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4,10-Dibromo-2,8-dimethyl-6*H*,12*H*-5,11-methanodibenzo[*b*,*f*][1,5]diazocine

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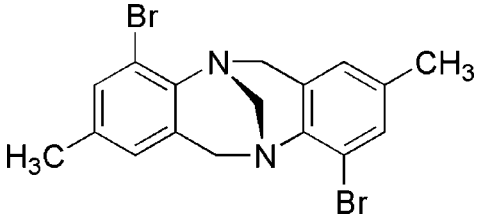
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.006 Å; R factor = 0.042; wR factor = 0.116; data-to-parameter ratio = 18.4.

In the molecule of the title compound, $C_{17}H_{16}Br_2N_2$, the 4,10-bromo-2,8-dimethyl analogue of Tröger's base, the two aryl rings are offset with respect to one another by virtue of the diazocine bridge. There are two crystallographically independent molecules in the unit cell and both of these have a dihedral angle of 95.4 (1)° between the two aryl rings.

Related literature

For related literature on the crystal structures of some other brominated Tröger's base analogues, see: Hansson *et al.* (2003); Bhuiyan *et al.* (2006); Lenev *et al.* (2006); Faroughi *et al.* (2006*a*,*b*, 2007).

For related literature, see: Hof *et al.* (2005); Jensen & Wärnmark (2001); Jensen, Strozyk & Wärnmark (2002); Jensen, Tejler & Wärnmark (2002); Kiehne & Lützen (2004); Solano *et al.* (2005).



Experimental

Crystal data

$C_{17}H_{16}Br_2N_2$
M_r = 408.14
Triclinic, $P\overline{1}$
a = 10.169 (4) Å
b = 11.477 (5) Å
c = 15.269 (6) Å
α = 104.259 (6)°
β = 106.185 (6)°
γ = 103.093 (6)°
V = 1573.1 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.15 mm^{-1}
T = 150 (2) K
0.35 × 0.16 × 0.05 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.351, T_{max} = 0.783
15349 measured reflections
7031 independent reflections
5002 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.116
S = 1.01
7031 reflections
383 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.35 e Å^{-3}
$\Delta\rho_{min}$ = −1.13 e Å^{-3}

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *TEXSAN* for Windows (Molecular Structure Corporation, 1998), *Xtal3.6* (Hall *et al.*, 1999), *ORTEPII* (Johnson, 1976) and *WinGX* (Farrugia, 1999); software used to prepare material for publication: *WinGX*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2032).

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supplementary materials

Acta Cryst. (2007). E**63**, o3030 [**doi:10.1107/S1600536807025007**]

4,10-Dibromo-2,8-dimethyl-6*H*,12*H*-5,11-methanodibenzo[*b*,*f*][1,5]diazocine

M. Faroughi, A. C. Try and P. Turner

Comment

The halogen substituents on Tröger's base analogues have been successfully converted into a range of other functionalities *via* exchange reactions (Jensen & Wärnmark, 2001; Jensen, Strozyk & Wärnmark, 2002; Jensen *et al.*, 2002; Kiehne & Lützen, 2004; Hof *et al.*, 2005). An important feature of this family of molecules is the methano-strapped diazocine bridge that creates the cavity present in these compounds. The bridge also imparts a twist within the compounds such that the two aryl rings are offset with respect to one another. The dihedral angle between these rings has been measured across a range of compounds to lie between 82° (Solano *et al.*, 2005) and 108° (Faroughi *et al.*, 2006*b*) for simple dibenzo Tröger's base analogues, and is dependant upon the nature of the substituents on the aromatic rings. We were interested in preparing a range of dihalo Tröger's base analogues as precursors for supramolecular recognition elements. The synthesis of (I) in racemic form was achieved by reacting 2-bromo-4-methylaniline with paraformaldehyde in trifluoroacetic acid (TFA) as shown in Fig. 2. The molecular structure of (I) is shown in Fig. 1.

Experimental

The title compound was prepared on a 2 g scale according to the literature procedure (Hansson *et al.*, 2003) in an almost quantitative yield. Single crystals of (I) were produced by slow evaporation of a dichloromethane solution.

Refinement

H atoms were positioned geometrically, with C—H = 0.95, 0.99 and 0.98 Å for aromatic, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H and x = 1.2 for all other H atoms. The methyl groups were free to rotate about their respective C—C bonds in the refinement.

Figures

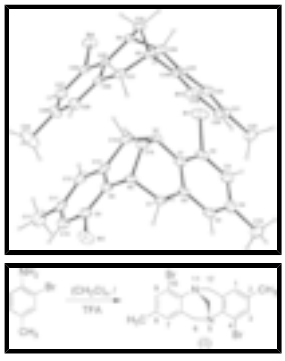


Fig. 1. Molecular structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are shown at the 50% probability level.

4,10-Dibromo-2,8-dimethyl-6*H*,12*H*-5,11- methanodibenzo[*b*,*f*][1,5]diazocine

Crystal data

$C_{17}H_{16}Br_2N_2$	$Z = 4$
$M_r = 408.14$	$F_{000} = 808$
Triclinic, $P\overline{1}$	$D_x = 1.723$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 465 K
$a = 10.169$ (4) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 11.477$ (5) Å	Cell parameters from 993 reflections
$c = 15.269$ (6) Å	$\theta = 2$–27º
$\alpha = 104.259$ (6)º	$\mu = 5.15$ mm^{-1}
$\beta = 106.185$ (6)º	$T = 150$ (2) K
$\gamma = 103.093$ (6)º	Blade, colourless
$V = 1573.1$ (11) Å^3	0.35 × 0.16 × 0.05 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	7031 independent reflections
Radiation source: fine-focus sealed tube	5002 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.036$
$T = 150$(2) K	$\theta_{max} = 28.2$º
ω scans	$\theta_{min} = 1.5$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -13\rightarrow12$
$T_{min} = 0.351$, $T_{max} = 0.783$	$k = -14\rightarrow14$
15349 measured reflections	$l = -20\rightarrow20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.116$	$w = 1/[\sigma^2(F_o^2) + (0.0675P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
7031 reflections	$\Delta\rho_{max} = 1.35$ e Å^{-3}
383 parameters	$\Delta\rho_{min} = -1.13$ 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}
Br1	0.57686 (5)	0.30388 (5)	−0.01862 (3)	0.03267 (13)
Br2	0.94459 (5)	0.21585 (5)	0.50648 (3)	0.03313 (13)
N1	0.6106 (3)	0.2665 (3)	0.1804 (2)	0.0207 (7)
N2	0.7408 (3)	0.2825 (3)	0.3459 (2)	0.0189 (7)
C1	0.7347 (4)	0.3580 (4)	0.1821 (3)	0.0196 (8)
C2	0.7393 (4)	0.3851 (4)	0.0987 (3)	0.0222 (9)
C3	0.8574 (4)	0.4732 (4)	0.0979 (3)	0.0253 (9)
H3	0.8576	0.4883	0.0395	0.030*
C4	0.9755 (4)	0.5392 (4)	0.1832 (3)	0.0254 (9)
C5	0.9709 (4)	0.5158 (4)	0.2672 (3)	0.0218 (9)
H5	1.0498	0.5626	0.3259	0.026*
C6	0.8530 (4)	0.4249 (4)	0.2682 (3)	0.0180 (8)
C7	0.8571 (4)	0.3987 (4)	0.3617 (3)	0.0207 (9)
H7A	0.9519	0.3895	0.3925	0.025*
H7B	0.8472	0.4721	0.4065	0.025*
C8	0.7727 (4)	0.1687 (4)	0.3088 (3)	0.0211 (9)
C9	0.8670 (4)	0.1269 (4)	0.3707 (3)	0.0234 (9)
C10	0.9076 (4)	0.0219 (4)	0.3362 (3)	0.0283 (10)
H10	0.9739	−0.0024	0.3798	0.034*
C11	0.8519 (4)	−0.0473 (4)	0.2384 (3)	0.0277 (10)
C12	0.7502 (4)	−0.0115 (4)	0.1770 (3)	0.0261 (10)
H12	0.7061	−0.0615	0.1106	0.031*
C13	0.7119 (4)	0.0953 (4)	0.2106 (3)	0.0219 (9)
C14	0.6071 (4)	0.1347 (4)	0.1393 (3)	0.0229 (9)
H14A	0.6321	0.1259	0.0803	0.027*
H14B	0.5079	0.0769	0.1203	0.027*
C15	0.6070 (4)	0.2845 (4)	0.2783 (3)	0.0208 (9)
H15A	0.5915	0.3667	0.3028	0.025*
H15B	0.5245	0.2166	0.2755	0.025*
C16	1.1084 (4)	0.6328 (4)	0.1831 (4)	0.0338 (11)
H16A	1.1496	0.7042	0.2438	0.051*
H16B	1.0807	0.6641	0.1287	0.051*
H16C	1.1803	0.5903	0.1767	0.051*

C17	0.9049 (5)	−0.1547 (4)	0.1984 (4)	0.0402 (13)
H17A	0.8292	−0.2154	0.1388	0.060*
H17B	0.9284	−0.1975	0.2461	0.060*
H17C	0.9914	−0.1206	0.1845	0.060*
Br3	0.34713 (4)	0.59722 (4)	0.47521 (3)	0.02297 (12)
Br4	0.16448 (4)	−0.06142 (4)	0.02942 (3)	0.02554 (12)
N3	0.1800 (3)	0.3402 (3)	0.3097 (2)	0.0164 (7)
N4	0.1316 (3)	0.1725 (3)	0.1605 (2)	0.0177 (7)
C18	0.2907 (4)	0.4193 (4)	0.2894 (3)	0.0158 (8)
C19	0.3825 (4)	0.5349 (4)	0.3593 (3)	0.0181 (8)
C20	0.4944 (4)	0.6110 (4)	0.3433 (3)	0.0211 (9)
H20	0.5574	0.6877	0.3928	0.025*
C21	0.5151 (4)	0.5760 (4)	0.2554 (3)	0.0224 (9)
C22	0.4201 (4)	0.4640 (4)	0.1838 (3)	0.0202 (9)
H22	0.4299	0.4413	0.1223	0.024*
C23	0.3105 (4)	0.3842 (4)	0.2005 (3)	0.0172 (8)
C24	0.2160 (4)	0.2581 (4)	0.1228 (3)	0.0189 (8)
H24A	0.1487	0.2739	0.0696	0.023*
H24B	0.2778	0.2159	0.0961	0.023*
C25	0.2166 (4)	0.1128 (4)	0.2146 (3)	0.0176 (8)
C26	0.2474 (4)	0.0074 (4)	0.1661 (3)	0.0182 (8)
C27	0.3334 (4)	−0.0503 (4)	0.2159 (3)	0.0242 (9)
H27	0.3553	−0.1197	0.1814	0.029*
C28	0.3875 (4)	−0.0067 (4)	0.3162 (3)	0.0260 (9)
C29	0.3515 (4)	0.0942 (4)	0.3655 (3)	0.0237 (9)
H29	0.3841	0.1215	0.4341	0.028*
C30	0.2689 (4)	0.1554 (4)	0.3161 (3)	0.0180 (8)
C31	0.2386 (4)	0.2689 (4)	0.3711 (3)	0.0174 (8)
H31A	0.1687	0.2398	0.4013	0.021*
H31B	0.3292	0.3265	0.4236	0.021*
C32	0.0695 (4)	0.2478 (4)	0.2201 (3)	0.0184 (8)
H32A	0.0175	0.2930	0.1826	0.022*
H32B	−0.0013	0.1902	0.2363	0.022*
C33	0.6416 (4)	0.6569 (4)	0.2401 (3)	0.0271 (10)
H33A	0.6500	0.6117	0.1796	0.041*
H33B	0.7306	0.6743	0.2941	0.041*
H33C	0.6257	0.7371	0.2369	0.041*
C34	0.4842 (6)	−0.0687 (5)	0.3711 (3)	0.0461 (14)
H34A	0.5715	−0.0031	0.4197	0.069*
H34B	0.5112	−0.1267	0.3257	0.069*
H34C	0.4321	−0.1161	0.4031	0.069*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0257 (2)	0.0465 (3)	0.0218 (2)	0.0129 (2)	0.00442 (19)	0.0076 (2)
Br2	0.0322 (3)	0.0439 (3)	0.0291 (3)	0.0202 (2)	0.0104 (2)	0.0149 (2)
N1	0.0111 (15)	0.0274 (19)	0.0235 (18)	0.0066 (14)	0.0089 (14)	0.0047 (15)

N2	0.0121 (15)	0.0241 (18)	0.0218 (18)	0.0095 (14)	0.0067 (14)	0.0055 (14)
C1	0.0152 (18)	0.022 (2)	0.023 (2)	0.0102 (16)	0.0077 (17)	0.0060 (17)
C2	0.0156 (19)	0.029 (2)	0.022 (2)	0.0126 (17)	0.0053 (17)	0.0056 (18)
C3	0.027 (2)	0.031 (2)	0.029 (2)	0.0175 (19)	0.0166 (19)	0.0135 (19)
C4	0.024 (2)	0.025 (2)	0.040 (3)	0.0138 (18)	0.020 (2)	0.016 (2)
C5	0.0170 (19)	0.019 (2)	0.029 (2)	0.0110 (16)	0.0064 (17)	0.0047 (18)
C6	0.0142 (18)	0.020 (2)	0.021 (2)	0.0118 (16)	0.0062 (16)	0.0042 (16)
C7	0.0123 (18)	0.024 (2)	0.024 (2)	0.0069 (16)	0.0044 (16)	0.0060 (17)
C8	0.0137 (18)	0.023 (2)	0.029 (2)	0.0059 (16)	0.0118 (17)	0.0067 (18)
C9	0.0162 (19)	0.026 (2)	0.031 (2)	0.0067 (17)	0.0118 (18)	0.0094 (18)
C10	0.018 (2)	0.030 (2)	0.048 (3)	0.0116 (18)	0.019 (2)	0.020 (2)
C11	0.017 (2)	0.016 (2)	0.054 (3)	0.0035 (17)	0.021 (2)	0.010 (2)
C12	0.021 (2)	0.019 (2)	0.034 (2)	0.0012 (17)	0.0157 (19)	−0.0001 (18)
C13	0.0135 (18)	0.020 (2)	0.034 (2)	0.0027 (16)	0.0155 (18)	0.0062 (18)
C14	0.0112 (18)	0.026 (2)	0.027 (2)	0.0031 (16)	0.0080 (17)	0.0013 (18)
C15	0.0128 (18)	0.027 (2)	0.025 (2)	0.0080 (16)	0.0092 (17)	0.0080 (18)
C16	0.023 (2)	0.031 (3)	0.058 (3)	0.011 (2)	0.023 (2)	0.021 (2)
C17	0.035 (3)	0.024 (2)	0.072 (4)	0.014 (2)	0.035 (3)	0.013 (2)
Br3	0.0167 (2)	0.0248 (2)	0.0216 (2)	0.00433 (16)	0.00694 (16)	−0.00018 (17)
Br4	0.0208 (2)	0.0270 (2)	0.0212 (2)	0.00706 (17)	0.00518 (17)	−0.00192 (17)
N3	0.0076 (14)	0.0220 (18)	0.0175 (17)	0.0034 (13)	0.0051 (13)	0.0036 (14)
N4	0.0100 (14)	0.0197 (17)	0.0204 (17)	0.0054 (13)	0.0042 (13)	0.0021 (14)
C18	0.0103 (17)	0.018 (2)	0.021 (2)	0.0081 (15)	0.0061 (15)	0.0058 (16)
C19	0.0118 (17)	0.020 (2)	0.022 (2)	0.0077 (15)	0.0063 (16)	0.0040 (16)
C20	0.0133 (18)	0.016 (2)	0.027 (2)	0.0018 (16)	0.0037 (17)	0.0027 (17)
C21	0.0149 (18)	0.022 (2)	0.035 (2)	0.0079 (16)	0.0113 (18)	0.0127 (19)
C22	0.0162 (19)	0.026 (2)	0.027 (2)	0.0132 (17)	0.0131 (17)	0.0110 (18)
C23	0.0106 (17)	0.022 (2)	0.020 (2)	0.0086 (15)	0.0043 (15)	0.0055 (16)
C24	0.0160 (19)	0.021 (2)	0.018 (2)	0.0063 (16)	0.0063 (16)	0.0040 (16)
C25	0.0092 (17)	0.020 (2)	0.022 (2)	0.0024 (15)	0.0060 (16)	0.0055 (16)
C26	0.0104 (17)	0.019 (2)	0.021 (2)	0.0011 (15)	0.0064 (16)	0.0025 (16)
C27	0.020 (2)	0.022 (2)	0.031 (2)	0.0068 (17)	0.0122 (18)	0.0052 (18)
C28	0.025 (2)	0.025 (2)	0.030 (2)	0.0136 (18)	0.0085 (19)	0.0092 (19)
C29	0.022 (2)	0.022 (2)	0.027 (2)	0.0080 (17)	0.0082 (18)	0.0081 (18)
C30	0.0101 (17)	0.017 (2)	0.022 (2)	0.0010 (15)	0.0064 (16)	0.0006 (16)
C31	0.0132 (18)	0.021 (2)	0.017 (2)	0.0040 (15)	0.0068 (16)	0.0042 (16)
C32	0.0085 (17)	0.021 (2)	0.021 (2)	0.0040 (15)	0.0040 (15)	0.0007 (16)
C33	0.017 (2)	0.028 (2)	0.041 (3)	0.0064 (18)	0.0155 (19)	0.014 (2)
C34	0.064 (4)	0.050 (3)	0.037 (3)	0.043 (3)	0.017 (3)	0.013 (3)

Geometric parameters (Å, °)

Br1—C2	1.907 (4)	Br3—C19	1.903 (4)
Br2—C9	1.910 (4)	Br4—C26	1.896 (4)
N1—C1	1.436 (5)	N3—C18	1.434 (5)
N1—C15	1.470 (5)	N3—C32	1.465 (4)
N1—C14	1.476 (5)	N3—C31	1.481 (5)
N2—C8	1.436 (5)	N4—C25	1.431 (5)
N2—C15	1.469 (5)	N4—C32	1.467 (4)

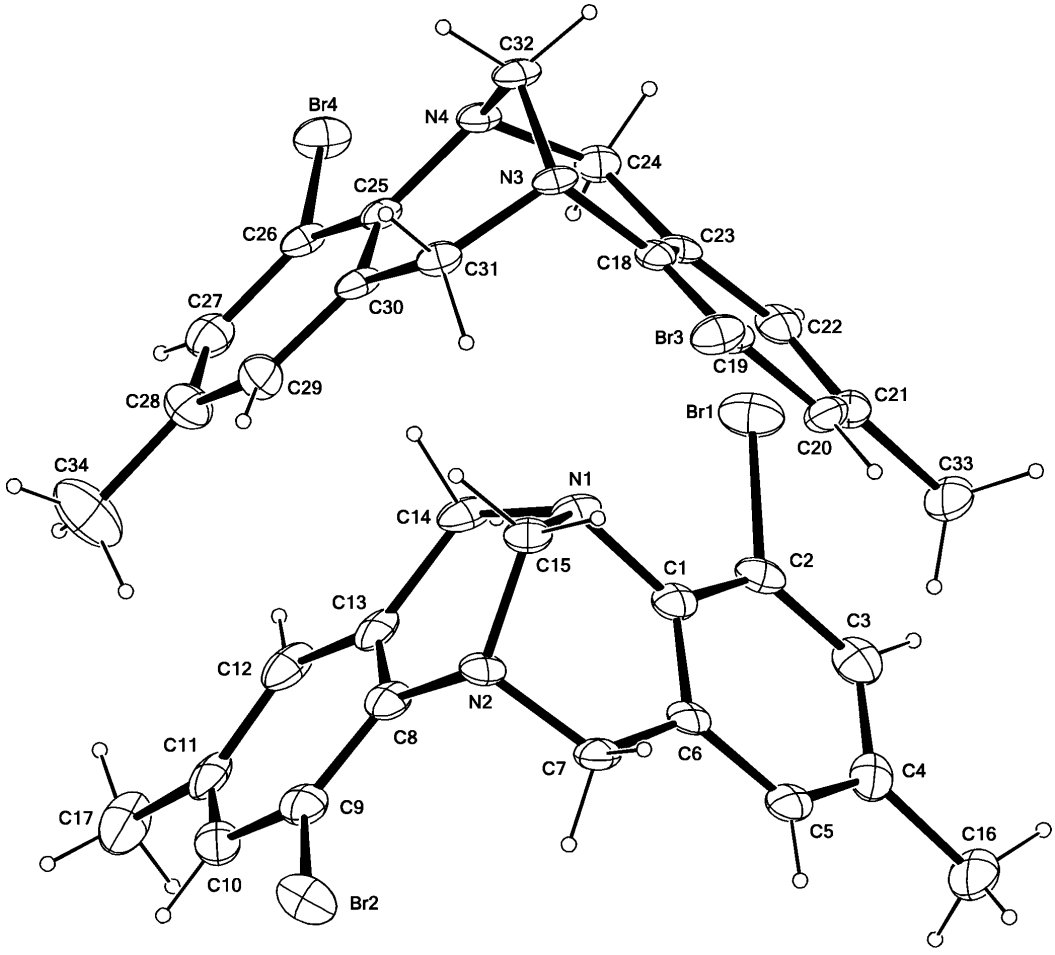
N2—C7	1.485 (5)	N4—C24	1.484 (5)
C1—C2	1.394 (6)	C18—C19	1.399 (5)
C1—C6	1.403 (5)	C18—C23	1.402 (5)
C2—C3	1.389 (6)	C19—C20	1.388 (5)
C3—C4	1.394 (6)	C20—C21	1.393 (5)
C3—H3	0.9500	C20—H20	0.9500
C4—C5	1.384 (6)	C21—C22	1.392 (5)
C4—C16	1.525 (6)	C21—C33	1.518 (5)
C5—C6	1.406 (5)	C22—C23	1.399 (5)
C5—H5	0.9500	C22—H22	0.9500
C6—C7	1.521 (5)	C23—C24	1.521 (5)
C7—H7A	0.9900	C24—H24A	0.9900
C7—H7B	0.9900	C24—H24B	0.9900
C8—C13	1.401 (6)	C25—C26	1.404 (5)
C8—C9	1.404 (6)	C25—C30	1.404 (5)
C9—C10	1.390 (6)	C26—C27	1.386 (5)
C10—C11	1.386 (6)	C27—C28	1.388 (6)
C10—H10	0.9500	C27—H27	0.9500
C11—C12	1.400 (6)	C28—C29	1.398 (5)
C11—C17	1.515 (6)	C28—C34	1.525 (6)
C12—C13	1.392 (5)	C29—C30	1.395 (5)
C12—H12	0.9500	C29—H29	0.9500
C13—C14	1.529 (6)	C30—C31	1.511 (5)
C14—H14A	0.9900	C31—H31A	0.9900
C14—H14B	0.9900	C31—H31B	0.9900
C15—H15A	0.9900	C32—H32A	0.9900
C15—H15B	0.9900	C32—H32B	0.9900
C16—H16A	0.9800	C33—H33A	0.9800
C16—H16B	0.9800	C33—H33B	0.9800
C16—H16C	0.9800	C33—H33C	0.9800
C17—H17A	0.9800	C34—H34A	0.9800
C17—H17B	0.9800	C34—H34B	0.9800
C17—H17C	0.9800	C34—H34C	0.9800
C1—N1—C15	111.0 (3)	C18—N3—C32	110.8 (3)
C1—N1—C14	112.6 (3)	C18—N3—C31	111.9 (3)
C15—N1—C14	107.8 (3)	C32—N3—C31	107.7 (3)
C8—N2—C15	110.6 (3)	C25—N4—C32	110.9 (3)
C8—N2—C7	112.5 (3)	C25—N4—C24	112.7 (3)
C15—N2—C7	107.4 (3)	C32—N4—C24	107.7 (3)
C2—C1—C6	118.1 (4)	C19—C18—C23	118.3 (3)
C2—C1—N1	120.9 (3)	C19—C18—N3	120.0 (3)
C6—C1—N1	121.0 (4)	C23—C18—N3	121.7 (3)
C3—C2—C1	122.3 (4)	C20—C19—C18	121.3 (3)
C3—C2—Br1	117.8 (3)	C20—C19—Br3	118.3 (3)
C1—C2—Br1	119.8 (3)	C18—C19—Br3	120.2 (3)
C2—C3—C4	119.7 (4)	C19—C20—C21	120.6 (4)
C2—C3—H3	120.2	C19—C20—H20	119.7
C4—C3—H3	120.2	C21—C20—H20	119.7
C5—C4—C3	118.7 (4)	C22—C21—C20	118.5 (4)

C5—C4—C16	120.9 (4)	C22—C21—C33	121.3 (4)
C3—C4—C16	120.4 (4)	C20—C21—C33	120.2 (4)
C4—C5—C6	121.9 (4)	C21—C22—C23	121.3 (4)
C4—C5—H5	119.0	C21—C22—H22	119.3
C6—C5—H5	119.0	C23—C22—H22	119.3
C1—C6—C5	119.2 (4)	C22—C23—C18	119.9 (4)
C1—C6—C7	121.1 (3)	C22—C23—C24	119.6 (3)
C5—C6—C7	119.6 (3)	C18—C23—C24	120.4 (3)
N2—C7—C6	112.5 (3)	N4—C24—C23	112.3 (3)
N2—C7—H7A	109.1	N4—C24—H24A	109.1
C6—C7—H7A	109.1	C23—C24—H24A	109.1
N2—C7—H7B	109.1	N4—C24—H24B	109.1
C6—C7—H7B	109.1	C23—C24—H24B	109.1
H7A—C7—H7B	107.8	H24A—C24—H24B	107.9
C13—C8—C9	117.5 (4)	C26—C25—C30	118.4 (4)
C13—C8—N2	122.0 (4)	C26—C25—N4	119.9 (3)
C9—C8—N2	120.6 (4)	C30—C25—N4	121.7 (3)
C10—C9—C8	122.0 (4)	C27—C26—C25	121.5 (4)
C10—C9—Br2	118.1 (3)	C27—C26—Br4	119.1 (3)
C8—C9—Br2	119.9 (3)	C25—C26—Br4	119.4 (3)
C11—C10—C9	120.3 (4)	C26—C27—C28	120.1 (4)
C11—C10—H10	119.9	C26—C27—H27	119.9
C9—C10—H10	119.9	C28—C27—H27	119.9
C10—C11—C12	118.1 (4)	C27—C28—C29	118.9 (4)
C10—C11—C17	120.9 (4)	C27—C28—C34	120.1 (4)
C12—C11—C17	120.9 (4)	C29—C28—C34	121.0 (4)
C13—C12—C11	121.8 (4)	C30—C29—C28	121.4 (4)
C13—C12—H12	119.1	C30—C29—H29	119.3
C11—C12—H12	119.1	C28—C29—H29	119.3
C12—C13—C8	120.1 (4)	C29—C30—C25	119.6 (4)
C12—C13—C14	119.6 (4)	C29—C30—C31	120.3 (3)
C8—C13—C14	120.2 (4)	C25—C30—C31	120.1 (4)
N1—C14—C13	112.3 (3)	N3—C31—C30	113.2 (3)
N1—C14—H14A	109.1	N3—C31—H31A	108.9
C13—C14—H14A	109.1	C30—C31—H31A	108.9
N1—C14—H14B	109.1	N3—C31—H31B	108.9
C13—C14—H14B	109.1	C30—C31—H31B	108.9
H14A—C14—H14B	107.9	H31A—C31—H31B	107.7
N2—C15—N1	112.4 (3)	N3—C32—N4	112.1 (3)
N2—C15—H15A	109.1	N3—C32—H32A	109.2
N1—C15—H15A	109.1	N4—C32—H32A	109.2
N2—C15—H15B	109.1	N3—C32—H32B	109.2
N1—C15—H15B	109.1	N4—C32—H32B	109.2
H15A—C15—H15B	107.9	H32A—C32—H32B	107.9
C4—C16—H16A	109.5	C21—C33—H33A	109.5
C4—C16—H16B	109.5	C21—C33—H33B	109.5
H16A—C16—H16B	109.5	H33A—C33—H33B	109.5
C4—C16—H16C	109.5	C21—C33—H33C	109.5
H16A—C16—H16C	109.5	H33A—C33—H33C	109.5

H16B—C16—H16C	109.5	H33B—C33—H33C	109.5
C11—C17—H17A	109.5	C28—C34—H34A	109.5
C11—C17—H17B	109.5	C28—C34—H34B	109.5
H17A—C17—H17B	109.5	H34A—C34—H34B	109.5
C11—C17—H17C	109.5	C28—C34—H34C	109.5
H17A—C17—H17C	109.5	H34A—C34—H34C	109.5
H17B—C17—H17C	109.5	H34B—C34—H34C	109.5
C15—N1—C1—C2	−160.4 (4)	C32—N3—C18—C19	161.6 (3)
C14—N1—C1—C2	78.6 (4)	C31—N3—C18—C19	−78.2 (4)
C15—N1—C1—C6	17.9 (5)	C32—N3—C18—C23	−18.5 (5)
C14—N1—C1—C6	−103.0 (4)	C31—N3—C18—C23	101.7 (4)
C6—C1—C2—C3	1.5 (6)	C23—C18—C19—C20	−2.7 (6)
N1—C1—C2—C3	179.9 (3)	N3—C18—C19—C20	177.3 (3)
C6—C1—C2—Br1	−176.5 (3)	C23—C18—C19—Br3	172.6 (3)
N1—C1—C2—Br1	1.9 (5)	N3—C18—C19—Br3	−7.5 (5)
C1—C2—C3—C4	−1.0 (6)	C18—C19—C20—C21	2.2 (6)
Br1—C2—C3—C4	176.9 (3)	Br3—C19—C20—C21	−173.1 (3)
C2—C3—C4—C5	−0.7 (6)	C19—C20—C21—C22	0.8 (6)
C2—C3—C4—C16	177.8 (4)	C19—C20—C21—C33	−177.4 (4)
C3—C4—C5—C6	2.1 (6)	C20—C21—C22—C23	−3.3 (6)
C16—C4—C5—C6	−176.5 (4)	C33—C21—C22—C23	174.8 (4)
C2—C1—C6—C5	−0.1 (5)	C21—C22—C23—C18	2.8 (6)
N1—C1—C6—C5	−178.5 (3)	C21—C22—C23—C24	−175.5 (4)
C2—C1—C6—C7	−178.8 (3)	C19—C18—C23—C22	0.2 (5)
N1—C1—C6—C7	2.8 (5)	N3—C18—C23—C22	−179.8 (3)
C4—C5—C6—C1	−1.6 (6)	C19—C18—C23—C24	178.5 (3)
C4—C5—C6—C7	177.1 (4)	N3—C18—C23—C24	−1.4 (5)
C8—N2—C7—C6	77.8 (4)	C25—N4—C24—C23	−77.5 (4)
C15—N2—C7—C6	−44.1 (4)	C32—N4—C24—C23	45.1 (4)
C1—C6—C7—N2	11.2 (5)	C22—C23—C24—N4	165.7 (3)
C5—C6—C7—N2	−167.5 (3)	C18—C23—C24—N4	−12.7 (5)
C15—N2—C8—C13	19.4 (5)	C32—N4—C25—C26	159.8 (3)
C7—N2—C8—C13	−100.8 (4)	C24—N4—C25—C26	−79.4 (4)
C15—N2—C8—C9	−160.6 (3)	C32—N4—C25—C30	−19.0 (5)
C7—N2—C8—C9	79.3 (4)	C24—N4—C25—C30	101.8 (4)
C13—C8—C9—C10	4.4 (6)	C30—C25—C26—C27	−3.4 (6)
N2—C8—C9—C10	−175.6 (4)	N4—C25—C26—C27	177.8 (3)
C13—C8—C9—Br2	−176.1 (3)	C30—C25—C26—Br4	174.6 (3)
N2—C8—C9—Br2	3.9 (5)	N4—C25—C26—Br4	−4.3 (5)
C8—C9—C10—C11	−1.8 (6)	C25—C26—C27—C28	2.2 (6)
Br2—C9—C10—C11	178.7 (3)	Br4—C26—C27—C28	−175.8 (3)
C9—C10—C11—C12	−2.6 (6)	C26—C27—C28—C29	1.1 (6)
C9—C10—C11—C17	174.5 (4)	C26—C27—C28—C34	−179.0 (4)
C10—C11—C12—C13	4.3 (6)	C27—C28—C29—C30	−3.2 (6)
C17—C11—C12—C13	−172.8 (4)	C34—C28—C29—C30	176.9 (4)
C11—C12—C13—C8	−1.7 (6)	C28—C29—C30—C25	2.0 (6)
C11—C12—C13—C14	176.3 (3)	C28—C29—C30—C31	−176.5 (4)
C9—C8—C13—C12	−2.7 (6)	C26—C25—C30—C29	1.3 (5)
N2—C8—C13—C12	177.4 (3)	N4—C25—C30—C29	−179.9 (3)

C9—C8—C13—C14	179.4 (3)	C26—C25—C30—C31	179.8 (3)
N2—C8—C13—C14	−0.5 (6)	N4—C25—C30—C31	−1.3 (5)
C1—N1—C14—C13	76.9 (4)	C18—N3—C31—C30	−77.8 (4)
C15—N1—C14—C13	−45.8 (4)	C32—N3—C31—C30	44.2 (4)
C12—C13—C14—N1	−163.5 (3)	C29—C30—C31—N3	166.5 (3)
C8—C13—C14—N1	14.5 (5)	C25—C30—C31—N3	−12.0 (5)
C8—N2—C15—N1	−54.2 (4)	C18—N3—C32—N4	54.5 (4)
C7—N2—C15—N1	68.9 (4)	C31—N3—C32—N4	−68.2 (4)
C1—N1—C15—N2	−54.8 (4)	C25—N4—C32—N3	54.7 (4)
C14—N1—C15—N2	68.9 (4)	C24—N4—C32—N3	−69.1 (4)

Fig. 1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C26
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C18
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Br3
C22
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C29
C21
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C13
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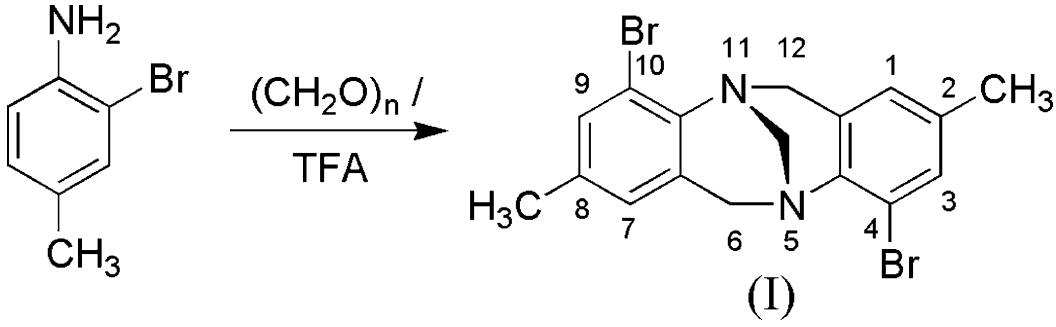
C10
Br2

Fig. 2



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