(a)   (b)

Fig. 2. Crystal packing diagrams of (1).H$_2$O with C—H H atoms omitted and hydrogen bonds drawn as thin lines. (a) View along the b axis, illustrating the base stacking and the hydrogen-bond linking of molecules through the water along the a axis. The interplanar spacings of the bases are 3·38 and 3·54 Å. (b) View along the a axis showing the partial base overlap.

Related literature. Henry *et al.* (1989) report the synthesis of the title compound and show that the immune system stimulatory effects are similar to those of 7-methyl-8-oxo-7,8-dihydroguanosine. The crystal structure of (1) is isomorphous to that of the 8-oxo nucleoside (Larson, Cottam & Robins, 1989). The C8—S13 bond length is 1·664 (2) Å; the r.m.s.d. of all other bond lengths involving non-H atoms is 0·006 Å. The r.m.s.d. of all bond angles is 0·54°. Structures of 8-substituted guanosines, most of which have immunomodulatory properties, show a predominance of *syn* conformation [*e.g.* 8-bromo-guanosine (Tavale & Sobell, 1970), 8-chloro-guanosine (Birnbaum, Lassota & Shugar, 1984), and 8-methylguanosine (Hamada, Honda, Fujii, Fujiwara & Tomita, 1985)] which may be partially responsible for such activity (Katze, 1985). Conformational parameters follow the conventions of Altona & Sundaralingam (1972).

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3-Hydroxy-1,3-bis(2-thienyl)prop-2-en-1-one

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Abstract. C$_{11}$H$_8$O$_2$S$_2$, M_r = 236·31, monoclinic, Cc, a = 27·172 (18), b = 5·282 (3), c = 21·835 (17) Å, β = 136·23 (3)°, V = 2168 Å^3, Z = 8, D_x = 1·448 Mg m^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ = 0·450 mm^{-1}, $F(000)$ = 976, T = 298 K, R = 0·0687 for 786 unique observed reflections. The two independent molecules in the asymmetric unit are essentially identical: both are approximately planar, with no non-H atom deviating by more than 0·10 Å from the molecular mean plane. The thiophene S atoms are *cis* to the O atoms of the central moiety, whose molecular parameters indicate

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a delocalized enol rather than a dione. The O-bound H atoms could not be located and are probably disordered.

Experimental. Colourless lath, $1.19 \times 0.35 \times 0.039$ mm, STADI-4 four-circle diffractometer, graphite-monochromated Mo $K\alpha$ radiation, cell parameters from 13 reflections with $20 < 2\theta < 25°$. For data collection, ω–2θ scans with ω-scan width $(2.10 + 0.347 \tan\theta)°$, $2\theta_{max} = 45°$, h $-28 \rightarrow 20$, k $0 \rightarrow 5$, l $0 \rightarrow 23$, no significant crystal movement or decay, no absorption correction, 1599 unique reflections, 786 with $F > 4\sigma(F)$ for structure solution [by automatic direct methods (Sheldrick, 1986)] and refinement [using full-matrix least squares on F (Sheldrick, 1976)]. Anisotropic thermal parameters for S and O, isotropic for C; H atoms in fixed, calculated positions. Despite the rather extreme β angle, there were no serious correlation problems. At convergence, $R = 0.0687$, $wR = 0.0900$, $w^{-1} = \sigma^2(F) + 0.0352F^2$, $S = 1.116$ for 159 parameters, max. shift/e.s.d. in final cycle 0.07, max. and min. residues in final difference Fourier synthesis 0.55, -0.37 e Å^{-3} respectively. Scattering factors were inlaid (Sheldrick, 1976). Atom coordinates and isotropic thermal parameters are given in Table 1 while selected bond lengths and angles appear in Table 2.* The atom-numbering scheme for the molecule is shown in Fig. 1, which was generated using *ORTEP* (Mallinson & Muir, 1985). Molecular geometry calculations were performed using *CALC* (Gould & Taylor, 1985).

Related literature. The present compound HL, upon deprotonation to L^-, gives the neutral complex ML_2 where $M = Cu^{2+}$, Pd^{2+}. We have determined the crystal structures of these (Baxter, Blake, Heath & Stephenson, 1990) and have shown that the thio-

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* Lists of structure factors, anisotropic thermal parameters, torsion angles and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52316 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
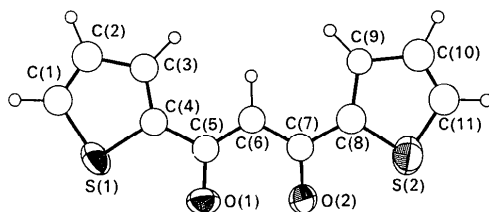

Fig. 1. View of one molecule of type A showing atom-numbering scheme; the atoms of the type-B molecule have the corresponding primed labels. Thermal ellipsoids are drawn at the 30% probability level, excepting those of H which have artificial radii of 0.10 Å for clarity.

Table 1. *Atomic coordinates and isotropic thermal parameters with e.s.d.'s*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}/U_{iso} (Å²)
S(1)	0.1405	0.3591 (10)	0.3813	0.092 (4)
O(1)	0.0430 (6)	−0.0460 (22)	0.2594 (7)	0.088 (6)
O(2)	−0.0588 (6)	−0.3510 (21)	0.1793 (7)	0.086 (6)
S(2)	−0.1811 (4)	−0.5916 (10)	0.1223 (5)	0.112 (4)
S(1')	0.2786 (3)	−1.5878 (11)	0.3428 (4)	0.100 (4)
O(1')	0.1741 (6)	−1.3794 (21)	0.1687 (7)	0.089 (6)
O(2')	0.0757 (6)	−1.0939 (20)	0.0437 (7)	0.089 (6)
S(2')	−0.0348 (3)	−0.7115 (12)	−0.0509 (4)	0.103 (4)
C(1)	0.1569 (8)	0.595 (3)	0.4496 (10)	0.055 (3)
C(2)	0.1133 (9)	0.587 (3)	0.4570 (11)	0.059 (3)
C(3)	0.0594 (8)	0.3901 (24)	0.4025 (10)	0.051 (3)
C(4)	0.0682 (8)	0.255 (3)	0.3580 (9)	0.050 (3)
C(5)	0.0230 (8)	0.0490 (24)	0.2939 (9)	0.048 (3)
C(6)	−0.0353 (8)	−0.0329 (24)	0.2741 (10)	0.048 (3)
C(7)	−0.0751 (8)	−0.2363 (24)	0.2147 (10)	0.049 (3)
C(8)	−0.1383 (9)	−0.3340 (25)	0.1902 (10)	0.059 (3)
C(9)	−0.1699 (8)	−0.2323 (24)	0.2166 (9)	0.043 (3)
C(10)	−0.2319 (9)	−0.408 (3)	0.1732 (11)	0.067 (3)
C(11)	−0.2411 (9)	−0.582 (3)	0.1251 (10)	0.062 (3)
C(1')	0.3202 (10)	−1.561 (3)	0.4477 (11)	0.069 (3)
C(2')	0.2957 (10)	−1.368 (3)	0.4587 (12)	0.068 (3)
C(3')	0.2414 (8)	−1.2239 (25)	0.3809 (9)	0.050 (3)
C(4')	0.2259 (8)	−1.3237 (24)	0.3112 (10)	0.048 (3)
C(5')	0.1725 (8)	−1.2499 (25)	0.2169 (10)	0.050 (3)
C(6')	0.1241 (9)	−1.054 (3)	0.1847 (11)	0.063 (3)
C(7')	0.0748 (7)	−0.9829 (23)	0.0948 (9)	0.043 (3)
C(8')	0.0247 (8)	−0.7892 (24)	0.0612 (9)	0.050 (3)
C(9')	0.0122 (7)	−0.6250 (24)	0.1031 (9)	0.042 (3)
C(10')	−0.0402 (10)	−0.453 (3)	0.0421 (12)	0.071 (3)
C(11')	−0.0705 (10)	−0.486 (3)	−0.0425 (12)	0.073 (3)

Table 2. *Bond lengths (Å) and angles (°) with e.s.d.'s*

S(1)—C(1)	1.738 (20)	S(1')—C(1')	1.675 (24)
S(1)—C(4)	1.726 (19)	S(1')—C(4')	1.746 (20)
C(1)—C(2)	1.31 (3)	C(1')—C(2')	1.33 (3)
C(2)—C(3)	1.46 (3)	C(2')—C(3')	1.42 (3)
C(3)—C(4)	1.36 (3)	C(3')—C(4')	1.36 (3)
C(4)—C(5)	1.47 (3)	C(4')—C(5')	1.48 (3)
C(5)—O(1)	1.308 (23)	C(5')—O(1')	1.283 (24)
C(5)—C(6)	1.38 (3)	C(5')—C(6')	1.40 (3)
C(6)—C(7)	1.41 (3)	C(6')—C(7')	1.41 (3)
C(7)—O(2)	1.286 (24)	C(7')—O(2')	1.278 (23)
C(7)—C(8)	1.47 (3)	C(7')—C(8')	1.41 (3)
C(8)—C(9)	1.44 (3)	C(8')—C(9')	1.47 (3)
C(8)—S(2)	1.706 (22)	C(8')—S(2')	1.750 (20)
C(9)—C(10)	1.51 (3)	C(9')—C(10')	1.37 (3)
C(10)—C(11)	1.28 (3)	C(10')—C(11')	1.39 (3)
C(11)—S(2)	1.677 (23)	C(11')—S(2')	1.626 (25)
C(1)—S(1)—C(4)	90.8 (9)	C(1')—S(1')—C(4')	91.3 (11)
S(1)—C(1)—C(2)	112.8 (16)	S(1')—C(1')—C(2')	112.3 (18)
C(1)—C(2)—C(3)	113.0 (18)	C(1')—C(2')—C(3')	114.6 (20)
C(2)—C(3)—C(4)	111.5 (17)	C(2')—C(3')—C(4')	110.2 (18)
S(1)—C(4)—C(3)	111.8 (14)	S(1')—C(4')—C(3')	111.5 (14)
S(1)—C(4)—C(5)	120.5 (14)	S(1')—C(4')—C(5')	117.4 (14)
C(3)—C(4)—C(5)	127.7 (17)	C(3')—C(4')—C(5')	131.0 (18)
C(4)—C(5)—O(1)	115.0 (16)	C(4')—C(5')—O(1')	114.9 (17)
C(4)—C(5)—C(6)	120.8 (17)	C(4')—C(5')—C(6')	121.1 (18)
O(1)—C(5)—C(6)	124.2 (17)	O(1')—C(5')—C(6')	124.0 (18)
C(5)—C(6)—C(7)	118.3 (17)	C(5')—C(6')—C(7')	120.0 (18)
C(6)—C(7)—O(2)	122.9 (18)	C(6')—C(7')—O(2')	119.7 (17)
C(6)—C(7)—C(8)	121.4 (17)	C(6')—C(7')—C(8')	120.4 (17)
O(2)—C(7)—C(8)	115.7 (17)	O(2')—C(7')—C(8')	119.9 (16)
C(7)—C(8)—C(9)	126.8 (18)	C(7')—C(8')—C(9')	132.4 (17)
C(7)—C(8)—S(2)	118.6 (15)	C(7')—C(8')—S(2')	117.8 (14)
C(9)—C(8)—S(2)	114.6 (15)	C(9')—C(8')—S(2')	109.7 (13)
C(8)—C(9)—C(10)	103.6 (16)	C(8')—C(9')—C(10')	109.2 (16)
C(9)—C(10)—C(11)	115.2 (19)	C(9')—C(10')—C(11')	114.4 (20)
C(10)—C(11)—S(2)	115.6 (17)	C(10')—C(11')—S(2')	114.5 (18)
C(8)—S(2)—C(11)	90.8 (11)	C(8')—S(2')—C(11')	92.1 (11)

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$\cdots M$ contact with another metal in the lattice.

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

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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) Å^3, $Z = 8$, $D_x = 1.495$ 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) Å^3, $Z = 8$, $D_x = 1.458$ 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 $(1.20 + 0.14 \tan\theta)°$, 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* (Å^2) *for* $C_9H_7NO_2S$

$$B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	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)