)	0.032 (3)	0.000 (2)	−0.002 (2)	−0.003 (2)
C22	0.022 (3)	0.022 (3)	0.025 (3)	0.001 (2)	0.003 (2)	0.001 (2)
C23	0.026 (3)	0.020 (3)	0.031 (3)	−0.002 (2)	0.001 (2)	−0.004 (2)
N23	0.028 (3)	0.022 (2)	0.023 (3)	0.0005 (19)	0.0008 (19)	0.0026 (19)
C24	0.024 (3)	0.015 (3)	0.029 (3)	−0.008 (2)	0.001 (2)	0.001 (2)
C25	0.028 (3)	0.016 (3)	0.029 (3)	0.004 (2)	0.002 (2)	0.003 (2)
C26	0.036 (4)	0.025 (3)	0.031 (3)	0.001 (3)	−0.001 (3)	0.006 (2)
C27	0.029 (3)	0.025 (3)	0.028 (3)	−0.002 (2)	0.003 (2)	−0.004 (2)
Br27	0.0473 (4)	0.0370 (3)	0.0278 (3)	−0.0073 (3)	0.0013 (3)	−0.0035 (3)
C28	0.028 (3)	0.020 (3)	0.039 (4)	−0.007 (2)	0.002 (3)	−0.003 (2)
C29	0.017 (3)	0.019 (3)	0.036 (3)	−0.003 (2)	0.002 (2)	0.003 (2)
C30	0.019 (3)	0.022 (3)	0.027 (3)	0.004 (2)	−0.002 (2)	−0.002 (2)
C31	0.023 (3)	0.018 (3)	0.041 (4)	−0.001 (2)	−0.002 (3)	0.002 (2)
C32	0.031 (3)	0.020 (3)	0.032 (3)	−0.002 (2)	−0.005 (3)	−0.003 (2)
C33	0.036 (4)	0.030 (3)	0.031 (3)	0.009 (3)	−0.003 (2)	−0.008 (3)
C34	0.038 (4)	0.019 (3)	0.036 (4)	0.005 (3)	−0.002 (3)	0.003 (3)
C35	0.018 (3)	0.024 (3)	0.034 (3)	0.008 (2)	−0.003 (2)	−0.001 (2)
C36	0.025 (3)	0.019 (3)	0.032 (3)	−0.006 (2)	−0.002 (2)	0.006 (2)

Geometric parameters (Å, °)

C1—C2	1.352 (7)	C21—C22	1.358 (7)
C1—C10	1.464 (7)	C21—C30	1.474 (7)
C1—H1A	0.9500	C21—H21A	0.9500
C2—C3	1.458 (7)	C22—C23	1.453 (7)
C2—C16	1.499 (7)	C22—C36	1.507 (7)
C3—N3	1.292 (6)	C23—N23	1.288 (6)
C3—H3A	0.9500	C23—H23A	0.9500
N3—C4	1.407 (6)	N23—C24	1.411 (7)
C4—C5	1.395 (7)	C24—C25	1.395 (7)
C4—C9	1.410 (7)	C24—C29	1.404 (7)
C5—C6	1.381 (7)	C25—C26	1.388 (7)
C5—H5A	0.9500	C25—H25A	0.9500
C6—C7	1.401 (7)	C26—C27	1.403 (7)
C6—H6A	0.9500	C26—H26A	0.9500
C7—C8	1.382 (7)	C27—C28	1.378 (8)
C7—Br7	1.894 (5)	C27—Br27	1.890 (5)
C8—C9	1.390 (7)	C28—C29	1.379 (7)
C8—H8A	0.9500	C28—H28A	0.9500
C9—H9A	0.9500	C29—H29A	0.9500
C10—C15	1.403 (7)	C30—C31	1.402 (7)
C10—C11	1.424 (7)	C30—C35	1.413 (7)
C11—C12	1.389 (7)	C31—C32	1.394 (7)
C11—H11A	0.9500	C31—H31A	0.9500
C12—C13	1.400 (7)	C32—C33	1.390 (7)
C12—H12A	0.9500	C32—H32A	0.9500
C13—C14	1.373 (7)	C33—C34	1.378 (7)
C13—H13A	0.9500	C33—H33A	0.9500
C14—C15	1.386 (7)	C34—C35	1.384 (7)

C14—H14A	0.9500	C34—H34A	0.9500
C15—H15A	0.9500	C35—H35A	0.9500
C16—H16A	0.9800	C36—H36A	0.9800
C16—H16B	0.9800	C36—H36B	0.9800
C16—H16C	0.9800	C36—H36C	0.9800
C2—C1—C10	129.9 (5)	C22—C21—C30	129.7 (5)
C2—C1—H1A	115.0	C22—C21—H21A	115.1
C10—C1—H1A	115.0	C30—C21—H21A	115.1
C1—C2—C3	115.5 (5)	C21—C22—C23	117.0 (5)
C1—C2—C16	127.0 (5)	C21—C22—C36	125.9 (5)
C3—C2—C16	117.5 (5)	C23—C22—C36	117.1 (4)
N3—C3—C2	123.1 (5)	N23—C23—C22	122.2 (5)
N3—C3—H3A	118.4	N23—C23—H23A	118.9
C2—C3—H3A	118.4	C22—C23—H23A	118.9
C3—N3—C4	117.8 (5)	C23—N23—C24	119.3 (4)
C5—C4—N3	118.3 (5)	C25—C24—C29	118.2 (5)
C5—C4—C9	118.4 (5)	C25—C24—N23	118.3 (5)
N3—C4—C9	123.3 (5)	C29—C24—N23	123.2 (5)
C6—C5—C4	121.4 (5)	C26—C25—C24	120.9 (5)
C6—C5—H5A	119.3	C26—C25—H25A	119.5
C4—C5—H5A	119.3	C24—C25—H25A	119.5
C5—C6—C7	119.2 (5)	C25—C26—C27	119.4 (5)
C5—C6—H6A	120.4	C25—C26—H26A	120.3
C7—C6—H6A	120.4	C27—C26—H26A	120.3
C8—C7—C6	120.7 (5)	C28—C27—C26	120.4 (5)
C8—C7—Br7	119.1 (4)	C28—C27—Br27	119.9 (4)
C6—C7—Br7	120.2 (4)	C26—C27—Br27	119.7 (4)
C7—C8—C9	119.7 (5)	C27—C28—C29	119.7 (5)
C7—C8—H8A	120.2	C27—C28—H28A	120.1
C9—C8—H8A	120.2	C29—C28—H28A	120.1
C8—C9—C4	120.6 (5)	C28—C29—C24	121.4 (5)
C8—C9—H9A	119.7	C28—C29—H29A	119.3
C4—C9—H9A	119.7	C24—C29—H29A	119.3
C15—C10—C11	116.5 (5)	C31—C30—C35	117.4 (5)
C15—C10—C1	118.3 (5)	C31—C30—C21	125.2 (5)
C11—C10—C1	125.1 (5)	C35—C30—C21	117.4 (5)
C12—C11—C10	121.2 (5)	C32—C31—C30	120.6 (5)
C12—C11—H11A	119.4	C32—C31—H31A	119.7
C10—C11—H11A	119.4	C30—C31—H31A	119.7
C11—C12—C13	120.5 (5)	C33—C32—C31	120.5 (5)
C11—C12—H12A	119.7	C33—C32—H32A	119.7
C13—C12—H12A	119.7	C31—C32—H32A	119.7
C14—C13—C12	118.7 (5)	C34—C33—C32	119.9 (5)
C14—C13—H13A	120.6	C34—C33—H33A	120.1
C12—C13—H13A	120.6	C32—C33—H33A	120.1
C13—C14—C15	121.5 (5)	C33—C34—C35	120.0 (5)
C13—C14—H14A	119.3	C33—C34—H34A	120.0
C15—C14—H14A	119.3	C35—C34—H34A	120.0
C14—C15—C10	121.6 (5)	C34—C35—C30	121.6 (5)

C14—C15—H15A	119.2	C34—C35—H35A	119.2
C10—C15—H15A	119.2	C30—C35—H35A	119.2
C2—C16—H16A	109.5	C22—C36—H36A	109.5
C2—C16—H16B	109.5	C22—C36—H36B	109.5
H16A—C16—H16B	109.5	H36A—C36—H36B	109.5
C2—C16—H16C	109.5	C22—C36—H36C	109.5
H16A—C16—H16C	109.5	H36A—C36—H36C	109.5
H16B—C16—H16C	109.5	H36B—C36—H36C	109.5
C10—C1—C2—C3	−179.4 (5)	C30—C21—C22—C23	178.4 (5)
C10—C1—C2—C16	2.9 (10)	C30—C21—C22—C36	−1.8 (10)
C1—C2—C3—N3	175.0 (5)	C21—C22—C23—N23	−177.0 (5)
C16—C2—C3—N3	−7.0 (8)	C36—C22—C23—N23	3.2 (8)
C2—C3—N3—C4	−176.6 (5)	C22—C23—N23—C24	172.5 (5)
C3—N3—C4—C5	−144.6 (5)	C23—N23—C24—C25	154.0 (5)
C3—N3—C4—C9	36.2 (7)	C23—N23—C24—C29	−33.0 (7)
N3—C4—C5—C6	−179.3 (5)	C29—C24—C25—C26	1.4 (8)
C9—C4—C5—C6	−0.1 (8)	N23—C24—C25—C26	174.8 (5)
C4—C5—C6—C7	−0.3 (8)	C24—C25—C26—C27	−1.4 (8)
C5—C6—C7—C8	0.6 (7)	C25—C26—C27—C28	0.4 (8)
C5—C6—C7—Br7	179.0 (4)	C25—C26—C27—Br27	−177.4 (4)
C6—C7—C8—C9	−0.4 (8)	C26—C27—C28—C29	0.5 (8)
Br7—C7—C8—C9	−178.8 (4)	Br27—C27—C28—C29	178.3 (4)
C7—C8—C9—C4	−0.1 (8)	C27—C28—C29—C24	−0.4 (8)
C5—C4—C9—C8	0.3 (8)	C25—C24—C29—C28	−0.5 (7)
N3—C4—C9—C8	179.5 (5)	N23—C24—C29—C28	−173.5 (5)
C2—C1—C10—C15	−156.0 (6)	C22—C21—C30—C31	−22.9 (9)
C2—C1—C10—C11	26.3 (9)	C22—C21—C30—C35	157.0 (6)
C15—C10—C11—C12	2.9 (8)	C35—C30—C31—C32	−1.3 (8)
C1—C10—C11—C12	−179.4 (5)	C21—C30—C31—C32	178.6 (5)
C10—C11—C12—C13	−2.5 (8)	C30—C31—C32—C33	0.0 (9)
C11—C12—C13—C14	1.4 (8)	C31—C32—C33—C34	1.2 (9)
C12—C13—C14—C15	−0.8 (8)	C32—C33—C34—C35	−1.2 (8)
C13—C14—C15—C10	1.4 (8)	C33—C34—C35—C30	−0.2 (8)
C11—C10—C15—C14	−2.4 (8)	C31—C30—C35—C34	1.4 (7)
C1—C10—C15—C14	179.8 (5)	C21—C30—C35—C34	−178.5 (5)

Fig. 1