# organic compounds

# 6H,12H-5,11-Methanodibenzo[b,f]-[1,5]diazocine

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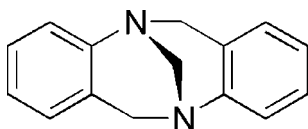Correspondence e-mail: andrew.try@mq.edu.au

In the molecule of the title compound, $C_{15}H_{14}N_2$, the unsubstituted analogue of Tröger's base, the two aromatic rings are offset with respect to one another. The dihedral angle between the two benzene rings is 95.42 (4)°.

## Related literature

For general background, see: Solano *et al.* (2005); Allen *et al.* (1987); Cremer & Pople (1975). For related literature, see: Pardo *et al.* (2006); Faroughi *et al.* (2006a,b); Faroughi *et al.* (2007); Cooper & Partridge (1955); Li *et al.* (2005); Jensen *et al.* (2002).



## Experimental

### Crystal data

$C_{15}H_{14}N_2$
$M_r$ = 222.28
Monoclinic, $P2_1/c$
$a$ = 12.266 (2) Å
$b$ = 7.362 (1) Å
$c$ = 12.759 (2) Å
$\beta$ = 104.457 (2)°

$V$ = 1115.7 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 150 (2) K
$0.50 \times 0.50 \times 0.42$ mm

### Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: integration [Gaussian (Coppens *et al.*, 1965) and *XPREP* (Siemens, 1995)]
$T_{min}$ = 0.964, $T_{max}$ = 0.976

10679 measured reflections
2701 independent reflections
2297 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.038

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.106
$S$ = 1.06
2701 reflections

154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001) and *SHELXTL* (Bruker, 2003); software used to prepare material for publication: *modiCIFer* (Guzei, 2005).

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**supplementary materials**

## 6*H*,12*H*-5,11-Methanodibenzo[*b*,*f*][1,5]diazocine

**M. Faroughi, P. Jensen and A. C. Try**

### Comment

Tröger's base analogues are chiral, cavity-containing compounds with a V-shaped structure where two aromatic rings define the walls of the cavity. An important feature of all Tröger's base analogues is the methano-strapped diazocine bridge that 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 to lie between 82° (Solano *et al.*, 2005) and 108.44 (4)° (Faroughi *et al.*, 2006*b*) for simple dibenzo Tröger's base analogues, and is dependent upon the nature of the substituents on the aromatic rings. We have previously reported that the dihedral angles in 2,8-Dichloro and 2,8-dibromo Tröger's bases are 95.64 (3)° (Faroughi *et al.*, 2007) and 94.45 (4)° (Faroughi *et al.*, 2006*a*), respectively, and now report that the title compound, (I), has a very similar structure. Compound (I) is devoid of any substitutents and in the minimum energy conformation, the dihedral angle of this compound was calculated to be 101.33 ° (Pardo *et al.*, 2006).

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 hydrogenolysis of the 2,8-dibromo analogue.

In the molecule of the title compound, (I), (Fig. 1) the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings B (N1/N2/C1/C6—C8) and C (N1/N2/C8/C9/C14/C15) are not planar, having total puckering amplitudes, $Q_T$, of 1.395 (3) and 0.668 (3) Å, respectively and twist conformations $\varphi = -116.62\ (3)°$, $\theta = 109.90\ (2)°$ and $\varphi = -51.67\ (3)°$, $\theta = 113.44\ (3)°$ (Cremer & Pople, 1975). Rings A (C1—C6) and D (C9—C14) are, of course, planar and the dihedral angle between them is 95.42 (4)°.

### Experimental

2,8-Dibromo-6*H*,12*H*-5,11-methanodibenzo[*b*,*f*][1,5] diazocine (5.0 g, 13.16 mmol) was dissolved in absolute ethanol (750 ml) and dichloromethane (200 ml). Palladium, 10 wt. % on activated carbon (0.2 g) was added and the mixture was stirred under hydrogen atmosphere in the dark for 7 d. The reaction mixture was washed through celite, evaporated to dryness to afford a pale yellow solid. The solid was dissolved in dichloromethane (450 ml), basified with sodium hydrogen carbonate (2 *x* 400 ml). The mixture was extracted into dichloromethane (2 *x* 100 ml). The combined organic layers were washed with brine (100 ml), dried over anhydrous sodium sulfate, filtered and evaporated to dryness to afford the title compound (yield; 2.86 g, 98%) as a white solid. No further purification was needed: m.p. 413.62 K (DSC) (411–412 K (Cooper & Partridge, 1955), 403–404 K (Li *et al.*, 2005), 409.5–410 K (Jensen *et al.*, 2002). Single crystals of (I) were produced from slow evaporation of a dichloromethane solution.

### Refinement

H atoms were positioned geometrically, with C—H = 0.95 and 0.99 Å for aromatic and methylene H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.
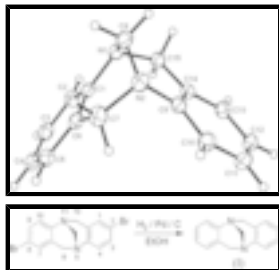
# supplementary materials

## Figures



Fig. 1. The molecular structure of (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

## 6*H*,12*H*-5,11-Methanodibenzo[*b*,*f*][1,5]diazocine

*Crystal data*

| | |
|---|---|
| $C_{15}H_{14}N_2$ | $F_{000} = 472$ |
| $M_r = 222.28$ | $D_x = 1.323$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Melting point: 413 K |
| Hall symbol: -P 2ybc | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 12.266$ (2) Å | Cell parameters from 6144 reflections |
| $b = 7.362$ (1) Å | $\theta = 3.2–28.4º$ |
| $c = 12.759$ (2) Å | $\mu = 0.08$ mm$^{-1}$ |
| $\beta = 104.457$ (2)º | $T = 150$ (2) K |
| $V = 1115.7$ (3) Å$^3$ | Prism, colorless |
| $Z = 4$ | $0.50 \times 0.50 \times 0.42$ mm |

*Data collection*

| | |
|---|---|
| Bruker SMART 1000 CCD area-detector diffractometer | 2701 independent reflections |
| Radiation source: fine-focus sealed tube | 2297 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.038$ |
| $T = 150(2)$ K | $\theta_{max} = 28.4º$ |
| $\omega$ scans | $\theta_{min} = 1.7º$ |
| Absorption correction: integration [Gaussian (Coppens *et al.*, 1965) and XPREP (Siemens, 1995)] | $h = -16 \rightarrow 16$ |
| $T_{min} = 0.964$, $T_{max} = 0.976$ | $k = -9 \rightarrow 9$ |
| 10679 measured reflections | $l = -16 \rightarrow 16$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | H-atom parameters constrained |

$wR(F^2) = 0.106$

$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.3391P]$

where $P = (F_o^2 + 2F_c^2)/3$

$S = 1.06$

$(\Delta/\sigma)_{max} < 0.001$

2701 reflections

$\Delta\rho_{max} = 0.32$ e Å$^{-3}$

154 parameters

$\Delta\rho_{min} = -0.15$ 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  | 0.18891 (7) | 0.28087 (13) | −0.03028 (7) | 0.0219 (2) |
| N2  | 0.26653 (8) | 0.18258 (13) | 0.15515 (7) | 0.0235 (2) |
| C1  | 0.15935 (8) | 0.09549 (15) | −0.05815 (8) | 0.0201 (2) |
| C2  | 0.12619 (9) | 0.04813 (16) | −0.16752 (9) | 0.0239 (2) |
| H2  | 0.1245 | 0.1383 | −0.2212 | 0.029* |
| C3  | 0.09587 (9) | −0.12837 (17) | −0.19852 (9) | 0.0280 (3) |
| H3  | 0.0740 | −0.1591 | −0.2732 | 0.034* |
| C4  | 0.09733 (9) | −0.26109 (16) | −0.12057 (10) | 0.0286 (3) |
| H4  | 0.0766 | −0.3826 | −0.1415 | 0.034* |
| C5  | 0.12936 (9) | −0.21395 (16) | −0.01225 (10) | 0.0263 (2) |
| H5  | 0.1288 | −0.3041 | 0.0409 | 0.032* |
| C6  | 0.16238 (8) | −0.03768 (15) | 0.02097 (9) | 0.0216 (2) |
| C7  | 0.20637 (9) | 0.00762 (16) | 0.13997 (9) | 0.0257 (2) |
| H7A | 0.1426 | 0.0132 | 0.1745 | 0.031* |
| H7B | 0.2580 | −0.0898 | 0.1759 | 0.031* |
| C8  | 0.19490 (9) | 0.31378 (16) | 0.08392 (9) | 0.0250 (2) |
| H8A | 0.2245 | 0.4376 | 0.1034 | 0.030* |
| H8B | 0.1181 | 0.3080 | 0.0953 | 0.030* |
| C9  | 0.37554 (9) | 0.17298 (15) | 0.13212 (8) | 0.0213 (2) |
| C10 | 0.46315 (9) | 0.08515 (16) | 0.20605 (9) | 0.0262 (2) |
| H10 | 0.4491 | 0.0277 | 0.2681 | 0.031* |
| C11 | 0.57021 (10) | 0.08172 (17) | 0.18908 (10) | 0.0294 (3) |
| H11 | 0.6292 | 0.0203 | 0.2390 | 0.035* |
| C12 | 0.59195 (9) | 0.16755 (17) | 0.09953 (10) | 0.0285 (3) |
| H12 | 0.6661 | 0.1691 | 0.0895 | 0.034* |

| | | | | |
|---|---|---|---|---|
| C13 | 0.50467 (10) | 0.25091 (15) | 0.02499 (9) | 0.0252 (2) |
| H13 | 0.5194 | 0.3079 | −0.0368 | 0.030* |
| C14 | 0.39554 (9) | 0.25259 (14) | 0.03911 (9) | 0.0211 (2) |
| C15 | 0.29950 (9) | 0.33096 (15) | −0.04816 (9) | 0.0236 (2) |
| H15A | 0.3063 | 0.4649 | −0.0485 | 0.028* |
| H15B | 0.3047 | 0.2854 | −0.1198 | 0.028* |

*Atomic displacement parameters ($Å^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0195 (4) | 0.0218 (5) | 0.0237 (4) | 0.0013 (3) | 0.0043 (3) | 0.0017 (3) |
| N2 | 0.0222 (5) | 0.0278 (5) | 0.0210 (4) | 0.0018 (4) | 0.0060 (3) | −0.0004 (4) |
| C1 | 0.0140 (4) | 0.0230 (5) | 0.0235 (5) | 0.0017 (4) | 0.0050 (4) | 0.0007 (4) |
| C2 | 0.0191 (5) | 0.0295 (6) | 0.0224 (5) | 0.0020 (4) | 0.0038 (4) | 0.0023 (4) |
| C3 | 0.0206 (5) | 0.0356 (6) | 0.0265 (5) | 0.0005 (5) | 0.0032 (4) | −0.0069 (5) |
| C4 | 0.0194 (5) | 0.0254 (6) | 0.0400 (7) | −0.0016 (4) | 0.0055 (4) | −0.0056 (5) |
| C5 | 0.0207 (5) | 0.0251 (6) | 0.0336 (6) | −0.0001 (4) | 0.0077 (4) | 0.0049 (5) |
| C6 | 0.0161 (5) | 0.0256 (5) | 0.0239 (5) | 0.0009 (4) | 0.0064 (4) | 0.0020 (4) |
| C7 | 0.0254 (5) | 0.0304 (6) | 0.0223 (5) | −0.0017 (4) | 0.0081 (4) | 0.0042 (4) |
| C8 | 0.0223 (5) | 0.0264 (6) | 0.0260 (5) | 0.0041 (4) | 0.0057 (4) | −0.0032 (4) |
| C9 | 0.0205 (5) | 0.0212 (5) | 0.0215 (5) | 0.0005 (4) | 0.0040 (4) | −0.0030 (4) |
| C10 | 0.0276 (6) | 0.0273 (6) | 0.0217 (5) | 0.0018 (4) | 0.0025 (4) | 0.0013 (4) |
| C11 | 0.0234 (5) | 0.0287 (6) | 0.0317 (6) | 0.0045 (5) | −0.0014 (4) | 0.0001 (5) |
| C12 | 0.0188 (5) | 0.0276 (6) | 0.0387 (6) | 0.0004 (4) | 0.0063 (5) | −0.0028 (5) |
| C13 | 0.0231 (5) | 0.0236 (6) | 0.0296 (6) | −0.0026 (4) | 0.0078 (4) | 0.0001 (4) |
| C14 | 0.0202 (5) | 0.0183 (5) | 0.0237 (5) | −0.0003 (4) | 0.0034 (4) | −0.0009 (4) |
| C15 | 0.0210 (5) | 0.0233 (5) | 0.0256 (5) | −0.0015 (4) | 0.0041 (4) | 0.0051 (4) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N1—C1 | 1.4340 (14) | C7—H7A | 0.9900 |
| N1—C8 | 1.4607 (14) | C7—H7B | 0.9900 |
| N1—C15 | 1.4774 (13) | C8—H8A | 0.9900 |
| N2—C9 | 1.4406 (13) | C8—H8B | 0.9900 |
| N2—C8 | 1.4602 (14) | C9—C10 | 1.3988 (15) |
| N2—C7 | 1.4730 (15) | C9—C14 | 1.3990 (15) |
| C1—C2 | 1.3967 (15) | C10—C11 | 1.3835 (16) |
| C1—C6 | 1.4010 (15) | C10—H10 | 0.9500 |
| C2—C3 | 1.3819 (17) | C11—C12 | 1.3885 (17) |
| C2—H2 | 0.9500 | C11—H11 | 0.9500 |
| C3—C4 | 1.3911 (18) | C12—C13 | 1.3853 (16) |
| C3—H3 | 0.9500 | C12—H12 | 0.9500 |
| C4—C5 | 1.3834 (17) | C13—C14 | 1.3945 (15) |
| C4—H4 | 0.9500 | C13—H13 | 0.9500 |
| C5—C6 | 1.3936 (16) | C14—C15 | 1.5184 (14) |
| C5—H5 | 0.9500 | C15—H15A | 0.9900 |
| C6—C7 | 1.5161 (15) | C15—H15B | 0.9900 |
| C1—N1—C8 | 110.60 (9) | N2—C8—N1 | 112.56 (9) |

| | | | |
|---|---|---|---|
| C1—N1—C15 | 112.60 (8) | N2—C8—H8A | 109.1 |
| C8—N1—C15 | 107.05 (8) | N1—C8—H8A | 109.1 |
| C9—N2—C8 | 110.51 (9) | N2—C8—H8B | 109.1 |
| C9—N2—C7 | 112.97 (9) | N1—C8—H8B | 109.1 |
| C8—N2—C7 | 107.02 (9) | H8A—C8—H8B | 107.8 |
| C2—C1—C6 | 119.60 (10) | C10—C9—C14 | 119.85 (10) |
| C2—C1—N1 | 118.55 (9) | C10—C9—N2 | 118.75 (10) |
| C6—C1—N1 | 121.85 (9) | C14—C9—N2 | 121.38 (9) |
| C3—C2—C1 | 120.74 (10) | C11—C10—C9 | 120.16 (11) |
| C3—C2—H2 | 119.6 | C11—C10—H10 | 119.9 |
| C1—C2—H2 | 119.6 | C9—C10—H10 | 119.9 |
| C2—C3—C4 | 120.08 (11) | C10—C11—C12 | 120.34 (10) |
| C2—C3—H3 | 120.0 | C10—C11—H11 | 119.8 |
| C4—C3—H3 | 120.0 | C12—C11—H11 | 119.8 |
| C5—C4—C3 | 119.20 (11) | C13—C12—C11 | 119.50 (10) |
| C5—C4—H4 | 120.4 | C13—C12—H12 | 120.3 |
| C3—C4—H4 | 120.4 | C11—C12—H12 | 120.3 |
| C4—C5—C6 | 121.73 (11) | C12—C13—C14 | 121.16 (10) |
| C4—C5—H5 | 119.1 | C12—C13—H13 | 119.4 |
| C6—C5—H5 | 119.1 | C14—C13—H13 | 119.4 |
| C5—C6—C1 | 118.62 (10) | C13—C14—C9 | 118.89 (10) |
| C5—C6—C7 | 120.88 (10) | C13—C14—C15 | 120.17 (9) |
| C1—C6—C7 | 120.43 (10) | C9—C14—C15 | 120.86 (9) |
| N2—C7—C6 | 111.43 (9) | N1—C15—C14 | 111.48 (9) |
| N2—C7—H7A | 109.3 | N1—C15—H15A | 109.3 |
| C6—C7—H7A | 109.3 | C14—C15—H15A | 109.3 |
| N2—C7—H7B | 109.3 | N1—C15—H15B | 109.3 |
| C6—C7—H7B | 109.3 | C14—C15—H15B | 109.3 |
| H7A—C7—H7B | 108.0 | H15A—C15—H15B | 108.0 |
| C8—N1—C1—C2 | 166.47 (9) | C1—N1—C8—N2 | 51.79 (12) |
| C15—N1—C1—C2 | −73.82 (11) | C15—N1—C8—N2 | −71.21 (11) |
| C8—N1—C1—C6 | −13.21 (13) | C8—N2—C9—C10 | 166.53 (10) |
| C15—N1—C1—C6 | 106.51 (11) | C7—N2—C9—C10 | −73.59 (12) |
| C6—C1—C2—C3 | 0.29 (15) | C8—N2—C9—C14 | −12.12 (14) |
| N1—C1—C2—C3 | −179.39 (9) | C7—N2—C9—C14 | 107.76 (11) |
| C1—C2—C3—C4 | 0.47 (16) | C14—C9—C10—C11 | 2.00 (16) |
| C2—C3—C4—C5 | 0.02 (16) | N2—C9—C10—C11 | −176.68 (10) |
| C3—C4—C5—C6 | −1.30 (16) | C9—C10—C11—C12 | 0.95 (18) |
| C4—C5—C6—C1 | 2.04 (16) | C10—C11—C12—C13 | −2.43 (18) |
| C4—C5—C6—C7 | −174.88 (10) | C11—C12—C13—C14 | 0.98 (17) |
| C2—C1—C6—C5 | −1.51 (15) | C12—C13—C14—C9 | 1.92 (16) |
| N1—C1—C6—C5 | 178.16 (9) | C12—C13—C14—C15 | −174.93 (10) |
| C2—C1—C6—C7 | 175.42 (9) | C10—C9—C14—C13 | −3.39 (15) |
| N1—C1—C6—C7 | −4.91 (15) | N2—C9—C14—C13 | 175.25 (10) |
| C9—N2—C7—C6 | −73.65 (11) | C10—C9—C14—C15 | 173.43 (10) |
| C8—N2—C7—C6 | 48.21 (11) | N2—C9—C14—C15 | −7.93 (15) |
| C5—C6—C7—N2 | 163.19 (9) | C1—N1—C15—C14 | −75.25 (11) |
| C1—C6—C7—N2 | −13.68 (13) | C8—N1—C15—C14 | 46.50 (11) |
| C9—N2—C8—N1 | 52.38 (12) | C13—C14—C15—N1 | 166.32 (9) |

| C7—N2—C8—N1 | −71.01 (11) | C9—C14—C15—N1 | −10.46 (14) |

**Fig. 1**

**Fig. 2**



(I)