3·39, C(2)···O(11′) 3·46 Å] occur between carbonyl units related by the crystallographic center of symmetry. All others conform to normal van der Waals contacts.

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Acta Cryst. (1986). C**42**, 1785–1787

Structure of 3-Isopropyl-1*H*-2,1,3-benzothiadiazin-4(3*H*)-one 2,2-Dioxide (Bentazon)

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(*Received* 28 *February* 1986; *accepted* 25 *June* 1986)

Abstract. $C_{10}H_{12}N_2O_3S$, $M_r = 240·3$, monoclinic, space group $P2_1/c$, $a = 11·658$ (2), $b = 7·406$ (1), $c = 13·296$ (3) Å, $\beta = 110·55$ (2)°, $V = 1074·9$ (3) Å^3, $Z = 4$, $F(000) = 504$, $D_x = 1·48$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0·71007$ Å (graphite monochromator using Si standard), $\mu = 2·81$ cm^{-1} (no correction), $T = 173$ K, $R = 0·045$ for 1002 unique reflections with $|F_o| > 3\sigma(F)$. The nitrogen and carbon atoms in the heterocyclic ring are nearly coplanar with the aromatic carbon ring. However, the sulfur is displaced from this plane by 0·70 Å.

Introduction. Bentazon is one of many compounds known to have herbicidal activity. It is believed to inhibit CO_2 fixation and to inhibit the Hill reaction (photosynthetic electron transport) by binding within the chloroplast (Mine & Matsunaki, 1975). Precise structural information about herbicides can aid in drawing inferences concerning the binding sites in the chloroplast and the mechanism for inhibition of CO_2 fixation.

Experimental. Crystal (obtained from Environmental Protection Agency) 0·10 mm on a side, 2815 intensities measured (fixed width ω-scan, each background being measured for one-half of the total scan time), at ~ 173 K on a modified Nicolet four-circle diffractometer ($2\theta \leq 50°$, diffracted-beam monochromated Mo $K\alpha$ radiation); one standard reflection with no appreciable decay; no absorption correction; octants hkl and $\bar{h}\bar{k}l$, h −13→12, k −8→8, l 0→15; 1170 reflections with $F \gtrsim 3\sigma(F)$, averaging equivalent reflections gave 1002 unique reflections ($R_{\rm int} = 0·024$); cell constants refined from 2θ values of 16 reflections in range 22–37°; systematic absences $0k0$, $k = 2n + 1$ and $h0l$, $l = 2n + 1$.

Non-hydrogen-atom positions were identified using *MULTAN*76 (Main, Lessinger, Woolfson, Germain & Declercq, 1976). Hydrogen atoms located in electron difference synthesis (Powell & Jacobson, 1980) or calculated assuming C—H = 1·05 Å and H—C—H = 109·54°. Full-matrix refinement (Lapp & Jacobson, 1979) on $|F|$ to $R = 0·045$ and $wR = 0·045$, $w = 1/\sigma(F)^2$, non-hydrogens anisotropic; hydrogens isotropic; average $\Delta/\sigma = 0·12$; max. and min. heights in

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final $\Delta\rho$ map +0·6 and −0·4 e Å^3; atomic scattering factors from *International Tables for X-ray Crystallography* (Cromer & Waber, 1974).

Table 1. *Refined atomic coordinates* (×10^4) *and thermal parameters* (*e.s.d.'s in parentheses*)

	x	y	z	B(Å^2)
S	2699 (1)	8957 (2)	−1048 (1)	3·05 (5)
O(1)	3670 (3)	8321 (5)	−1351 (3)	5·4 (2)
O(2)	2746 (3)	10730 (4)	−648 (2)	4·0 (2)
O(3)	1312 (4)	6803 (5)	826 (2)	5·6 (2)
N(1)	1450 (3)	8606 (5)	−2036 (3)	3·6 (2)
N(2)	2516 (3)	7567 (5)	−131 (3)	3·3 (2)
C(1)	330 (4)	8590 (6)	−1873 (3)	2·8 (2)
C(2)	−744 (4)	8991 (6)	−2715 (3)	3·3 (2)
C(3)	−1846 (4)	8943 (7)	−2537 (4)	3·6 (2)
C(4)	−1888 (5)	8531 (7)	−1529 (4)	3·7 (2)
C(5)	−833 (5)	8116 (6)	−721 (4)	2·9 (2)
C(6)	298 (4)	8105 (6)	−866 (3)	4·0 (2)
C(7)	1400 (5)	7478 (6)	13 (3)	4·5 (3)
C(8)	3666 (6)	6816 (8)	703 (5)	6·1 (3)
C(9)	4413 (5)	8064 (9)	1427 (5)	6·0 (4)
C(10)	3735 (6)	4925 (8)	692 (5)	6·3 (3)
H(N1)	1484 (36)	8531 (55)	−2716 (31)	2 (1)
H(2)	−615 (34)	9335 (55)	−3426 (30)	2 (1)
H(3)	−2726 (37)	9323 (59)	−3166 (32)	2 (1)
H(4)	−2763 (37)	8496 (58)	−1433 (32)	2 (1)
H(5)	−852 (33)	7855 (51)	−45 (27)	1 (1)
H(9A)	5155 (41)	7479 (65)	1968 (34)	3 (1)
H(9B)	4000 (71)	8787 (115)	1519 (61)	15 (3)
H(9C)	4610 (68)	9033 (114)	1033 (60)	15 (3)
H(10A)	4499 (34)	4503 (55)	1110 (30)	2 (1)
H(10B)	3395 (50)	4212 (87)	244 (45)	8 (2)
H(10C)	3235 (96)	4816 (175)	1339 (84)	18 (4)

Thermal parameters for the hydrogens are isotropic as refined; those for the non-hydrogen atoms are given in the form of equivalent isotropic B's defined by:

$$B_{\text{eq}} = \tfrac{4}{3}[a^2\beta_{11} + b^2\beta_{22} + c^2\beta_{33} + 2ab(\cos\gamma)\beta_{12} + 2ac(\cos\beta)\beta_{13} + 2bc(\cos\alpha)\beta_{23}].$$

Table 2. *Selected distances* (Å) *and angles* (°) (*e.s.d.'s in parentheses*)

S—O(1)	1·409 (4)	C(4)—C(5)	1·355 (7)
S—O(2)	1·411 (4)	C(5)—C(6)	1·398 (7)
S—N(1)	1·603 (4)	C(6)—C(7)	1·476 (6)
S—N(2)	1·666 (4)	C(7)—O(3)	1·227 (5)
N(1)—C(1)	1·397 (6)	C(7)—N(2)	1·381 (6)
C(1)—C(2)	1·388 (6)	N(2)—C(8)	1·514 (7)
C(1)—C(6)	1·398 (6)	C(8)—C(9)	1·397 (9)
C(2)—C(3)	1·386 (6)	C(8)—C(10)	1·403 (8)
C(3)—C(4)	1·392 (7)		
O(1)—S—O(2)	119·4 (2)	C(4)—C(5)—C(6)	122·0 (4)
O(1)—S—N(1)	107·6 (2)	C(5)—C(6)—C(1)	118·3 (4)
O(1)—S—N(2)	108·9 (2)	C(5)—C(6)—C(7)	119·5 (4)
O(2)—S—N(1)	111·4 (2)	C(1)—C(6)—C(7)	122·1 (4)
O(2)—S—N(2)	107·3 (2)	C(6)—C(7)—N(2)	118·4 (4)
N(1)—S—N(2)	100·8 (2)	C(6)—C(7)—O(3)	120·5 (4)
S—N(1)—C(1)	120·2 (3)	N(2)—C(7)—O(3)	121·0 (4)
N(1)—C(1)—C(2)	120·1 (4)	C(7)—N(2)—S	120·0 (3)
N(1)—C(1)—C(6)	119·4 (4)	C(7)—N(2)—C(8)	121·1 (4)
C(2)—C(1)—C(6)	120·5 (4)	C(8)—N(2)—S	117·1 (3)
C(1)—C(2)—C(3)	119·0 (4)	N(2)—C(8)—C(9)	116·0 (5)
C(2)—C(3)—C(4)	121·2 (4)	N(2)—C(8)—C(10)	113·5 (5)
C(3)—C(4)—C(5)	119·0 (5)	C(9)—C(8)—C(10)	130·1 (6)

Discussion. All refined fractional coordinates are given in Table 1 along with equivalent isotropic thermal parameters.* A perspective view of the molecule and the atomic numbering are illustrated in Fig. 1. All C—C bond distances and angles (Table 2) in the ring system are, within standard deviations, equal to the expected values. The S—N(2) distance is longer than S—N(1) [1·666 (4) and 1·603 (4) Å, respectively], indicating less double-bond character in the S—N(2) bond. This is in accord with the involvement of N(2) in amide resonance with the C(7)—O(3) carbonyl. C(7)—N(2) [1·381 (6) Å] is somewhat long relative to normal amides, which is consistent with competition between S and C(7) for the electrons of N(2).

As expected, the aromatic ring containing atoms C(1)—C(6) is very nearly planar. The r.m.s. deviation for the least-squares plane defined by these atoms is 0·010 Å. Atoms N(1), N(2) and C(7) all lie near the plane with perpendicular displacements of 0·056, 0·010 and 0·002 Å, respectively. The 0·698 Å displacement of the sulfur atom from this plane clearly illustrates the puckered nature of the neighboring fused ring containing S, N(1), N(2), C(1), C(6) and C(7). The interplanar angle between the aromatic ring and the plane containing atoms S, O(1) and O(2) is 87·1°. Atoms C(8), C(9) and C(10) define a plane which forms dihedral angles of 92·6 and 69·3° with respect to the aromatic ring and the plane containing the sulfur and two oxygens. The exocyclic isopropyl group, however, appears to be significantly distorted. The C(8) atom lies very close (0·053 Å) to the N(2)—C(9)—C(10) plane, and the angles involving C(8) as the central atom are all considerably larger than normal tetrahedral angles.

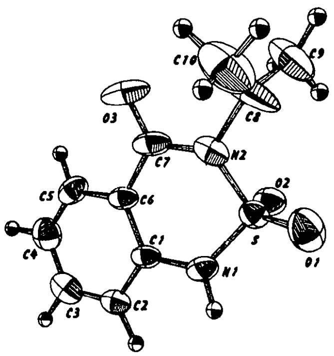

Fig. 1. A perspective view of the title compound, showing atomic numbering.

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* Lists of anisotropic thermal parameters, structure factors and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43185 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Also, the C(8)—C(9) and C(8)—C(10) distances [1·397 (9) and 1·403 (8) Å, respectively] are shorter than expected, while the C(8)—N(2) distance [1·514 (7) Å] is somewhat longer. These atoms were not as well behaved as the others during the refinement, due either to extreme thermal motion or to disorder. Thus the H associated with C(8) has been omitted.

This research was supported by the National Science Foundation URP Program (LEM) and in part by the US Department of Energy under Contract No. W-7405-Eng-82, Office of Basic Energy Sciences, Materials Science Division.

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Acta Cryst. (1986). C**42**, 1787–1789

Structure of Terpin

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(*Received* 27 *May* 1986; *accepted* 27 *June* 1986)

Abstact. *trans*-4-(1-Hydroxyisopropyl)-1-methylcyclohexan-1-ol monohydrate, $C_{10}H_{20}O_2.H_2O$, $M_r = 190{\cdot}28$, monoclinic, *Cc*, $a = 10{\cdot}912$ (3), $b = 22{\cdot}791$ (4), $c = 10{\cdot}705$ (2) Å, $\beta = 120{\cdot}64$ (2)°, $V = 2290{\cdot}85$ Å^3, $Z = 8$, $D_m = 1{\cdot}10$ (2), $D_x = 1{\cdot}11$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·7093 Å, μ(Mo $K\alpha$) = 0·077 mm^{-1}, $F(000) = 848$, $T = 298$ K, final $R = 0{\cdot}047$ for 1665 observed reflections. The title compound has the *trans* configuration with two molecules in the asymmetric unit. The water and *trans*-terpin molecules form a three-dimensional network connected by hydrogen bonding. C—C bonds range from 1·513 (6) to 1·554 (5) Å and C—O bonds from 1·427 (5) to 1·463 (6) Å; bond angles are normal.

Introduction. *Dendrocalamus latiflorus* Munro (Ma Bamboo) also called *Sinocalamus latiflorus* (Munro) or *Bambusa latiflorus* (Munro) is one of the major natural resources in Taiwan.

Tjon Sie Fat (1978), Chao, Ku, Huang, Lin, Lin & Pan (1963), Wu, Liu & Chen (1983), Chen & Juang (1982) and Lou (1983) have reported studies on the constituents of *D. latiflorus*. The chemical constituents were reported to be taxiphyllin and β-cellulose.

We have studied the methanol extract of the stem of *D. latiflorus* Munro collected at Chia-Yi, Taiwan. The following compounds were isolated and characterized: long-chain alkanes, allantoin, tricin, *p*-hydroxybenzaldehyde, long-chain carboxylic acids, β-sitosterol, stigmasterol, β-sitosteroyl-β-glycopyranoside, stigmasteroyl-β-glycopyranoside, acacetin, 2,2′,4,4′-tetramethyl-*trans*-stilbene, and an unknown crystal *X*, $C_{10}H_{22}O_3$, m.p. 375·5 K. The ^{1}H NMR spectrum of compound *X* shows signals between 1·1 and 1·8 p.p.m. (in $CDCl_3$), its IR spectrum indicates the presence of O—H stretching (3240, 3480 cm^{-1}) and C—H stretching (2940 cm^{-1}), and its mass spectrum shows a base peak at 96 and a largest peak at 154 (2%). Since the spectroscopic data were insufficient for structural identification, a single crystal of compound *X* was prepared and an X-ray diffraction study was carried out. The unknown *X* was determined to be *trans*-terpin.

Experimental. IR spectra were recorded with a JASCO model IRA-1 spectrometer, NMR spectra were recorded at 90 MHz on the Varian EM-390 spectrometer, and mass spectra were obtained with a JEOL JMS-300 mass spectrometer. Separations by column chromatography were carried out on silica gel (Merck, Kieselgel 60, 70–230 mesh).

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