

normal ranges. Similarly, the 'cyclohexenone' ring has normal bond lengths and angles, with the C—B bond shared with the cage having a normal carborane bond length [1.710 (4) Å].

The exocage ring in (1) does exert an influence on the detailed structure of the carborane in the vicinity of the ring. For instance, the bonds to the C and B atoms shared with the exocage ring are slightly longer than the related bonds on the other side of the molecule. Table 4 summarizes the situation and provides a comparison of all bond lengths with the results of calculations by Ott & Gimarc (1986) on *o*-carborane itself.

As noted earlier, compound (2) is rotationally disordered, and therefore some distances reported in Table 3 represent averaged B—C, C—C or B—C B—B distances. Nevertheless, it is possible to say that the bond distances and angles in the exocyclic ring are normal, with a single exception. Because of our earlier structural assignment which showed that the ring connects carbon and boron as shown in (2), (Wu & Jones, 1986), we can identify with certainty the framework bond making up part of the five-membered ring. Its length is 1.662 (5) Å, shorter than the corresponding bond in (1) [1.710 (4) Å] and other carboranes (Beall, 1975). Presumably, this reflects the inability of the three-carbon bridge to span a 'normal' C—B distance of about 1.70 Å.

This work was supported by the National Science Foundation through grants CHE 83-18345 and 86-17590. We thank Professor Robert A. Pascal Jr for helpful advice on crystallization.

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Acta Cryst. (1990). **C46**, 660–663

5-(2-Bromo-4,5-dimethoxyphenyl)-4-(2-hydroxy-3,4-dimethoxyphenyl)pyrimidine

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(Received 30 March 1989; accepted 19 July 1989)

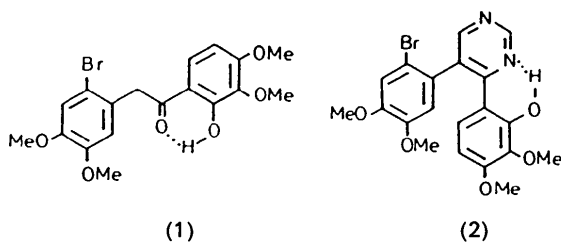
Abstract. 6-[5-(2-Bromo-4,5-dimethoxyphenyl)-4-pyrimidinyl]-2,3-dimethoxyphenol, C₂₀H₁₉BrN₂O₅, *M_r* = 447.3, triclinic, *P* $\bar{1}$, *a* = 9.360 (2), *b* = 11.771 (3), *c* = 10.236 (3) Å, α = 78.23 (2), β = 65.28 (2), γ = 72.19 (2)°, *V* = 971.5 (5) Å³, *Z* = 2, *D_x* = 1.52 Mg m⁻³, Mo *K*α radiation, λ = 0.71069 Å, μ = 2.13 mm⁻¹, *F*(000) = 456, *T* = 293 K, *R* = 0.050

for 2123 observed reflections. The crystal structure is in agreement with that predicted from IR and NMR spectral studies in solution. The bromobenzene ring at C(7) is nearly perpendicular [105.8 (2)°] to the heterocyclic ring, while the other aryl substituent at C(12) is rotated out of the pyrimidine ring plane by 20.8 (2)°. An intramolecular OH⋯N bond is observed with the distance O⋯N = 2.55 (1) Å and the angle O—H⋯N = 150 (7)°.

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Introduction. During our studies on the synthesis of nitrogen heterocycles (Dominguez, Lete, Villa & Iriondo, 1984; Villa, Dominguez & Lete, 1986), the reductive amination (formamide, formic acid and ammonium formate) of the phenolic deoxybenzoin (1) afforded (after flash column chromatographic separation of the mixture of products) a yellow crystalline component of m.p. 435–436 K, homogeneous on thin-layer chromatography.

On the basis of the usual spectra and analytical data, this compound was formulated as 5-(2-bromo-4,5-dimethoxyphenyl)-4-(2-hydroxy-3,4-dimethoxyphenyl)pyrimidine (2). In order to confirm this assignment, we have carried out an X-ray crystal structure analysis.



Experimental. Yellow plate-like crystals were grown from ethanol. The chemical analyses for C, H, N and Br gave the following calculated (experimental) results: C 53.68 (53.65); H 4.25 (4.45); N 6.26 (6.34); Br 17.90% (18.22%). The IR and ^1H NMR data suggested a strong intramolecular hydrogen bond. In the IR spectrum of solid pyrimidine a broad and shallow absorption band is found at 3100 cm^{-1} and assigned to the $\nu_s(\text{OH}\cdots\text{N})$ vibration. The ^1H NMR spectrum in deuterated chloroform solution showed a singlet at 13.0 p.p.m., almost completely invariant with concentration. Data were collected from a crystal approximately $0.08 \times 0.08 \times 0.1\text{ mm}$; cell parameters were determined by least squares from the setting angles of 23 reflections ($20 \leq 2\theta \leq 34^\circ$); 2877 independent reflections were measured; Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ radiation, ω scans up to $2\theta = 47^\circ$; one standard reflection (004), measured every 50, showed only small random deviations from its mean intensity; Lp applied but not absorption correction; 2123 reflections [$I \geq 2.5\sigma(I)$] considered observed and included in refinement; index range $h -9 \rightarrow 10$, $k -12 \rightarrow 13$, $l 0 \rightarrow 11$; structure solved with Patterson and Fourier methods with *MULTAN*11/84 (Main, Germain & Woolfson, 1984); refinement by least squares with *SHELX76* (Sheldrick, 1976), $\sum w(\Delta F)^2$ minimized $\{w = k/[\sigma^2(F) + 0.00077F^2]\}$, completed with anisotropic thermal parameters for non-H atoms; H atoms included in calculation with an overall isotropic temperature factor in idealized positions, except H(28) which was found from ΔF synthesis and

Table 1. Fractional coordinates ($\times 10^4$ for C, N, Br and O) and B_{eq} values, calculated according to Willis & Pryor (1975)

	x	y	z	$B_{\text{eq}}(\text{\AA}^2)$
C(1)	6510 (5)	1870 (4)	9383 (5)	2.79
C(2)	7742 (5)	1334 (4)	8202 (5)	2.99
C(3)	7436 (6)	798 (4)	7285 (5)	3.44
C(4)	5892 (6)	762 (4)	7578 (5)	3.04
C(5)	4602 (6)	1273 (4)	8799 (5)	2.73
C(6)	4929 (6)	1821 (4)	9684 (5)	2.85
C(7)	6852 (5)	2458 (4)	10352 (5)	2.76
C(8)	6872 (6)	1840 (5)	11643 (5)	3.53
N(9)	7337 (5)	2214 (4)	12529 (4)	4.06
C(10)	7868 (6)	3198 (5)	12023 (6)	3.81
N(11)	7848 (5)	3887 (4)	10828 (4)	3.44
C(12)	7294 (5)	3556 (4)	9979 (5)	2.62
C(13)	7220 (6)	4405 (4)	8721 (5)	2.86
C(14)	6224 (6)	4429 (4)	8002 (5)	3.38
C(15)	6160 (6)	5220 (4)	6828 (6)	3.65
C(16)	7110 (6)	6048 (4)	6311 (5)	3.56
C(17)	8070 (6)	6084 (4)	7020 (5)	3.40
C(18)	8140 (6)	5285 (4)	8202 (5)	3.07
Br(19)	9944 (1)	1270 (1)	7802 (1)	5.01
O(20)	5459 (4)	245 (3)	6763 (4)	4.01
C(21)	6759 (8)	-265 (5)	5481 (6)	5.08
O(22)	3104 (4)	1172 (3)	9015 (4)	3.69
C(23)	1761 (6)	1742 (5)	10183 (6)	4.52
O(24)	7160 (5)	6858 (3)	5152 (4)	4.96
C(25)	6316 (9)	6811 (6)	4292 (7)	5.92
O(26)	8962 (5)	6940 (3)	6575 (4)	4.46
C(27)	10457 (8)	6628 (6)	5378 (6)	5.56
O(28)	9124 (5)	5379 (3)	8816 (4)	4.31

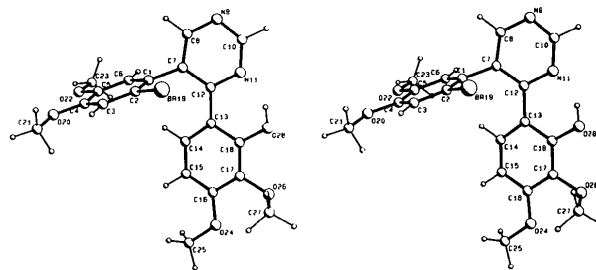


Fig. 1. Stereoscopic view of the molecule with the atom numbering.

refined with an individual isotropic temperature factor; final $R = 0.050$, $wR = 0.049$; scattering factors from *SHELX76* (Sheldrick, 1976); max. Δ/σ (for non-H atoms) = 0.41; max. and min. electron densities in final difference map $+0.75$ and -0.93 e \AA^{-3} .

Discussion. The fractional atomic coordinates with their B_{eq} values (Willis & Pryor, 1975) are given in Table 1.* Other parameters of interest were calculated with *PARST* (Nardelli, 1983). Fig. 1 shows a stereoscopic view of the molecule and the atom numbering (Motherwell & Clegg, 1978).

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, bond lengths and bond angles involving H atoms, least-squares-planes data and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52440 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The bond lengths and bond angles are unexceptional in comparison with standard values (*International Tables for X-ray Crystallography*, 1974), and are given in Table 2. The bond length C(12)—C(13) [1.472 (6) Å] could indicate that the resonance between the aryl group at C(12) and the pyrimidine ring bestows some double bond character on this bond. As may be seen from Table 2, the lengthening and shortening of the C—N and C—C bond lengths within the pyrimidine ring is likely to be related to this resonance system. Thus, the averaged values* of the C(10)—N(9), C(10)—N(11) and C(8)—N(9), C(12)—N(11) bond lengths are 1.324 (6, 2, 2, 2) and 1.346 (6, 1, 1, 2) Å respectively, and the C(7)—C(8) and C(7)—C(12) distances 1.377 (7) and 1.408 (6) Å. These results are in agreement with values found previously in similar heterocyclic systems (Martinez-Ripoll & Lorentz, 1973, 1974). The angles at the N and C atoms compare well with those found in other pyrimidine derivatives. The values of the C—C and C—O bond lengths are of the usual order of magnitude (Martinez-Ripoll & Lorenz, 1973, 1974; Koetzle & Williams, 1976, 1978; Cody, 1984; Bryan, Haltiwanger & Woode, 1987).

The heterocyclic ring of the molecule shows significant deviations from planarity; much smaller distortions are seen in the aryl groups attached to C(7) and C(12). The values of Ω^2 [$\Omega^2 = \sum(\Delta/\sigma)^2$, where $\Delta \equiv$ atomic deviation from the calculated mean plane and $\sigma \equiv$ standard deviation of Δ] are 156.8 (six atoms), 18.7 (six atoms) and 28.7 (six atoms) respectively. The aryl group at C(12) is rotated out of the pyrimidine ring plane by 20.8 (2)°, while the bromobenzene ring at C(7) lies nearly perpendicular to the heterocyclic ring plane with a dihedral angle of 105.8 (2)°.

The torsion angles given in Table 2 show that the methoxy groups at C(4) and C(5) are, as expected, coplanar with the benzene ring (Caillet, 1982). The methoxy group at C(16) (see Table 2) is also coplanar with the ring, but the remaining methoxy group at C(17) is directed away from the benzene ring. This behaviour has been reported to be typical for an arrangement of three adjacent methoxy groups (Miravittles, Solans, Bladé-Font, Germain & Declercq, 1982).

The C(18) OH group is nearly coplanar with the aromatic ring and forms an intramolecular hydrogen bond O(28)—H(28)···N(11), with distances N(11)—O(28), O(28)—H(28) and H(28)···N(11) 2.55 (1), 0.84 (6) and 1.79 (7) Å respectively, and the

* The first number in parentheses following an averaged value of a bond length is the root-mean-square estimated standard deviation of an individual datum. The second and third numbers are the average and the maximum deviations from the averaged value, respectively. The fourth number represents the number of individual measurements that are included in the averaged value.

Table 2. Bond lengths (Å), bond angles (°) and selected torsion angles (°)

C(1)—C(2)	1.374 (6)	N(11)—C(12)	1.346 (6)
C(1)—C(6)	1.397 (6)	C(12)—C(13)	1.472 (6)
C(1)—C(7)	1.499 (6)	C(13)—C(14)	1.401 (7)
C(2)—C(3)	1.392 (6)	C(13)—C(18)	1.427 (6)
C(2)—Br(19)	1.906 (4)	C(14)—C(15)	1.382 (7)
C(3)—C(4)	1.360 (6)	C(15)—C(16)	1.395 (7)
C(4)—C(5)	1.408 (6)	C(16)—C(17)	1.385 (7)
C(4)—O(20)	1.368 (5)	C(16)—O(24)	1.356 (6)
C(5)—C(6)	1.386 (6)	C(17)—C(18)	1.384 (7)
C(5)—O(22)	1.365 (5)	C(17)—O(26)	1.388 (6)
C(7)—C(8)	1.377 (7)	C(18)—O(28)	1.352 (6)
C(7)—C(12)	1.408 (6)	O(20)—C(21)	1.450 (6)
C(8)—N(9)	1.348 (6)	O(22)—C(23)	1.419 (6)
N(9)—C(10)	1.323 (6)	O(24)—C(25)	1.425 (7)
C(10)—N(11)	1.326 (6)	O(26)—C(27)	1.425 (7)
C(6)—C(1)—C(7)	120.6 (4)	C(7)—C(12)—N(11)	118.5 (4)
C(2)—C(1)—C(7)	121.1 (4)	N(11)—C(12)—C(13)	115.2 (4)
C(2)—C(1)—C(6)	118.2 (4)	C(7)—C(12)—C(13)	126.2 (4)
C(1)—C(2)—Br(19)	120.5 (3)	C(12)—C(13)—C(18)	120.7 (4)
C(1)—C(2)—C(3)	121.6 (4)	C(12)—C(13)—C(14)	122.9 (4)
C(3)—C(2)—Br(19)	117.9 (3)	C(14)—C(13)—C(18)	116.3 (4)
C(2)—C(3)—C(4)	119.9 (4)	C(13)—C(14)—C(15)	122.8 (5)
C(3)—C(4)—C(20)	124.7 (4)	C(14)—C(15)—C(16)	119.8 (5)
C(3)—C(4)—C(5)	120.2 (4)	C(15)—C(16)—O(24)	124.9 (5)
C(5)—C(4)—O(20)	115.1 (4)	C(15)—C(16)—C(17)	119.3 (5)
C(4)—C(5)—O(22)	115.8 (4)	C(17)—C(16)—O(24)	115.8 (5)
C(4)—C(5)—C(6)	119.1 (4)	C(16)—C(17)—O(26)	120.5 (5)
C(6)—C(5)—O(22)	125.2 (4)	C(16)—C(17)—C(18)	120.9 (4)
C(1)—C(6)—C(5)	121.0 (4)	C(18)—C(17)—O(26)	118.5 (4)
C(1)—C(7)—C(12)	124.4 (4)	C(13)—C(18)—C(17)	120.7 (4)
C(1)—C(7)—C(8)	118.0 (4)	C(17)—C(18)—O(28)	116.8 (4)
C(8)—C(7)—C(12)	117.4 (4)	C(13)—C(18)—O(28)	122.5 (4)
C(7)—C(8)—N(9)	123.4 (4)	C(4)—O(20)—C(21)	116.2 (4)
C(8)—N(9)—C(10)	114.5 (4)	C(5)—O(22)—C(23)	117.3 (4)
N(9)—C(10)—N(11)	126.9 (4)	C(16)—O(24)—C(25)	119.1 (4)
C(10)—N(11)—C(12)	118.7 (4)	C(17)—O(26)—C(27)	113.3 (4)
C(6)—C(5)—O(22)—C(23)	4.4 (8)	C(4)—C(5)—O(22)—C(23)	-176.1 (5)
C(5)—C(4)—O(20)—C(21)	178.7 (5)	C(3)—C(4)—O(20)—C(21)	-1.7 (8)
C(15)—C(16)—O(24)—C(25)	-6.4 (8)	C(17)—C(16)—O(24)—C(25)	174.7 (5)
C(16)—C(17)—O(26)—C(27)	-81.6 (6)	C(18)—C(17)—O(26)—C(27)	99.6 (6)

bond angle O(28)—H(28)···N(11) 150 (7)°. These results are in good agreement with the analytical and spectroscopic data.

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Acta Cryst. (1990). C46, 663–666

Structure of the Opioid κ -Agonist (–)-(1*R*,5*R*,9*R*,2''*S*)-2'-Hydroxy-2-(2-methoxypropyl)-5,9-dimethyl-6,7-benzomorphan Hydrobromide (I) and its Inactive (–)-(1*R*,5*R*,9*R*,2''*R*) Diastereomer (II)*†

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(Received 26 April 1989; accepted 1 August 1989)

Abstract. (I) C₁₈H₂₈NO₂⁺.Br[−], *M_r* = 370.33, monoclinic, *P*2₁, *a* = 8.446 (1), *b* = 13.137 (3), *c* = 8.6953 (4) Å, β = 113.73 (1)°, *V* = 883.2 (2) Å³, *Z* = 2, *D_m* = 1.37 (2), *D_x* = 1.390 Mg m^{−3}, $\lambda(\text{Cu } K\alpha)$ = 1.54178 Å, μ = 2.31 mm^{−1}, *F*(000) = 388, room temperature, final *R* = 0.041 for 1523 observed reflections. (II) C₁₈H₂₈NO₂⁺.Br[−], *M_r* = 370.33, monoclinic, *P*2₁, *a* = 8.623 (2), *b* = 13.570 (3), *c* = 8.005 (2) Å, β = 107.71 (2)°, *V* = 892.3 (4) Å³, *Z* = 2, *D_m* = 1.36 (2), *D_x* = 1.378 Mg m^{−3}, $\lambda(\text{Mo } K\alpha)$ = 0.71069 Å, μ = 2.29 mm^{−1}, *F*(000) = 388, room temperature, final *R* = 0.046 for 2885 observed reflections. The NCCO conformations in the two molecules are each other's mirror image: (+)-synclinal for (I) and (–)-synclinal for (II). Also, in (I) an intramolecular hydrogen bond is present between H(1) and the O of the *N*-side chain. These observations fit nicely the hypothesis of the κ -opioid pharmacophore.

Introduction. The title compound (I) emerged from a series of *N*-[(tetrahydrofuryl)alkyl] and *N*-(alkoxyalkyl) derivatives of the 6,7-benzomorphan (–)-normetazocine as the most potent opioid compound of the series (at least more than 100 times more active than morphine) and the least toxic one (therapeutic ratio is 27 times that of morphine);

furthermore, the action profile was that of a κ -opioid (Merz & Stockhaus, 1979). In the same study the title compound (II), which is a diastereomer of (I), was found to be completely inactive. Subsequently the κ -opioid properties of these compounds were reassessed *in vitro*: (I) was identified as a full agonist, (II) was inactive (Verlinde & De Ranter, 1988). This pronounced stereoselectivity with regard to the configuration at C2'' was also observed with the *N*-tetrahydrofurfuryl compounds in the series (Merz & Stockhaus, 1979) and has already been evaluated through crystal-structure analysis (Peeters, De Ranter & Blaton, 1982). The crystal structures of (I) and (II) are an essential part of the further analysis of the phenomenon.

Experimental. (I) Crystals obtained at room temperature from a methanol/diethyl ether solution. Density measured by flotation in *n*-heptane/CCl₄, crystal dimensions ~0.6 × 0.4 × 0.4 mm, Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Cu *K*α radiation, $\omega/2\theta$ -scan technique ($2\theta_{\text{max}} = 130^\circ$, $0 \leq h \leq 9$, $0 \leq k \leq 15$, $-10 \leq l \leq 10$), cell dimensions by least-squares refinement of the θ values of 15 reflections with $38 < 2\theta < 43^\circ$, space group *P*2₁ from systematic absences *0k0* for *k* odd (optically active compound). One standard reflection (493) monitored every 30 reflections did not reveal a significant change in intensity. 1572 independent reflections measured, 1523 observed reflections [*I* > 2.5σ(*I*)], Lorentz-polarization corrections, absorption ignored, scattering factors from Cromer & Mann (1968), and Stewart, Davidson & Simpson (1965) (for H), anomalous-dispersion correction for Br

* *Chemical Abstracts* names: (2*R*,6*R*,11*R*,2''*S*)- and (2*R*,6*R*,11*R*,2''*R*)-1,2,3,4,5,6-hexahydro-3-(2-methoxypropyl)-6,11-dimethyl-2,6-methano-3-benzazocin-8-ol.

† Structural Studies of Substituted 6,7-Benzomorphan Compounds. XVI. Part XV: Verlinde, Blaton, Peeters & De Ranter (1989).

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