

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Editors: W. Clegg and D. G. Watson

2,8-Dichloro-6*H*,12*H*-5,11-ethanodibenzo[*b,f*][1,5]diazocine

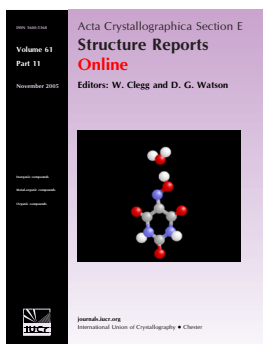
Masoud Faroughi, Andrew C. Try and Peter Turner

Acta Cryst. (2008). E64, o39

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2,8-Dichloro-6H,12H-5,11-ethano-dibenzo[*b,f*][1,5]diazocineMasoud Faroughi,^a Andrew C. Try^{a*} and Peter Turner^b^aDepartment of Chemistry and Biomolecular Sciences, Building F7B, Macquarie University, NSW 2109, Australia, and ^bCrystal Structure Analysis Facility, School of Chemistry, F11, The University of Sydney, NSW 2006, Australia

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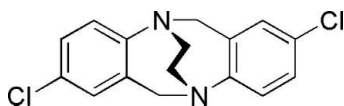
Received 23 November 2007; accepted 23 November 2007

Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.031; wR factor = 0.089; data-to-parameter ratio = 17.6.

In the molecule of the title compound, $\text{C}_{16}\text{H}_{14}\text{Cl}_2\text{N}_2$, the ethano-strapped 2,8-dichloro analogue of Tröger's base, the dihedral angle between the two benzene rings is $87.01(3)^\circ$.

Related literature

For related literature, see: Tröger (1887); Hamada & Mukai (1996); Ishida *et al.* (2005). For related structures, see: Spielman (1935); Larson & Wilcox (1986); Solano *et al.* (2005); Faroughi *et al.* (2006a,b); Faroughi, Try, Klepetko & Turner (2007); Faroughi, Try & Turner (2007).



Experimental

Crystal data

$\text{C}_{16}\text{H}_{14}\text{Cl}_2\text{N}_2$
 $M_r = 305.19$
 Triclinic, $P\bar{1}$
 $a = 6.8801(11)$ Å
 $b = 10.1951(17)$ Å
 $c = 10.2466(16)$ Å
 $\alpha = 85.320(3)^\circ$
 $\beta = 84.956(2)^\circ$

$\gamma = 76.470(3)^\circ$
 $V = 694.70(19)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.46$ mm⁻¹
 $T = 150(2)$ K
 $0.63 \times 0.44 \times 0.41$ mm

Data collection

Bruker SMART 1000 CCD diffractometer
 Absorption correction: Gaussian (*XPREP*; Coppens *et al.*, 1965; Siemens, 1995)
 $T_{\min} = 0.773$, $T_{\max} = 0.869$

6876 measured reflections
 3188 independent reflections
 2992 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.089$
 $S = 1.06$
 3188 reflections

181 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.34$ e Å⁻³
 $\Delta\rho_{\min} = -0.27$ e Å⁻³

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT* and *XPREP* (Siemens, 1995); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *Xtal3.6* (Hall *et al.*, 1999), *ORTEPII* (Johnson, 1976) and *WinGX* (Farrugia, 1999); software used to prepare material for publication: *WinGX*.

The authors thank the Australian Research Council for a Discovery Project grant to ACT (grant No. DP0345180) and Macquarie University for the award of a Macquarie University Research Development grant.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2402).

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supplementary materials

Acta Cryst. (2008). E64, o39 [doi:10.1107/S1600536807062642]

2,8-Dichloro-6*H*,12*H*-5,11-ethanodibenzo[*b,f*][1,5]diazocine

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

Comment

Tröger's base was first prepared in 1887 (Tröger, 1887) and its structure was elucidated until over 30 years latter (Spielman, 1935). The structural assignment was confirmed by X-ray crystallography (Larson & Wilcox, 1986). Since then large number of related compounds have been reported and the dihedral angle, between the least-squares planes through the aromatic rings, has been measured across a range of simple dibenzo Tröger's base analogues and found to lie between 82° (Solano *et al.*, 2005) and 108° (Faroughi *et al.*, 2006*b*). A common structural feature in all of these compounds is the methano-strapped diazocine bridge. The conversion of methano-strapped compounds to ethano-strapped analogues of Tröger's base have been reported for 2,8-dimethyl- and 2,8-dimethoxy- (Hamada & Mukai, 1996) as well as 2,8-dibromo- (Ishida *et al.*, 2005; Faroughi, Try, Klepetko & Turner, 2007) substitution patterns. We have previously reported that the dihedral angle in methano-strapped 2,8-dibromo Tröger's base is 94.5° (Faroughi *et al.*, 2006*a*) whilst the corresponding angle in the ethano-strapped 2,8-dibromo analogue is 86.1° (Faroughi, Try, Klepetko & Turner, 2007). In the present case, the dihedral angle of ethano-strapped 2,8-dichloro Tröger's base (I), whose molecular structure is shown in Fig. 1, was also found to be reduced [87.01 (3)°] in comparison with the methano-strapped analogue, which has a dihedral angle of 95.6° (Faroughi, Try & Turner *et al.*, 2007).

Experimental

The title compound was prepared according to the literature procedure (Hamada & Mukai, 1996) in 72% yield. 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 $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

- Fig. 1. View of (I), showing the atomic numbering scheme. Displacement ellipsoids are shown at the 50% probability level.
- Fig. 2. Synthetic scheme for the synthesis of (I) showing the numbering system used in naming the compound.

2,8-Dichloro-6*H*,12*H*-5,11-ethanodibenzo[*b,f*][1,5]diazocine

Crystal data

C₁₆H₁₄Cl₂N₂

Z = 2

supplementary materials

$M_r = 305.19$	$F_{000} = 316$
Triclinic, $P\bar{1}$	$D_x = 1.459 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Melting point: 454-455 K
$a = 6.8801 (11) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 10.1951 (17) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$c = 10.2466 (16) \text{ \AA}$	Cell parameters from 925 reflections
$\alpha = 85.320 (3)^\circ$	$\theta = 3.5\text{--}27.9^\circ$
$\beta = 84.956 (2)^\circ$	$\mu = 0.46 \text{ mm}^{-1}$
$\gamma = 76.470 (3)^\circ$	$T = 150 (2) \text{ K}$
$V = 694.70 (19) \text{ \AA}^3$	Prism, colorless
	$0.63 \times 0.44 \times 0.41 \text{ mm}$

Data collection

Bruker SMART 1000 CCD diffractometer	3188 independent reflections
Radiation source: fine-focus sealed tube	2992 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.033$
$T = 150(2) \text{ K}$	$\theta_{\text{max}} = 28.3^\circ$
ω scans	$\theta_{\text{min}} = 2.0^\circ$
Absorption correction: Gaussian (XPREP; Coppens <i>et al.</i> , 1965; Siemens, 1995)	$h = -8 \rightarrow 9$
$T_{\text{min}} = 0.773$, $T_{\text{max}} = 0.869$	$k = -13 \rightarrow 13$
6876 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.031$	H-atom parameters constrained
$wR(F^2) = 0.089$	$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 0.1729P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
3188 reflections	$(\Delta/\sigma)_{\text{max}} = 0.002$
181 parameters	$\Delta\rho_{\text{max}} = 0.34 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.27 \text{ e \AA}^{-3}$
	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 $F^2 > 2\sigma(F^2)$ is used only for calculat-

ing 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	-0.33151 (5)	0.87520 (3)	1.11085 (3)	0.03317 (10)
Cl2	0.19414 (5)	1.02485 (3)	0.31142 (3)	0.03303 (10)
N1	0.43135 (15)	0.61940 (11)	0.81861 (11)	0.0288 (2)
N2	0.19355 (15)	0.52439 (10)	0.65450 (10)	0.0249 (2)
C1	0.24125 (17)	0.67773 (12)	0.88354 (11)	0.0256 (2)
C2	0.23827 (19)	0.77730 (13)	0.96964 (13)	0.0300 (3)
H2	0.3590	0.8039	0.9806	0.036*
C3	0.0642 (2)	0.83825 (12)	1.03940 (12)	0.0297 (3)
H3	0.0645	0.9057	1.0981	0.036*
C4	-0.11108 (18)	0.79898 (12)	1.02196 (11)	0.0261 (2)
C5	-0.11437 (17)	0.70205 (12)	0.93531 (11)	0.0242 (2)
H5	-0.2366	0.6777	0.9238	0.029*
C6	0.06195 (17)	0.64005 (11)	0.86481 (11)	0.0231 (2)
C7	0.04879 (17)	0.53679 (12)	0.76854 (11)	0.0247 (2)
H7A	0.0654	0.4472	0.8169	0.030*
H7B	-0.0876	0.5605	0.7367	0.030*
C8	0.19502 (17)	0.64895 (11)	0.57911 (11)	0.0229 (2)
C9	0.05736 (18)	0.68840 (12)	0.48295 (11)	0.0250 (2)
H9	-0.0354	0.6346	0.4732	0.030*
C10	0.05307 (18)	0.80449 (12)	0.40135 (11)	0.0267 (2)
H10	-0.0423	0.8310	0.3370	0.032*
C11	0.19158 (18)	0.88103 (12)	0.41608 (11)	0.0256 (2)
C12	0.32586 (18)	0.84588 (12)	0.51236 (12)	0.0265 (2)
H12	0.4170	0.9009	0.5220	0.032*
C13	0.32901 (17)	0.73018 (12)	0.59568 (11)	0.0250 (2)
C14	0.48177 (18)	0.69776 (14)	0.69929 (13)	0.0317 (3)
H14A	0.6103	0.6474	0.6582	0.038*
H14B	0.5042	0.7841	0.7254	0.038*
C15	0.47175 (18)	0.47337 (13)	0.80467 (13)	0.0324 (3)
H15A	0.4103	0.4303	0.8826	0.039*
H15B	0.6183	0.4358	0.8017	0.039*
C16	0.39027 (19)	0.43836 (13)	0.68131 (13)	0.0319 (3)
H16A	0.4863	0.4477	0.6052	0.038*
H16B	0.3797	0.3428	0.6914	0.038*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.03691 (18)	0.03002 (17)	0.03158 (17)	-0.00488 (12)	-0.00344 (12)	-0.00303 (12)
Cl2	0.0492 (2)	0.02418 (16)	0.02644 (16)	-0.01157 (13)	-0.00413 (12)	0.00531 (11)
N1	0.0231 (5)	0.0311 (5)	0.0321 (5)	-0.0078 (4)	-0.0082 (4)	0.0091 (4)
N2	0.0270 (5)	0.0203 (5)	0.0266 (5)	-0.0053 (4)	-0.0019 (4)	0.0024 (4)

supplementary materials

C1	0.0256 (5)	0.0257 (6)	0.0264 (5)	-0.0078 (4)	-0.0101 (4)	0.0080 (4)
C2	0.0314 (6)	0.0291 (6)	0.0333 (6)	-0.0125 (5)	-0.0160 (5)	0.0065 (5)
C3	0.0403 (7)	0.0237 (6)	0.0279 (6)	-0.0100 (5)	-0.0145 (5)	0.0035 (4)
C4	0.0316 (6)	0.0228 (5)	0.0231 (5)	-0.0051 (4)	-0.0069 (4)	0.0042 (4)
C5	0.0269 (5)	0.0242 (5)	0.0232 (5)	-0.0094 (4)	-0.0072 (4)	0.0047 (4)
C6	0.0264 (5)	0.0219 (5)	0.0223 (5)	-0.0085 (4)	-0.0075 (4)	0.0055 (4)
C7	0.0261 (5)	0.0239 (5)	0.0258 (5)	-0.0097 (4)	-0.0039 (4)	0.0020 (4)
C8	0.0253 (5)	0.0198 (5)	0.0231 (5)	-0.0048 (4)	-0.0006 (4)	0.0001 (4)
C9	0.0291 (5)	0.0244 (6)	0.0231 (5)	-0.0089 (4)	-0.0026 (4)	-0.0028 (4)
C10	0.0326 (6)	0.0266 (6)	0.0213 (5)	-0.0064 (5)	-0.0058 (4)	-0.0006 (4)
C11	0.0333 (6)	0.0203 (5)	0.0222 (5)	-0.0060 (4)	0.0001 (4)	0.0011 (4)
C12	0.0277 (5)	0.0252 (6)	0.0277 (6)	-0.0096 (4)	-0.0012 (4)	0.0009 (4)
C13	0.0235 (5)	0.0254 (6)	0.0262 (5)	-0.0064 (4)	-0.0033 (4)	0.0019 (4)
C14	0.0240 (5)	0.0366 (7)	0.0358 (7)	-0.0120 (5)	-0.0081 (5)	0.0104 (5)
C15	0.0252 (6)	0.0308 (6)	0.0376 (7)	-0.0019 (5)	-0.0051 (5)	0.0099 (5)
C16	0.0311 (6)	0.0236 (6)	0.0367 (6)	-0.0012 (5)	0.0003 (5)	0.0053 (5)

Geometric parameters (\AA , $^\circ$)

C11—C4	1.7477 (13)	C7—H7B	0.9900
C12—C11	1.7471 (12)	C8—C9	1.3968 (16)
N1—C1	1.4334 (16)	C8—C13	1.4043 (16)
N1—C15	1.4657 (17)	C9—C10	1.3882 (17)
N1—C14	1.4659 (16)	C9—H9	0.9500
N2—C8	1.4332 (14)	C10—C11	1.3901 (17)
N2—C7	1.4608 (15)	C10—H10	0.9500
N2—C16	1.4653 (16)	C11—C12	1.3795 (17)
C1—C2	1.3937 (18)	C12—C13	1.3956 (16)
C1—C6	1.4077 (15)	C12—H12	0.9500
C2—C3	1.3802 (19)	C13—C14	1.5223 (16)
C2—H2	0.9500	C14—H14A	0.9900
C3—C4	1.3865 (17)	C14—H14B	0.9900
C3—H3	0.9500	C15—C16	1.5269 (19)
C4—C5	1.3866 (17)	C15—H15A	0.9900
C5—C6	1.3980 (17)	C15—H15B	0.9900
C5—H5	0.9500	C16—H16A	0.9900
C6—C7	1.5230 (16)	C16—H16B	0.9900
C7—H7A	0.9900		
C1—N1—C15	115.51 (10)	C10—C9—C8	121.47 (11)
C1—N1—C14	113.66 (10)	C10—C9—H9	119.3
C15—N1—C14	114.24 (11)	C8—C9—H9	119.3
C8—N2—C7	114.43 (9)	C9—C10—C11	118.43 (11)
C8—N2—C16	115.99 (9)	C9—C10—H10	120.8
C7—N2—C16	113.67 (9)	C11—C10—H10	120.8
C2—C1—C6	119.43 (11)	C12—C11—C10	121.14 (11)
C2—C1—N1	116.75 (10)	C12—C11—C12	119.53 (9)
C6—C1—N1	123.82 (11)	C10—C11—C12	119.33 (9)
C3—C2—C1	121.62 (11)	C11—C12—C13	120.58 (11)
C3—C2—H2	119.2	C11—C12—H12	119.7

C1—C2—H2	119.2	C13—C12—H12	119.7
C2—C3—C4	118.57 (11)	C12—C13—C8	119.04 (10)
C2—C3—H3	120.7	C12—C13—C14	117.56 (10)
C4—C3—H3	120.7	C8—C13—C14	123.39 (10)
C3—C4—C5	121.36 (12)	N1—C14—C13	116.80 (10)
C3—C4—Cl1	118.71 (10)	N1—C14—H14A	108.1
C5—C4—Cl1	119.92 (9)	C13—C14—H14A	108.1
C4—C5—C6	120.10 (10)	N1—C14—H14B	108.1
C4—C5—H5	120.0	C13—C14—H14B	108.1
C6—C5—H5	120.0	H14A—C14—H14B	107.3
C5—C6—C1	118.91 (11)	N1—C15—C16	112.65 (10)
C5—C6—C7	117.90 (10)	N1—C15—H15A	109.1
C1—C6—C7	123.18 (11)	C16—C15—H15A	109.1
N2—C7—C6	116.32 (9)	N1—C15—H15B	109.1
N2—C7—H7A	108.2	C16—C15—H15B	109.1
C6—C7—H7A	108.2	H15A—C15—H15B	107.8
N2—C7—H7B	108.2	N2—C16—C15	112.95 (11)
C6—C7—H7B	108.2	N2—C16—H16A	109.0
H7A—C7—H7B	107.4	C15—C16—H16A	109.0
C9—C8—C13	119.27 (10)	N2—C16—H16B	109.0
C9—C8—N2	117.29 (10)	C15—C16—H16B	109.0
C13—C8—N2	123.43 (10)	H16A—C16—H16B	107.8
C15—N1—C1—C2	140.54 (11)	C16—N2—C8—C13	-39.77 (16)
C14—N1—C1—C2	-84.57 (13)	C13—C8—C9—C10	1.50 (18)
C15—N1—C1—C6	-39.47 (15)	N2—C8—C9—C10	-177.27 (10)
C14—N1—C1—C6	95.42 (14)	C8—C9—C10—C11	0.77 (18)
C6—C1—C2—C3	1.36 (18)	C9—C10—C11—C12	-2.32 (18)
N1—C1—C2—C3	-178.64 (11)	C9—C10—C11—Cl2	178.13 (9)
C1—C2—C3—C4	-0.33 (18)	C10—C11—C12—C13	1.56 (18)
C2—C3—C4—C5	-0.88 (18)	Cl2—C11—C12—C13	-178.90 (9)
C2—C3—C4—Cl1	179.63 (9)	C11—C12—C13—C8	0.77 (18)
C3—C4—C5—C6	1.03 (17)	C11—C12—C13—C14	179.84 (11)
Cl1—C4—C5—C6	-179.48 (8)	C9—C8—C13—C12	-2.26 (17)
C4—C5—C6—C1	0.03 (16)	N2—C8—C13—C12	176.43 (10)
C4—C5—C6—C7	-178.54 (10)	C9—C8—C13—C14	178.73 (11)
C2—C1—C6—C5	-1.19 (17)	N2—C8—C13—C14	-2.57 (18)
N1—C1—C6—C5	178.82 (10)	C1—N1—C14—C13	-54.36 (15)
C2—C1—C6—C7	177.30 (10)	C15—N1—C14—C13	81.12 (14)
N1—C1—C6—C7	-2.70 (17)	C12—C13—C14—N1	153.32 (12)
C8—N2—C7—C6	-54.43 (13)	C8—C13—C14—N1	-27.67 (18)
C16—N2—C7—C6	82.00 (12)	C1—N1—C15—C16	86.66 (13)
C5—C6—C7—N2	150.29 (10)	C14—N1—C15—C16	-47.97 (14)
C1—C6—C7—N2	-28.21 (15)	C8—N2—C16—C15	86.98 (12)
C7—N2—C8—C9	-85.65 (13)	C7—N2—C16—C15	-48.75 (14)
C16—N2—C8—C9	138.96 (11)	N1—C15—C16—N2	-39.74 (14)
C7—N2—C8—C13	95.62 (13)		

Fig. 1

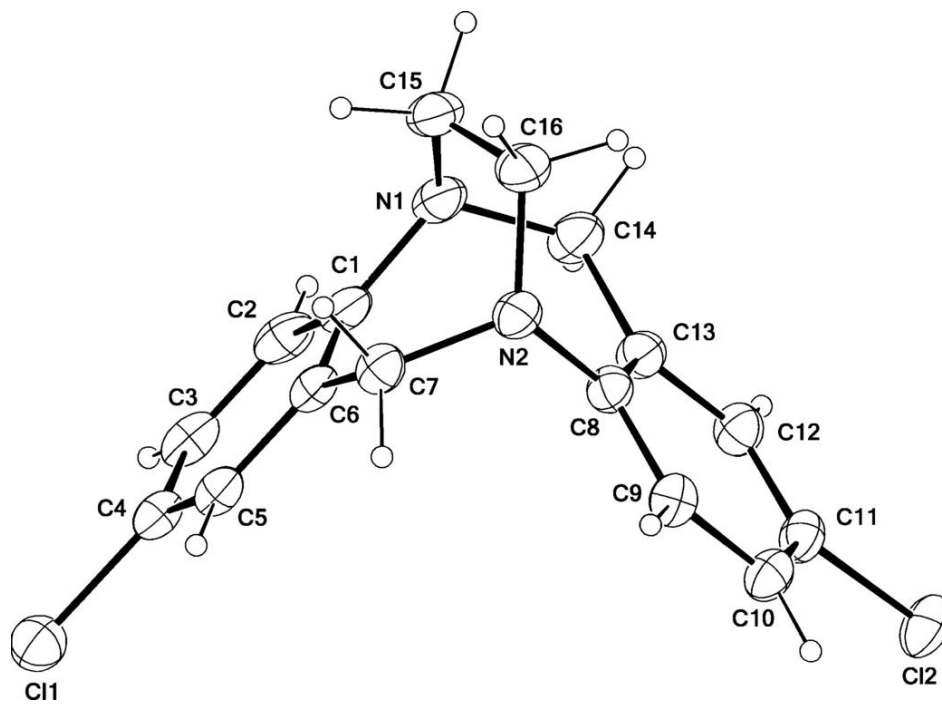


Fig. 2

