

phene ring, whose S atom is not involved in primary coordination to the metal centre, can rotate by 180° from the orientation found here to form a secondary S...M contact with another metal in the lattice.

References

BAXTER, L. A. M., BLAKE, A. J., HEATH, G. A. & STEPHENSON, T. A. (1990). *J. Chem. Soc. Dalton Trans.* In preparation.

GOULD, R. O. & TAYLOR, P. (1985). *CALC.* Program for molecular geometry calculations. Fortran77 version. Univ. of Edinburgh, Scotland.

MALLINSON, P. D. & MUIR, K. W. (1985). *J. Appl. Cryst.* **18**, 51–53.

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

SHELDRIK, G. M. (1986). *SHELX86.* Program for crystal structure solution. Univ. of Göttingen, Federal Republic of Germany.

Acta Cryst. (1990). **C46**, 510–512

The Structures of Two Auxin-Like Compounds: 1,2-Benzisothiazol-3-yl- and 1,2-Benzisoxazol-3-ylacetic Acid

BY P. DOMIANO

*Istituto di Strutturistica Chimica, Università degli Studi di Parma,
Centro di Studio per la Strutturistica Diffraattometrica, Viale delle Scienze, I-43100 Parma, Italy*

AND C. BRANCA

Istituto di Botanica, Università degli Studi di Parma, Viale delle Scienze, I-43100 Parma, Italy

(Received 17 July 1989; accepted 25 September 1989)

Abstract. (I) $C_9H_7NO_2S$, $M_r = 193.22$, monoclinic, space group $C2/c$, $a = 12.263$ (3), $b = 8.989$ (1), $c = 16.779$ (3) Å, $\beta = 111.87$ (1)°, $V = 1716.5$ (6) Å³, $Z = 8$, $D_x = 1.495$ g cm⁻³, $\mu = 30.0$ cm⁻¹, $F(000) = 800$, $R = 0.061$ for 1391 unique observed reflections. (II) $C_9H_7NO_3$, $M_r = 177.16$, monoclinic, space group $P2_1/c$, $a = 19.274$ (3), $b = 5.805$ (1), $c = 15.755$ (3) Å, $\beta = 113.68$ (1)°, $V = 1614.3$ (5) Å³, $Z = 8$, $D_x = 1.458$ g cm⁻³, $\mu = 8.9$ cm⁻¹, $F(000) = 736$, $R = 0.061$ for 2669 unique observed reflections. Data collection was performed at room temperature using Cu $K\alpha$ radiation ($\lambda = 1.54184$ Å) for both compounds. The benzisoxazole and benzisothiazole moieties are planar, the angles between the five- and six-membered rings being 0.6 (1)° for (I) and 1.0 (1) and 1.8 (1)° for the two independent molecules of (II). The plane through the carboxylic acid chain forms with the isothiazole ring in (I) an angle of 77.8 (2)°, corresponding values for angles with the isoxazole ring of molecules A and A' of (II) are 72.5 (2) and 81.9 (2)°; the different conformations of the two independent molecules in the crystal of (II) can be confirmed from the pertinent torsion angles. Bond distances and angles compare well with those found in similar compounds. The N—C distances display typical double-bond character in both compounds. Possible hydrogen bonds occur between the two independent molecules of (II): $O3 \cdots N1' = 2.777$ (3), $O3' \cdots N1^i = 2.812$ (2) Å. In (I) the hydrogen bond

involves the O2 and N1 atoms: $O2 \cdots N1^{ii} = 2.774$ (3) Å [symmetry code: (i) $x, \frac{1}{2} - y, \frac{1}{2} + z$; (ii) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$].

Experimental. Prismatic crystals $0.10 \times 0.10 \times 0.06$ and $0.20 \times 0.20 \times 0.08$ mm for (I) and (II), respectively; cell parameters and orientation matrices were obtained by least-squares refinement using 22 and 29 reflections in the 2θ range 20–40°. Intensities were collected at room temperature on a Siemens AED diffractometer, using $\theta/2\theta$ scan mode, scan speed 3–12° min⁻¹, scan width $(1.20 + 0.14 \tan \theta)^\circ$, θ range 3–70°. The integrated intensities were obtained by a

Table 1. *Final atomic coordinates* ($\times 10^4$, for S $\times 10^5$) *and equivalent isotropic B values* (Å²) for $C_9H_7NO_2S$

	$B_{eq} = (4/3) \sum_i \sum_j B_{ij} a_i a_j$			
	x	y	z	B_{eq}
S1	28153 (5)	935 (7)	50146 (4)	3.36 (2)
N1	2897 (2)	130 (2)	4039 (1)	3.08 (6)
C1	3901 (2)	1402 (2)	5438 (1)	2.57 (6)
C2	4358 (2)	2014 (3)	6272 (2)	3.14 (7)
C3	5226 (2)	3058 (3)	6433 (2)	3.34 (7)
C4	5659 (2)	3514 (3)	5803 (2)	3.43 (7)
C5	5212 (2)	2909 (3)	4992 (2)	3.01 (7)
C6	4317 (2)	1847 (2)	4804 (1)	2.52 (6)
C7	3695 (2)	1070 (2)	4011 (1)	2.61 (6)
C8	3901 (2)	1311 (3)	3193 (2)	2.97 (6)
C9	3322 (2)	2715 (3)	2735 (1)	2.75 (6)
O1	2798 (2)	3591 (2)	3007 (1)	3.96 (6)
O2	3444 (2)	2870 (3)	1989 (1)	4.28 (6)

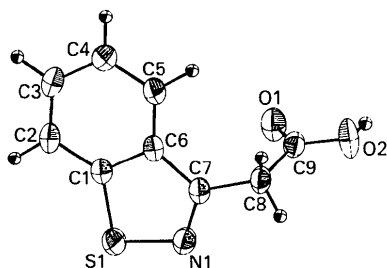
Table 2. Final atomic coordinates ($\times 10^4$) and equivalent isotropic B values (\AA^2) for $\text{C}_9\text{H}_7\text{NO}_3$

$$B_{\text{eq}} = (4/3)\sum_j \beta_j a_j^2$$

	x	y	z	B_{eq}
O1	9504 (1)	-3308 (2)	250 (1)	3.52 (4)
N1	8857 (1)	-1859 (3)	-76 (1)	3.50 (4)
C1	10048 (1)	-2206 (3)	979 (1)	2.84 (5)
C2	10781 (1)	-2993 (3)	1493 (1)	3.41 (5)
C3	11228 (1)	-1554 (4)	2194 (1)	3.82 (5)
C4	10962 (1)	562 (4)	2381 (1)	3.92 (5)
C5	10237 (1)	1301 (3)	1863 (1)	3.35 (5)
C6	9772 (1)	-121 (3)	1138 (1)	2.73 (5)
C7	9014 (1)	-30 (3)	439 (1)	2.85 (5)
C8	8442 (1)	1853 (3)	258 (1)	3.17 (5)
C9	7829 (1)	1292 (3)	593 (1)	3.00 (5)
O2	7726 (1)	-538 (3)	860 (2)	5.58 (7)
O3	7421 (1)	3139 (3)	549 (1)	4.40 (5)
O1'	5576 (1)	1918 (2)	776 (1)	3.99 (4)
N1'	6228 (1)	3324 (3)	1111 (1)	3.97 (5)
C1'	5029 (1)	3042 (3)	957 (1)	2.96 (5)
C2'	4290 (1)	2305 (3)	717 (1)	3.60 (5)
C3'	3838 (1)	3771 (4)	954 (1)	3.72 (5)
C4'	4107 (1)	5865 (4)	1418 (1)	3.80 (5)
C5'	4843 (1)	6546 (3)	1650 (1)	3.30 (5)
C6'	5310 (1)	5100 (3)	1407 (1)	2.73 (4)
C7	6078 (1)	5157 (3)	1476 (1)	3.23 (5)
C8'	6662 (1)	6975 (4)	1887 (2)	4.09 (6)
C9'	7194 (1)	6453 (3)	2874 (1)	3.42 (5)
O2'	7176 (1)	4717 (3)	3271 (1)	5.05 (5)
O3'	7681 (1)	8143 (3)	3239 (1)	4.62 (5)

Table 3. Selected bond distances (\AA), bond angles ($^\circ$) and torsion angles ($^\circ$) with their e.s.d.'s for $\text{C}_9\text{H}_7\text{NO}_2\text{S}$

S1—N1	1.678 (3)	S1—C1	1.719 (2)
N1—C7	1.307 (3)	C1—C2	1.411 (3)
C1—C6	1.399 (4)	C2—C3	1.367 (4)
C3—C4	1.410 (4)	C4—C5	1.376 (4)
C5—C6	1.399 (3)	C6—C7	1.443 (3)
C7—C8	1.500 (4)	C8—C9	1.510 (3)
C9—O1	1.208 (3)	C9—O2	1.324 (4)
N1—S1—C1	94.1 (1)	S1—N1—C7	111.5 (2)
S1—C1—C6	109.1 (2)	S1—C1—C2	129.6 (2)
C2—C1—C6	121.3 (2)	C1—C2—C3	117.2 (2)
C2—C3—C4	122.3 (2)	C3—C4—C5	120.3 (3)
C4—C5—C6	118.8 (2)	C1—C6—C5	120.1 (2)
C5—C6—C7	129.7 (2)	C1—C6—C7	110.2 (2)
N1—C7—C6	115.2 (2)	C6—C7—C8	124.2 (2)
N1—C7—C8	120.6 (2)	C7—C8—C9	112.2 (2)
C8—C9—O2	111.8 (2)	C8—C9—O1	124.6 (2)
O1—C9—O2	123.6 (2)		
S1—N1—C7—C8	-178.6 (2)	C5—C6—C7—C8	-1.4 (4)
C1—C6—C7—C8	178.4 (2)	C6—C7—C8—C9	-77.8 (3)
N1—C7—C8—C9	100.8 (3)	C7—C8—C9—O1	3.3 (4)
C7—C8—C9—O2	-176.0 (2)		

Fig. 1. Drawing of compound $\text{C}_9\text{H}_7\text{NO}_2\text{S}$ with thermal ellipsoids at the 50% probability level.Table 4. Selected bond distances (\AA), bond angles ($^\circ$) and torsion angles ($^\circ$) with their e.s.d.'s for $\text{C}_9\text{H}_7\text{NO}_3$

O1—N1	1.418 (2)	O1—C1	1.364 (2)
N1—C7	1.297 (2)	C1—C2	1.394 (2)
C1—C6	1.384 (3)	C2—C3	1.376 (3)
C3—C4	1.407 (3)	C4—C5	1.375 (3)
C5—C6	1.402 (2)	C6—C7	1.434 (2)
C7—C8	1.497 (3)	C8—C9	1.511 (3)
C9—O2	1.189 (3)	C9—O3	1.315 (2)
O1'—N1'	1.411 (2)	O1'—C1'	1.364 (3)
N1'—C7'	1.296 (3)	C1'—C2'	1.387 (3)
C1'—C6'	1.383 (2)	C2'—C3'	1.373 (3)
C3'—C4'	1.405 (3)	C4'—C5'	1.373 (3)
C5'—C6'	1.393 (3)	C6'—C7'	1.440 (3)
C7'—C8'	1.489 (3)	C8'—C9'	1.510 (3)
C9'—O2'	1.194 (3)	C9'—O3'	1.319 (2)
N1—O1—C1	107.1 (1)	O1—N1—C7	108.0 (2)
O1—C1—C6	109.9 (2)	O1—C1—C2	126.4 (2)
C2—C1—C6	123.7 (2)	C1—C2—C3	115.4 (2)
C2—C3—C4	122.3 (2)	C3—C4—C5	121.1 (2)
C4—C5—C6	117.7 (2)	C1—C6—C5	119.8 (2)
C5—C6—C7	136.4 (2)	C1—C6—C7	103.9 (1)
N1—C7—C6	111.1 (1)	C6—C7—C8	128.2 (2)
N1—C7—C8	120.6 (2)	C7—C8—C9	113.3 (2)
C8—C9—O3	110.0 (2)	C8—C9—O2	125.6 (2)
O2—C9—O3	124.5 (2)		
N1'—O1'—C1'	107.0 (1)	O1'—N1'—C7'	108.5 (2)
O1'—C1'—C6'	110.1 (2)	O1'—C1'—C2'	126.2 (2)
C2'—C1'—C6'	123.7 (2)	C1'—C2'—C3'	115.4 (2)
C2'—C3'—C4'	122.4 (2)	C3'—C4'—C5'	120.9 (2)
C4'—C5'—C6'	117.8 (2)	C1'—C6'—C5'	119.8 (2)
C5'—C6'—C7'	136.4 (2)	C1'—C6'—C7'	103.8 (2)
N1'—C7'—C6'	110.7 (2)	C6'—C7'—C8'	128.7 (2)
N1'—C7'—C8'	120.7 (2)	C7'—C8'—C9'	112.8 (2)
C8'—C9'—O3'	111.7 (2)	C8'—C9'—O2'	123.9 (2)
O2'—C9'—O3'	124.4 (2)		

O1—N1—C7—C8	179.2 (2)	C5—C6—C7—C8	1.2 (4)
C1—C6—C7—C8	-178.8 (2)	C6—C7—C8—C9	-104.3 (2)
N1—C7—C8—C9	77.0 (2)	C7—C8—C9—O2	-10.0 (3)
C7—C8—C9—O3	169.9 (2)		
O1'—N1'—C7'—C8'	-179.8 (2)	C5'—C6'—C7'—C8'	1.0 (4)
C1'—C6'—C7'—C8'	179.3 (2)	C6'—C7'—C8'—C9'	96.7 (2)
N1'—C7'—C8'—C9'	-83.8 (3)	C7'—C8'—C9'—O2'	3.6 (3)
C7'—C8'—C9'—O3'	-176.7 (2)		

modified version (Belletti, Uguzzoli, Cantoni & Pasquinelli, 1979) of the Lehmann & Larsen (1974) procedure. Standard reflections [00 $\bar{4}$ for (I), $\bar{1}\bar{1}$.2.10 for (II)] measured after every 100 reflections showed variations of 0.3 and 0.2%. Intensities [1789 for (I) in index range $h \pm 13$, k 0–10, l 0–20 and 3481 for (II) in index range $h \pm 21$, k 0–7, l 0–19] were corrected for Lorentz and polarization effects but not for absorption. The structures were solved by direct methods with *SHELX86* (Sheldrick, 1986) and refined by anisotropic full-matrix least squares (all H atoms from difference synthesis, refined isotropically) on *F* using *SHELX76* (Sheldrick, 1976), to an *R* value of 0.061 [$wR = 0.064$; 1391 unique observed reflections with $I > 2\sigma(I)$] for (I) and of 0.061 [$wR = 0.069$; 2669 unique observed reflections with $I > 2\sigma(I)$] for (II); $w = 1/\sigma^2(F)$. The refined parameters were 146 and 291 with corresponding data/parameter ratios of 9.5 and 9.2 for (I) and (II), respectively. Goodness of fit 0.760 and 0.665 for (I) and (II), respectively. Max. $\Delta/\sigma = 0.17$ for (I), 0.13 for (II). Max., min. heights in

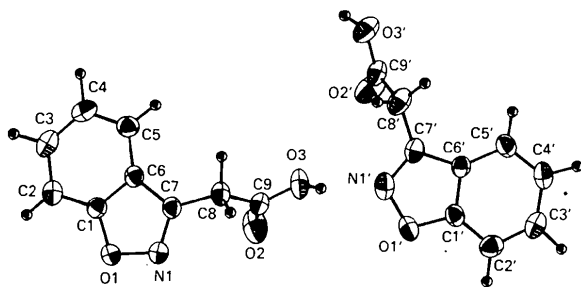


Fig. 2. Drawing of compound C₉H₇NO₃ with thermal ellipsoids at the 50% probability level.

final difference Fourier synthesis 0.62, -0.50 e Å⁻³ for (I), 0.26, -0.35 e Å⁻³ for (II). Scattering factors from *International Tables for X-ray Crystallography* (1974). All standard calculations were performed with *CRYSRULER* (Rizzoli, Sangermano, Calestani & Andreotti, 1987) on an XT IBM 286 computer. Final atomic coordinates are given in Tables 1 and 2,* selected bond distances and angles are in Tables 3 and 4. Figs. 1 and 2 are *ORTEP* (Johnson, 1976) drawings of the molecules for (I) and (II), respectively.

Related literature. With the aim to understand better the auxin activity of several classes of compounds (3-indolylacetic, 1-naphthaleneacetic, 3-indolylbutyric and 2,4-chlorophenoxyacetic acids), an intensive search of the Cambridge Structural Database System (CSDS) (Allen *et al.*, 1979), accessed through the Servizio Italiano di Diffusione Dati Cristallografici (CNR, Parma), was performed. Since neither benzisothiazole nor benzisoxazole derivatives of acetic acid were found from this search, the crystal

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52311 (33 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Acta Cryst. (1990). **C46**, 512-515

Structure of Sulfonosine

BY STEVEN B. LARSON,* NAEEM B. HANNA, GANAPATHI R. REVANKAR AND ROLAND K. ROBINS

ICN Nucleic Acid Research Institute, 3300 Hyland Avenue, Costa Mesa, CA 92626, USA

(Received 11 August 1989; accepted 13 October 1989)

Abstract. 2-Amino-9-(β-D-ribofuranosyl)-9H-purine-6-sulfonamide (I) (sulfonosine), C₁₀H₁₄N₆O₆S, *M_r* =

structure determinations of the title compounds were undertaken in order to gain more information so that a complete series of structural data could be correlated. Details on the correlation between structure and biological activity on six different auxins in *in vitro* regeneration of tomato plants are reported elsewhere (Branca, Bucci, Domiano, Ricci, Torelli & Bassi, 1989).

Other structurally similar molecules have been studied by Allen, Kennard, Watson, Brammer, Orpen & Taylor (1987); Gaetani, Vitali, Mangia, Nardelli & Pelizzi (1972); Lisgarten & Palmer (1988).

References

- ALLEN, F. H., BELLARD, S., BRICE, M. D., CARTWRIGHT, B. A., DOUBLEDAY, A., HIGGS, H., HUMMELINK, T., HUMMELINK-PETERS, B. G., KENNARD, O., MOTHERWELL, W. D. S., RODGERS, J. R. & WATSON, D. G. (1979). *Acta Cryst.* **B35**, 2331-2339.
- ALLEN, F. H., KENNARD, O., WATSON, D. G., BRAMMER, L., ORPEN, A. G. & TAYLOR, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1-S19.
- BELLETTI, D., UGOZZOLI, F., CANTONI, A. & PASQUINELLI, G. (1979). Internal Report No. 1-3/79. Centro di Studio per la Strutturistica Diffraattometrica del CNR, Univ. of Parma, Italy.
- BRANCA, C., BUCCI, G., DOMIANO, P., RICCI, A., TORELLI, A. & BASSI, M. (1989). *Plant Sci.* Submitted.
- GAETANI, E., VITALI, T., MANGIA, A., NARDELLI, M. & PELIZZI, G. (1972). *J. Chem. Soc. Perkin Trans. 2*, pp. 2125-2129.
- International Tables for X-ray Crystallography* (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
- JOHNSON, C. K. (1976). *ORTEP*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- LEHMANN, M. S. & LARSEN, F. K. (1974). *Acta Cryst.* **A30**, 580-584.
- LISGARTEN, J. N. & PALMER, R. A. (1988). *Acta Cryst.* **C44**, 2013-2016.
- RIZZOLI, C., SANGERMANO, V., CALESTANI, G. & ANDREOTTI, G. D. (1987). *J. Appl. Cryst.* **20**, 436-439.
- SHELDRIK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.
- SHELDRIK, G. M. (1986). *SHELX86*. Program for crystal structure solution. Univ. of Göttingen, Federal Republic of Germany.

346.32, monoclinic, *P*2₁, *a* = 6.2899 (12), *b* = 13.276 (3), *c* = 8.4161 (14) Å, β = 105.686 (16)°, *V* = 676.6 (2) Å³, *Z* = 2, *D_x* = 1.700 g cm⁻³, Mo *K*α (λ = 0.71073 Å), μ = 2.723 cm⁻¹, *F*(000) = 360, *T* =

* To whom correspondence should be addressed.