Acta Cryst. (1988). C**44**, 1857–1858

Structure of 2-Amino-5-bromopyrimidine

BY H. L. L. WATTON, J. N. LOW AND P. TOLLIN

Department of Applied Physics, Electronics and Manufacturing Engineering, University of Dundee, Dundee DD1 4HN, Scotland

AND R. ALAN HOWIE

Department of Chemistry, University of Aberdeen, Meston Walk, Old Aberdeen AB9 2UE, Scotland

(*Received* 14 *March* 1988; *accepted* 20 *June* 1988)

Abstract. $C_4H_4BrN_3$, $M_r = 174{\cdot}01$, orthorhombic, *Cmca*, $a = 7{\cdot}702\ (3)$, $b = 8{\cdot}215\ (3)$, $c = 17{\cdot}733\ (12)$ Å, $U = 1122{\cdot}0$ Å^3, $Z = 8$, $D_x = 2{\cdot}06$ g cm^{-3}, Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71069$ Å, $\mu = 71{\cdot}4$ cm^{-1}, $F(000) = 672$, $T = 293$ K, $R = 0{\cdot}060$ for 578 unique observed $[F > 5\sigma(F)]$ reflections. Atoms Br, C5, C2 and N2 lie on the mirror plane at $x = 0$; atoms N3 and C4 are therefore symmetry equivalents of N1 and C6. The numbering system conforms to that for pyrimidine nucleobases. The molecules of the title compound form self-base-paired ribbons which run parallel to the *a* axis. The hydrogen bond involved in the base-pairing between symmetry related molecules is N2···N1 ($-0{\cdot}5-x$, $1{\cdot}5-y$, $-z$) 3·10 (3) Å.

Experimental. Crystals were obtained from aqueous solution as very thin micaceous plates. Space group and initial cell dimensions were obtained from Weissenberg photographs. Data were collected on a Nicolet *P*3 (four-circle) diffractometer in Aberdeen by RAH. The crystal had dimensions 0·04 × 0·4 × 0·6 mm. Cell parameters were measured on the diffractometer using 14 reflections in the 2θ range 17–21°. Range of indices: $0 \le h \le 12$; $0 \le k \le 12$; $0 \le l \le 24$. Data measured using $\omega/2\theta$ scans in the range $0 < 2\theta < 60°$. Standard reflections, 020 and 120, were measured every 50 reflections. No changes greater than 2σ from the mean of the intensities of these reflections were found throughout data collection. 783 independent reflections measured, giving 578 observed $[F > 5\sigma(F)]$ reflections used in the refinement. Lorentz and polarization factors were applied. A ψ-scan absorption correction was used. Maximum and minimum transmission factors were 0·3748 and 0·0567. The structure was solved by the heavy-atom method using the *SHELXS*86 program (Sheldrick, 1986).

Blocked full-matrix refinement (on *F*) was carried out using the program *SHELX*76 (Sheldrick, 1976). The hydrogen atoms were included at calculated positions. All hydrogen atoms were given isotropic temperature factors 1·5 times that of the parent atom and allowed to ride on that atom. All other atoms were refined anisotropically. The refinement converged at $R = 0{\cdot}060$, $wR = 0{\cdot}071$, $w = 2{\cdot}5097[\sigma^2(F) + 0{\cdot}001511F^2]^{-1}$. 51 refined parameters; max. shift/e.s.d. <0·01; max. difference peak 1·29, min. difference peak −1·36 e Å^{-3}. The largest of these difference peaks were associated with the Br atom.

Scattering factors and anomalous-dispersion corrections were taken from *International Tables for X-ray Crystallography* (1974). Also used were the program packages *XANADU* (Roberts & Sheldrick, 1975) and *PLUTO* (Motherwell & Clegg, 1978). All calculations were carried out on the Dundee University Prime

Table 1. *Coordinates* ($\times 10^4$) *and* U_{eq} *values* (Å$^2 \times 10^3$) *for non-hydrogen atoms with e.s.d.'s in parentheses*

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	*y*	*z*	U_{eq}
Br	0	2636 (1)	2251 (1)	46 (1)
N1	−1557 (6)	6200 (5)	773 (2)	35 (1)
C2	0	6755 (9)	548 (4)	32 (2)
N2	0	8003 (9)	48 (5)	42 (1)
C6	−1541 (8)	4997 (6)	1283 (3)	35 (1)
C5	0	4362 (9)	1539 (4)	35 (2)

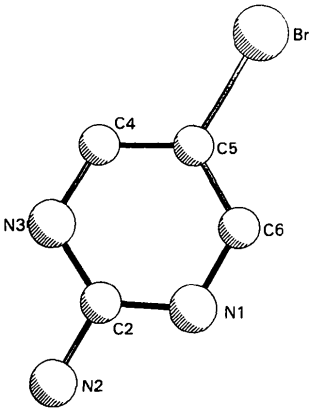

Fig. 1. Perspective view of the molecule showing atomic numbering (see *Abstract*).

0108-2701/88/101857-02$03.00

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

C5—Br	1·899 (7)	C2—N1	1·344 (5)
C6—N1	1·339 (6)	N2—C2	1·355 (12)
C5—C6	1·374 (7)		
C6—N1—C2	116·3 (5)	N1—C2—N1	126·3 (7)
N2—C2—N1	116·8 (4)	C5—C6—N1	120·8 (6)
C6—C5—C6	119·5 (7)	C6—C5—Br	120·2 (3)

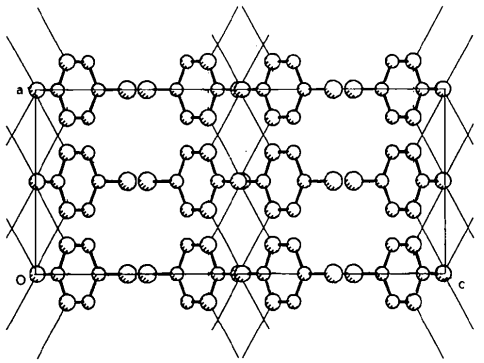

Fig. 2. The contents of the unit cell viewed down the *b* axis, showing hydrogen bonding between the bases.

computer. The atomic numbering is shown in the perspective drawing (Fig. 1), and tables of atomic parameters, bond lengths and angles are given (Tables 1 and 2). Fig. 2 shows a view of the molecular packing.*

Related literature. Base-pairing between nucleosides, nucleotides and nucleobases has been reviewed by Wilson & Tollin (1987).

* 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 51167 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

MOTHERWELL, W. D. S. & CLEGG, W. (1978). *PLUTO*. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.

ROBERTS, P. & SHELDRICK, G. M. (1975). *XANADU*. Program for torsion angle, mean plane and libration correction calculations. Univ. of Cambridge, England.

SHELDRICK, G. M. (1976). *SHELX76*. Program for structure determination. Univ. of Cambridge, England.

SHELDRICK, G. M. (1986). *SHELXS86*. In *Crystallographic Computing* 3, edited by G. M. SHELDRICK, C. KRUGER & R. GODDARD, pp. 175–189. Oxford Univ. Press.

WILSON, C. C. & TOLLIN, P. (1987). *Nucleosides Nucleotides*, **6**(3), 643–653.

Acta Cryst. (1988). C**44**, 1858–1860

Structure of Intrasil Brilliant Yellow*

BY N. N. DHANESHWAR, S. S. TAVALE AND T. N. GURU ROW†

Physical Chemistry Division, National Chemical Laboratory, Pune 411 008, *India*

(*Received* 26 *November* 1987; *accepted* 10 *June* 1988)

Abstract. 3-(5-Chloro-2-benzoxazolyl)-7-(diethylamino)-2*H*-1-benzopyran-2-one, $C_{20}H_{17}ClN_2O_3$, M_r = 369, monoclinic, $P2_1/a$, a = 9·262 (2), b = 13·282 (2), c = 14·453 (2) Å, β = 104·16 (2)°, V = 1724 (1) Å^3, Z = 4, D_m (flotation in KI solution) = 1·43, D_x = 1·42 Mg m^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, μ = 2·51 cm^{-1}, $F(000)$ = 768, T = 293 K, R = 0·056 for 1071 observed reflections. The dihedral angle between the benzoxazoline and the benzopyrone moieties is 5·9°, showing significant deviation from planarity. The two ring systems are planar.

Experimental. The title compound is a commercial dye. It was dissolved in chloroform and purified by column chromatography using 20% chloroform and 80% petroleum ether and recrystallized from acetone. Crystal approx. 0·20 × 0·05 × 1·00 mm. Nonius CAD-4F-11M diffractometer, graphite-monochromated radiation, $\omega/2\theta$ scan mode, scan speed 1° min^{-1},

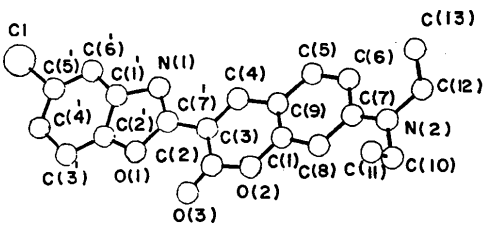

Fig. 1. A perspective view of the molecule with atomic numbering.

* NCL Communication No. 4333.

† To whom correspondence is to be addressed.

0108-2701/88/101858-03$03.00