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Acta Cryst. (1995). C**51**, 2304–2305

1,2-Bis(4-pyridyl)ethane

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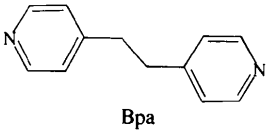
(*Received* 13 *February* 1995; *accepted* 13 *April* 1995)

Abstract

The 1,2-bis(4-pyridyl)ethane [$C_{12}H_{12}N_2$ (Bpa)] molecule lies on a centre of symmetry. Bond distances and angles have values within the normal ranges. The value of the torsion angle C2—C3—C6—C6′ [−99.5 (3)°] shows that the Bpa molecule is not planar.

Comment

The synthesis of Bpa has been reported by Asword & Burkhardt (1928) and Kutlu (1978). It is of special interest since it is used as a disinfectant in dental hygiene preparations (Edwards, 1973) and dry heat sterilization indicators (Cheng, 1972), and to simulate asphaltenes of coal hydroliquefaction (Smith, Romine & El-Sheikh, 1980).



Bpa

The purpose of the X-ray analysis was to characterize the features of the molecular geometry and conformation. Fig. 1 shows the molecular structure of Bpa and gives the numbering system used. Bond distances and angles lie within the expected ranges and compare well with those found in the structures of [1,2-bis(*N*-ethyl-4-pyridinium)ethane]$^{4+}_2$ (7,7,8,8-tetracyanoquinodimethane)$^{4-}_5$ (Ashwell *et al.*, 1977), 1,2-di(4-pyridyl)-ethylene–7,7,8,8-tetracyano-*p*-quinodimethane (Ashwell, Kennedy & Nowell, 1983) and TCNQ salts of 1,2-bis(4-pyridinium)ethane (Ashwell, Allen, Cross & Nowell, 1983). The crystal structure viewed along **b** is shown in Fig. 2. The Bpa molecule is on a centre of symmetry.

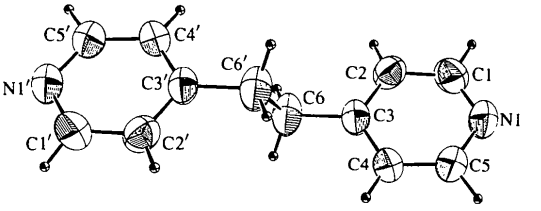


Fig. 1. View of the title molecule. The non-H atoms are shown with displacement ellipsoids drawn at the 50% probability level. For clarity, the H atoms are drawn as small spheres of arbitrary size.

The C6—C6′ bond distance and C6′—C6—C3 bond angle are 1.498 (4) Å and 112.6 (2)°, respectively. The C2—C3—C6—C6′ and C4—C3—C6—C6′ torsion angles [−99.5 (3) and 78.0 (3)°, respectively] indicate that the Bpa molecule is not planar.

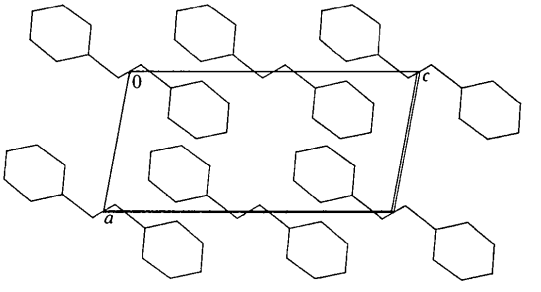


Fig. 2. Projection of the Bpa molecules along **b**.

Experimental

Bpa, from Aldrich Chemical Company, was purified by recrystallization from benzene–cyclohexane (1:3) mixed solvent; m.p. 383 K (literature m.p. 383–384 K).

Crystal data

$C_{12}H_{12}N_2$
M_r = 184.2
Mo $K\alpha$ radiation
λ = 0.71073 Å

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Monoclinic
$P2_1/c$
$a = 5.561\ (2)$ Å
$b = 8.159\ (3)$ Å
$c = 11.353\ (4)$ Å
$\beta = 100.73\ (4)°$
$V = 506.1\ (3)$ Å^3
$Z = 2$
$D_x = 1.209$ Mg m^{-3}

Cell parameters from 16 reflections
$\theta = 17–19°$
$\mu = 0.0730$ mm^{-1}
$T = 293$ K
Prism
0.40 × 0.24 × 0.16 mm
White

Data collection

Enraf–Noinus CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
796 measured reflections
754 independent reflections
391 observed reflections $[F > 3\sigma(F)]$

$R_{int} = 0.035$
$\theta_{max} = 34°$
$h = -6 \rightarrow 6$
$k = -9 \rightarrow 0$
$l = -12 \rightarrow 0$
3 standard reflections monitored every 200 reflections
intensity decay: none

Refinement

Refinement on F
$R = 0.035$
$wR = 0.038$
$S = 1.20$
391 reflections
88 parameters
Unit weights applied
$(\Delta/\sigma)_{max} = 0.0002$

$\Delta\rho_{max} = 0.10$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV) and Cromer & Mann (1968)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
C4	0.6678 (4)	0.1880 (4)	0.8366 (2)	4.18 (7)
C2	0.9312 (5)	0.0328 (4)	0.7416 (2)	4.56 (7)
C3	0.8810 (4)	0.0980 (3)	0.8459 (2)	3.79 (7)
C5	0.5236 (5)	0.2098 (4)	0.7266 (2)	4.68 (7)
N1	0.5683 (4)	0.1479 (3)	0.6252 (2)	5.07 (6)
C1	0.7714 (5)	0.0618 (4)	0.6349 (2)	5.23 (8)
C6	1.0472 (5)	0.0663 (4)	0.9647 (2)	5.14 (8)

Table 2. *Selected geometric parameters* (Å, °)

C4—C3	1.382 (4)	C3—C6	1.509 (3)
C4—C5	1.364 (3)	C5—N1	1.323 (4)
C2—C3	1.373 (4)	N1—C1	1.317 (4)
C2—C1	1.383 (3)		
C3—C4—C5	119.3 (3)	C2—C3—C6	121.0 (2)
C3—C2—C1	119.2 (3)	C4—C5—N1	125.0 (3)
C4—C3—C2	116.7 (2)	C5—N1—C1	115.3 (2)
C4—C3—C6	122.2 (2)	C2—C1—N1	124.5 (3)

The structure was solved by direct methods and refined by full-matrix least squares. H atoms were found by a difference Fourier synthesis and refined isotropically.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Cell refinement: *CAD-4 Software*. Data reduction: *MolEN PROCESS* (Fair, 1990). Program(s) used to solve structure: *MULTAN*80 (Main *et al.*, 1980). Program(s) used to refine structure: *MolEN LSFM*. Molecular graphics: *ORTEP*II (Johnson, 1976).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and bond distances, angles and torsion angles involving H atoms have been deposited with the IUCr (Reference: NA1166). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1995). C**51**, 2305–2307

(±)-2-Oxocyclohexaneacetic Acid: Structure and Hydrogen-Bonding Pattern of a γ-Keto Acid

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(*Received* 6 *July* 1994; *accepted* 17 *May* 1995)

Abstract

In the title compound, $C_8H_{12}O_3$, enantiomeric pairs of molecules form centrosymmetric dimers by mutual hydrogen bonding of carboxyl groups, with the ketone not involved in the hydrogen bonding. The dimers are of four types, centered on the three edges and the center of the cell. The carboxyl C—O bond lengths and angles are substantially disordered. There is a 2.551 (3) Å intermolecular contact between methine H and ketone O atoms.

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