Table 1. *Positional parameters and equivalent isotropic thermal parameters of non-H atoms with e.s.d.'s in parentheses*

$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$.

	x	y	z	B_{eq} (Å^2)
Cl	0·1704 (1)	0·2234 (1)	0·5867 (0)	5·8 (0)
C(1)	0·4527 (3)	0·3117 (5)	0·7460 (1)	4·1 (1)
C(2)	0·4793 (4)	0·3142 (5)	0·7963 (1)	4·8 (1)
C(3)	0·4105 (4)	0·2293 (6)	0·8303 (2)	5·0 (1)
C(4)	0·3126 (4)	0·1449 (6)	0·8145 (1)	4·8 (1)
C(5)	0·2854 (4)	0·1421 (5)	0·7648 (1)	4·4 (1)
C(6)	0·3558 (3)	0·2242 (4)	0·7291 (1)	3·7 (1)
C(7)	0·3158 (3)	0·2187 (5)	0·6774 (2)	4·0 (1)
C(8)	0·3768 (3)	0·2314 (5)	0·6345 (1)	3·8 (1)
C(9)	0·5046 (3)	0·2471 (6)	0·6326 (1)	4·7 (1)
C(10)	0·5535 (4)	0·1636 (8)	0·5856 (2)	6·0 (1)
C(11)	0·5014 (4)	0·2465 (9)	0·5401 (2)	6·3 (2)
C(12)	0·3744 (4)	0·2490 (5)	0·5423 (1)	4·8 (1)
C(13)	0·3182 (3)	0·2332 (5)	0·5862 (1)	4·2 (1)
C(14)	0·3138 (5)	0·2709 (8)	0·4951 (2)	6·7 (2)
O(14)	0·3615 (3)	0·2909 (3)	0·4560 (1)	8·9 (1)

Table 2. *Bond lengths* (Å), *bond angles* (°) *and selected torsion angles* (°) *with e.s.d.'s in parentheses*

Cl—C(14)	1·740 (3)	C(8)—C(9)	1·505 (5)
C(1)—C(2)	1·390 (4)	C(8)—C(13)	1·471 (4)
C(1)—C(6)	1·388 (5)	C(9)—C(10)	1·523 (6)
C(2)—C(3)	1·375 (6)	C(10)—C(11)	1·503 (8)
C(3)—C(4)	1·378 (6)	C(11)—C(12)	1·491 (7)
C(4)—C(5)	1·376 (4)	C(12)—C(13)	1·358 (4)
C(5)—C(6)	1·408 (5)	C(12)—C(14)	1·465 (6)
C(6)—C(7)	1·469 (6)	C(14)—O(14)	1·201 (6)
C(7)—C(8)	1·362 (6)		

Cl—C(13)—C(8)	117·3 (2)	C(5)—C(6)—C(7)	116·6 (3)
Cl—C(13)—C(12)	119·6 (2)	C(1)—C(6)—C(7)	125·8 (3)
C(3)—C(1)—C(6)	91·2 (2)	C(6)—C(7)—C(9)	99·8 (2)
C(2)—C(1)—C(6)	120·6 (3)	C(6)—C(7)—C(8)	129·3 (4)
C(1)—C(2)—C(3)	120·7 (3)	C(5)—C(7)—C(9)	127·2 (2)
C(2)—C(3)—C(4)	119·7 (4)	C(7)—C(8)—C(13)	120·3 (3)
C(3)—C(4)—C(5)	120·0 (4)	C(7)—C(8)—C(9)	123·9 (3)
C(4)—C(5)—C(6)	121·4 (4)	C(9)—C(8)—C(13)	115·8 (3)
C(3)—C(5)—C(7)	123·9 (2)	C(8)—C(9)—C(10)	111·8 (3)
C(1)—C(6)—C(5)	117·5 (2)	C(7)—C(9)—C(11)	117·6 (2)

C(8)—C(9)—C(10)—C(11)	−51·7 (5)	C(11)—C(12)—C(13)—C(8)	5·9 (6)
C(9)—C(10)—C(11)—C(12)	−46·2 (5)	C(12)—C(13)—C(8)—C(9)	−0·3 (5)
C(10)—C(11)—C(12)—C(13)	18·1 (6)	C(13)—C(8)—C(9)—C(10)	−28·3 (4)

Final difference Fourier map featureless with $\Delta\rho$ within $\pm 0{\cdot}19$ e Å^{-3}. The atomic scattering factors used for all atoms were as provided in the *SHELX*76 program. Computer programs: *PARST* (Nardelli, 1983) for geometrical calculations, *MOLDRAW* (Ugliengo, Borzani & Viterbo, 1988) for molecular illustrations. A view of the molecule with the adopted atom numbering is shown in Fig. 1. Table 1* lists the final atomic coordinates and equivalent isotropic thermal parameters of non-H atoms. The bond lengths, bond angles and selected torsion angles are shown in Table 2.

Related literature. The compound has antifungal activity. The X-ray crystal structure analysis of similar compounds has not so far been reported in the literature.

We thank Professor Frank R. Fronczek, Department of Chemistry, Louisiana State Univeristy, for helping in data collection.

* Lists of structure factors, anisotropic thermal parameters least-squares-planes calculations, bond lengths and angles involving H atoms and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53004 (11 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of 5,5′-Dibromo-2,2′-bipyridine

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(*Received* 16 *May* 1990; *accepted* 18 *July* 1990)

Abstract. $C_{10}H_6Br_2N_2$, $M_r = 313{\cdot}99$, monoclinic, $P2_1/a$, $a = 21{\cdot}072$ (4), $b = 5{\cdot}956$ (1), $c = 3{\cdot}997$ (1) Å, $\beta = 91{\cdot}78$ (2)°, $V = 501{\cdot}4$ (2) Å^3, $Z = 2$, $D_x = 2{\cdot}08$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71068 Å, $\mu = 79{\cdot}65$ cm^{-1}, $F(000) = 300$, room temperature, $R = 0{\cdot}037$ for 830 reflections. The molecule has crystallo-

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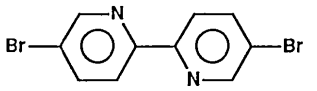
0108-2701/91/020454-02$03.00

graphic $\bar{1}$ symmetry. The bipyridine moiety has a coplanar *anti* conformation, which is similar to that reported for other bipyridines.



Experimental. The title compound was prepared (Yamamoto, Zhou, Kanbara & Maruyama, 1990) by modifying a method reported for the preparation of 5,5′-dichloro-2,2′-bipyridine (Oae, Kawai & Furukawa, 1987). Colorless prisms from benzene, 0·15 × 0·15 × 0·32 mm, Rigaku automated four-circle diffractometer (AFC-5), graphite-monochromated Mo $K\alpha$ radiation, unit-cell dimensions by least squares from the 2θ values of 20 reflections with $19 \le 2\theta \le 22°$; intensities in the range $3 < 2\theta < 55°$ measured with $\omega/2\theta$ scan technique ($-26 \le h \le 26$, $0 \le k \le 7$, $0 \le l \le 5$), scan rate 4° $(2\theta)\,\text{min}^{-1}$, scan width 1·30° plus $\alpha_1 - \alpha_2$ divergence; three reflections monitored periodically showed no significant intensity deterioration; 1114 measured independent reflections, 284 with no net intensities, $I \le 3\sigma(I)$; absorption correction by Gaussian integration (8 × 8 × 8); standard deviations estimated by $\sigma^2(F_o) = \sigma_p^2(F_o) + qF_o^2$ with $\sigma_p(F_o)$ evaluated from counting statistics and q ($2{\cdot}70 \times 10^{-3}$) from variations of monitored reflections; structure solved by direct methods, anisotropic block-diagonal least-squares refinement, $\sum w(|F_o| - |F_c|)^2$ minimized with $w = 1/\sigma^2(F_o)$; H atoms from a difference map, isotropic; final $R = 0{\cdot}037$ for 830 reflections with $F_o \ge 3\sigma(F_o)$ ($wR = 0{\cdot}043$, $S = 1{\cdot}519$), $[\Delta x_i/\sigma(x_i)]_{\max} = 0{\cdot}4$; atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV); programs *SAPI*85 (Fan, 1985, unpublished), *ORTEP* (Johnson, 1971) and *DABEX* (Toriumi & Ohba, 1981, unpublished).

Atomic parameters are listed in Table 1.* Fig. 1 shows the structure of the molecule having crystallographic $\bar{1}$ symmetry. Bond lengths and bond angles are given in Table 2.

Related literature. Crystal structures of 2,2′-bipyridine (Merritt & Schroeder, 1956) and a derivative (Fronczek, Taylor, Gupta & Newkome, 1985) have been reported. Both reports show a coplanar anti conformation of the bipyridine moiety of the compounds which is similar to that of the title compound.

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53424 (10 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional coordinates and isotropic temperature factors of non-*H *atoms*

$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	B_{eq}(Å^2)
Br1	0·80387 (2)	0·48581 (7)	0·10503 (13)	3·99
N2	0·9822 (2)	0·7408 (5)	0·2867 (9)	3·25
C3	0·9719 (2)	0·9348 (6)	0·4474 (10)	2·59
C4	0·9104 (2)	1·0081 (6)	0·5105 (13)	3·13
C5	0·8586 (2)	0·8756 (7)	0·4103 (11)	3·30
C6	0·8710 (2)	0·6762 (7)	0·2518 (10)	2·89
C7	0·9321 (2)	0·6145 (7)	0·1943 (11)	3·31

Table 2. *Bond distances* (Å) *and angles* (°)

Br1—C6	1·892 (4)	C3—C3′	1·468 (8)
C3—C4	1·399 (6)	C6—C7	1·367 (6)
C5—C6	1·375 (6)	N2—C7	1·339 (5)
N2—C3	1·343 (5)	C4—C5	1·395 (6)

C3—N2—C7	118·5 (4)	N2—C3—C4	121·3 (4)
N2—C3—C3′	116·8 (5)	C4—C3—C3′	121·9 (4)
C3—C4—C5	119·5 (4)	C4—C5—C6	117·6 (4)
C5—C6—C7	120·2 (4)	C5—C6—Br1	120·7 (3)
C7—C6—Br1	119·1 (3)	N2—C7—C6	122·8 (4)

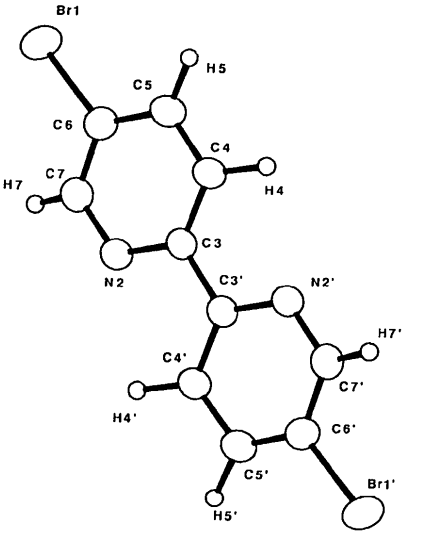


Fig. 1. Atomic numbering and molecular structure of 5,5′-dibromo-2,2′-bipyridine.

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