

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

O(1)—C(2)	1.325 (3)	O(1)—C(1')	1.473 (2)
C(2)—C(3)	1.485 (3)	C(2)—O(21)	1.196 (3)
C(3)—C(4)	1.330 (4)	C(3)—N(31)	1.393 (3)
C(4)—C(41)	1.472 (3)	N(31)—C(32)	1.153 (4)
C(41)—C(42)	1.381 (4)	C(41)—C(46)	1.392 (4)
C(42)—C(43)	1.386 (4)	C(43)—C(44)	1.362 (4)
C(44)—C(45)	1.370 (5)	C(45)—C(46)	1.395 (4)
C(1')—C(2')	1.515 (3)	C(1')—C(6')	1.523 (3)
C(2')—C(3')	1.523 (3)	C(3')—C(3'')	1.529 (4)
C(3')—C(4')	1.514 (4)	C(4')—C(5')	1.519 (3)
C(5')—C(6')	1.543 (3)	C(6')—C(7')	1.575 (3)
C(7')—C(8')	1.546 (3)	C(7')—C(9')	1.532 (3)
C(7')—C(71')	1.534 (3)	C(71')—C(72')	1.388 (3)
C(71')—C(76')	1.387 (3)	C(72')—C(73')	1.372 (4)
C(73')—C(74')	1.371 (4)	C(74')—C(75')	1.372 (5)
C(75')—C(76')	1.386 (4)		
C(2)—O(1)—C(1')	118.1 (2)	O(1)—C(2)—C(3)	112.0 (2)
O(1)—C(2)—O(21)	125.3 (2)	C(3)—C(2)—O(21)	122.7 (2)
C(2)—C(3)—C(4)	125.0 (2)	C(2)—C(3)—N(31)	112.5 (2)
C(4)—C(3)—N(31)	122.4 (2)	C(3)—C(4)—C(41)	129.9 (2)
C(3)—N(31)—C(32)	176.7 (3)	C(4)—C(41)—C(42)	117.8 (2)
C(4)—C(41)—C(46)	123.9 (2)	C(42)—C(41)—C(46)	118.4 (2)
C(41)—C(42)—C(43)	121.5 (2)	C(42)—C(43)—C(44)	119.7 (3)
C(43)—C(44)—C(45)	120.1 (3)	C(44)—C(45)—C(46)	120.8 (3)
C(41)—C(46)—C(45)	119.6 (3)	O(1)—C(1')—C(2')	106.4 (2)
O(1)—C(1')—C(6')	108.4 (2)	C(2')—C(1')—C(6')	113.6 (2)
C(1')—C(2')—C(3')	112.3 (2)	C(2')—C(3')—C(3'')	110.6 (2)
C(2')—C(3')—C(4')	108.3 (2)	C(3'')—C(3')—C(4')	112.9 (2)
C(3')—C(4')—C(5')	112.1 (2)	C(4')—C(5')—C(6')	113.2 (2)
C(1')—C(6')—C(5')	108.6 (2)	C(1')—C(6')—C(7')	113.8 (2)
C(5')—C(6')—C(7')	112.7 (2)	C(6')—C(7')—C(8')	110.3 (2)
C(6')—C(7')—C(9')	111.2 (2)	C(8')—C(7')—C(9')	106.8 (2)
C(6')—C(7')—C(71')	110.7 (2)	C(8')—C(7')—C(71')	106.1 (2)
C(9')—C(7')—C(71')	111.5 (2)	C(7')—C(71')—C(72')	120.1 (2)
C(7')—C(71')—C(76')	123.8 (2)	C(72')—C(71')—C(76')	116.1 (2)
C(71')—C(72')—C(73')	122.6 (2)	C(72')—C(73')—C(74')	120.4 (3)
C(73')—C(74')—C(75')	118.5 (3)	C(74')—C(75')—C(76')	121.0 (3)
C(71')—C(76')—C(75')	121.3 (2)		
C(1')—O(1)—C(2)—C(3)	176.4 (2)	C(2)—C(3)—C(4)—C(41)	-175.7 (3)
O(1)—C(2)—C(3)—C(4)	-5.9 (4)	N(31)—C(3)—C(4)—C(41)	-0.7 (4)
O(21)—C(2)—C(3)—N(31)	-1.5 (3)	C(3)—C(4)—C(41)—C(46)	-26.6 (5)

blocked-cascade refinement (on F) of 263 parameters with *SHELXTL* (Sheldrick, 1983) converged at $R = 0.043$, $wR = 0.047$ [$w^{-1} = \sigma^2(F) + 0.0005F^2$], $S = 1.34$, $(\Delta/\sigma)_{\max} = 0.02$ in the last cycle; $-0.11 < \Delta\rho < 0.12 \text{ e } \text{Å}^{-3}$ in the final difference map. Scattering factors were obtained from *International Tables for X-ray Crystallography* (1974, Vol. IV).

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Structures of Two Acylpyridinium Salts and One Simple Pyridinium Salt

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Abstract. *N*-Phenoxycarbonyl-4-dimethylamino-pyridinium chloride (I), $\text{C}_{14}\text{H}_{15}\text{N}_2\text{O}_2^+\text{Cl}^-$, $M_r =$

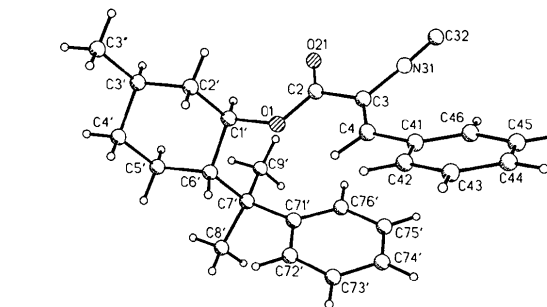


Fig. 1. Perspective view with the atom numbering.

Final atomic parameters are listed in Table 1,* bond lengths and angles, as well as selected torsion angles, in Table 2. Fig. 1 shows the molecular conformation.

Related literature. The title compound is an educt for the diastereoselective 1,4-addition of organocopper reagents (Oppolzer & Löher, 1981) because one face of the double bond is shielded.

We thank Professor U. Schöllkopf (University of Göttingen) for providing the sample.

* 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 55196 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: SE1000]

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278.7, monoclinic, $P2_1/c$, $a = 17.397(4)$, $b = 5.865(2)$, $c = 13.482(5)$ Å, $\beta = 104.26(2)^\circ$, $V = 1333.2 \text{ Å}^3$, $Z = 4$, $D_x = 1.389 \text{ g cm}^{-3}$, $\lambda(\text{Mo K}\alpha) = 0.71069 \text{ Å}$, $\mu = 2.83 \text{ cm}^{-1}$, $F(000) = 584$, $T = 198 \text{ K}$,

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Table 1. *Experimental details*

	(I)	(II)	(III)
Crystal			
Habit	Needles	Prisms	Prisms
Size (mm)	0.45 × 0.10 × 0.08	0.56 × 0.20 × 0.20	0.42 × 0.30 × 0.25
Lattice parameters			
No. of reflections	20	28	38
2θ range (°)	10.1–27.5	6.9–21.9	13.4–40.1
Reflection range			
<i>h</i>	–22 to 21	–11 to 11	–12 to 22
<i>k</i>	–7 to 0	–12 to 12	–8 to 9
<i>l</i>	0 to 17	–25 to 25	–18 to 16
Maximum sinθ/λ (Å ^{–1})	0.650	0.650	0.650
Check reflections	204,015,215	023,115,322	311,400,206
Variation (%)	5,6,6	7,8,8	5,5,6
Reflections			
Collected	3452	13350	4087
Unique observed	2631	5033	1501
<i>R</i> _{int}	0.017	0.026	0.038
Observed criterion	<i>I</i> > 2σ(<i>I</i>)	<i>I</i> > 4σ(<i>I</i>)	<i>I</i> > 3σ(<i>I</i>)
No. of parameters	173	380	92
<i>R</i>	0.049	0.0511	0.0462
<i>wR</i>	0.055	0.0584	0.0523
<i>S</i>	1.73	1.98	1.49
Secondary-extinction parameter, <i>χ</i> , in $F^* = F[1 + 0.002\chi F^2/\sin(2\theta)]^{-1/4}$	0.0010 (3)	0.0006 (2)	0.00002 (14)
Weighting factor, <i>g</i> , in $w^{-1} = \sigma^2(F) + gF^2$	0.0003	0.0002	0.0005
Fourier differences peaks			
Minimum (e Å ^{–3})	–0.29	–0.21	–0.28
Maximum (e Å ^{–3})	0.50	0.34	0.44
Maximum Δσ	0.002	0.220	0.052

$R = 0.0486$ for 2631 unique reflections with $I > 2\sigma(I)$. *N*-Benzoyl-4-dimethylaminopyridinium tetraphenylborate (II), C₁₄H₁₅N₂O⁺.B(C₆H₅)₄[–], $M_r = 546.5$, triclinic, PI , $a = 9.086$ (2), $b = 9.328$ (2), $c = 19.494$ (5) Å, $\alpha = 79.03$ (2), $\beta = 78.83$ (2), $\gamma = 64.53$ (2)°, $V = 1452.6$ Å³, $Z = 2$, $D_x = 1.249$ g cm^{–3}, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 0.69$ cm^{–1}, $F(000) = 580$, $T = 172$ K, $R = 0.0511$ for 5033 unique reflections with $I > 4\sigma(I)$. 4-Dimethylaminopyridinium chloride (III), C₇H₁₁N₂⁺.Cl[–], $M_r = 158.6$, monoclinic, $C2/c$, $a = 17.113$ (3), $b = 7.460$ (2), $c = 14.570$ (3) Å, $\beta = 120.84$ (1)°, $V = 1597.0$ Å³, $Z = 8$, $D_x = 1.319$ g cm^{–3}, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 4.03$ cm^{–1}, $F(000) = 672$, $T = 192$ K, $R = 0.0462$ for 1501 unique reflections with $I > 3\sigma(I)$. (I) and (II) are *N*-acylpyridinium salts; (III) is a pyridinium salt for comparative purposes. In compound (I), the C(9) atom of the phenyl ring, the oxycarbonyl group [O(2)—C(8)—O(1)] and the pyridinium moiety are all essentially coplanar; this is demonstrated in the torsional angles: O(1)—C(8)—N(1)—C(7) = –6.7 (3), C(1)—N(1)—C(8)—O(2) = –1.1 (3), C(9)—O(2)—C(8)—O(1) = 6.1 (4) and C(9)—O(2)—C(8)—N(1) = –176.8 (2)°. The coplanarity of the carbonyl group with the pyridinium moiety in (I) is in contrast to that observed in (II); the torsional angle in (II) for O(1)—C(8)—N(1)—C(7) is –18.9 (2)°. The benzoyl group of (II) is non-planar with a torsional angle C(14)—C(9)—C(8)—O(1) = –32.3 (3)°. The phenyl group in (I) is rotated out of the plane defined by the oxycarbonyl group: C(14)—C(9)—O(2)—C(8) = 61.4 (3)°. The simple pyridinium salt (III) is unexceptional. The only interesting feature is the position of the Cl anion relative to the N

Table 2. *Atom coordinates (× 10⁴) and equivalent isotropic temperature factors (Å² × 10³)*

Compound (I)	U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.			U_{eq}
	<i>x</i>	<i>y</i>	<i>z</i>	
Cl(1)	1639 (1)	1736 (1)	478 (1)	21 (1)
N(1)	7452 (1)	3245 (3)	5743 (1)	17 (1)
C(1)	7892 (1)	1302 (3)	5771 (2)	19 (1)
C(2)	8473 (1)	761 (4)	6603 (2)	19 (1)
C(3)	8657 (1)	2221 (3)	7480 (2)	16 (1)
N(2)	9282 (1)	1841 (3)	8256 (1)	17 (1)
C(4)	9802 (1)	–114 (4)	8251 (2)	23 (1)
C(5)	9438 (1)	3155 (4)	9205 (2)	21 (1)
C(6)	8152 (1)	4158 (4)	7452 (2)	18 (1)
C(7)	7582 (1)	4624 (4)	6589 (2)	19 (1)
C(8)	6881 (1)	3952 (4)	4840 (2)	20 (1)
O(1)	6464 (1)	5567 (3)	4809 (1)	25 (1)
O(2)	6888 (1)	2447 (3)	4100 (1)	23 (1)
C(9)	6402 (1)	2821 (4)	3110 (2)	20 (1)
C(10)	5891 (1)	1077 (4)	2711 (2)	24 (1)
C(11)	5449 (1)	1258 (4)	1698 (2)	27 (1)
C(12)	5536 (1)	3142 (4)	1121 (2)	27 (1)
C(13)	6059 (1)	4875 (4)	1544 (2)	26 (1)
C(14)	6502 (1)	4729 (4)	2557 (2)	23 (1)
Compound (II)				
N(1)	858 (2)	993 (2)	3197 (1)	24 (1)
C(1)	1701 (2)	1803 (2)	2757 (1)	25 (1)
C(2)	2051 (2)	1684 (2)	2058 (1)	25 (1)
C(3)	1505 (2)	758 (2)	1752 (1)	22 (1)
C(6)	625 (2)	–56 (2)	2221 (1)	26 (1)
C(7)	331 (2)	82 (2)	2916 (1)	27 (1)
N(2)	1777 (2)	673 (2)	1063 (1)	26 (1)
C(4)	2725 (3)	1468 (3)	581 (1)	36 (1)
C(5)	1088 (2)	–174 (3)	753 (1)	31 (1)
C(8)	365 (2)	1179 (2)	3942 (1)	28 (1)
O(1)	–795 (2)	895 (2)	4229 (1)	38 (1)
C(9)	1329 (3)	1680 (2)	4297 (1)	30 (1)
C(10)	3025 (3)	1196 (2)	4142 (1)	33 (1)
C(11)	3849 (3)	1633 (3)	4538 (1)	41 (1)
C(12)	2984 (4)	2551 (3)	5082 (1)	51 (1)
C(13)	1308 (4)	3033 (3)	5226 (1)	60 (1)
C(14)	474 (3)	2599 (3)	4844 (1)	47 (1)
B(1)	–2553 (2)	6967 (2)	2158 (1)	19 (1)
C(15)	–2782 (2)	6314 (2)	1477 (1)	20 (1)
C(16)	–4279 (2)	7051 (2)	1193 (1)	23 (1)
C(17)	–4535 (2)	6552 (2)	614 (1)	26 (1)
C(18)	–3310 (2)	5282 (2)	297 (1)	26 (1)
C(19)	–1837 (2)	4494 (2)	573 (1)	27 (1)
C(20)	–1594 (2)	5004 (2)	1153 (1)	24 (1)
C(21)	–3661 (2)	6449 (2)	2847 (1)	19 (1)
C(22)	–5196 (2)	7497 (2)	3139 (1)	23 (1)
C(23)	–6081 (2)	7046 (2)	3741 (1)	26 (1)
C(24)	–5468 (2)	5502 (2)	4072 (1)	28 (1)
C(25)	–3986 (2)	4400 (2)	3784 (1)	29 (1)
C(26)	–3120 (2)	4873 (2)	3183 (1)	26 (1)
C(27)	–624 (2)	6270 (2)	2296 (1)	20 (1)
C(28)	–164 (2)	5933 (2)	2973 (1)	26 (1)
C(29)	1430 (2)	5525 (2)	3099 (1)	29 (1)
C(30)	2663 (2)	5401 (2)	2542 (1)	27 (1)
C(31)	2264 (2)	5710 (2)	1862 (1)	26 (1)
C(32)	657 (2)	6154 (2)	1746 (1)	23 (1)
C(33)	–3104 (2)	8912 (2)	2035 (1)	20 (1)
C(34)	–3356 (2)	9771 (2)	2600 (1)	23 (1)
C(35)	–3688 (2)	11389 (2)	2510 (1)	27 (1)
C(36)	–3755 (2)	12235 (2)	1841 (1)	27 (1)
C(37)	–3501 (2)	11430 (2)	1270 (1)	28 (1)
C(38)	–3193 (2)	9814 (2)	1370 (1)	24 (1)
Compound (III)				
Cl(1)	3471 (1)	774 (1)	5286 (1)	19 (1)
N(1)	2984 (1)	–3343 (3)	2028 (2)	21 (1)
C(1)	3829 (2)	–2636 (3)	2598 (2)	21 (1)
C(2)	4296 (2)	–2626 (3)	3687 (2)	19 (1)
C(3)	3896 (2)	–3357 (3)	4252 (2)	17 (1)
N(2)	4344 (1)	–3438 (3)	5319 (2)	17 (1)
C(4)	5216 (2)	–2539 (4)	5983 (2)	22 (1)
C(5)	3892 (2)	–4086 (4)	5874 (2)	24 (1)
C(6)	2992 (2)	–4050 (3)	3616 (2)	20 (1)
C(7)	2577 (2)	–4025 (4)	2534 (2)	22 (1)

Table 3. Selected bond lengths (Å) and angles (°)

	(I)	(II)	(III)
N—C _{carbonyl}	1.430 (2)	1.456 (1)	—
O(1)—C(8)	1.187 (3)	1.203 (1)	—
O—C _{carbonyl} —N	108.2 (2)	118.0 (2)	—
O _{carbonyl} —C _{carbonyl} —N	123.5 (2)	117.5 (2)	—
C(2)—C(3)—N(2)—C(4)	-1.0 (3)	3.0 (2)	9.2 (5)
C(2)—C(3)—N(2)—C(5)	-173.5 (2)	-174.8 (1)	175.6 (2)

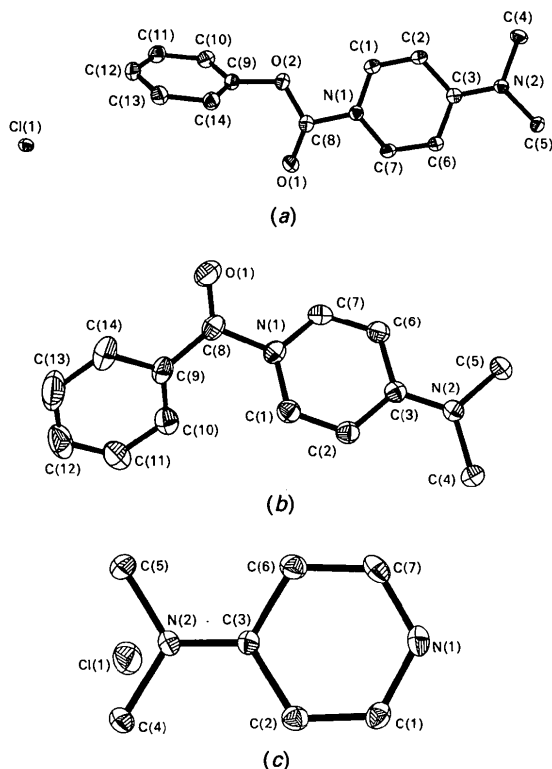
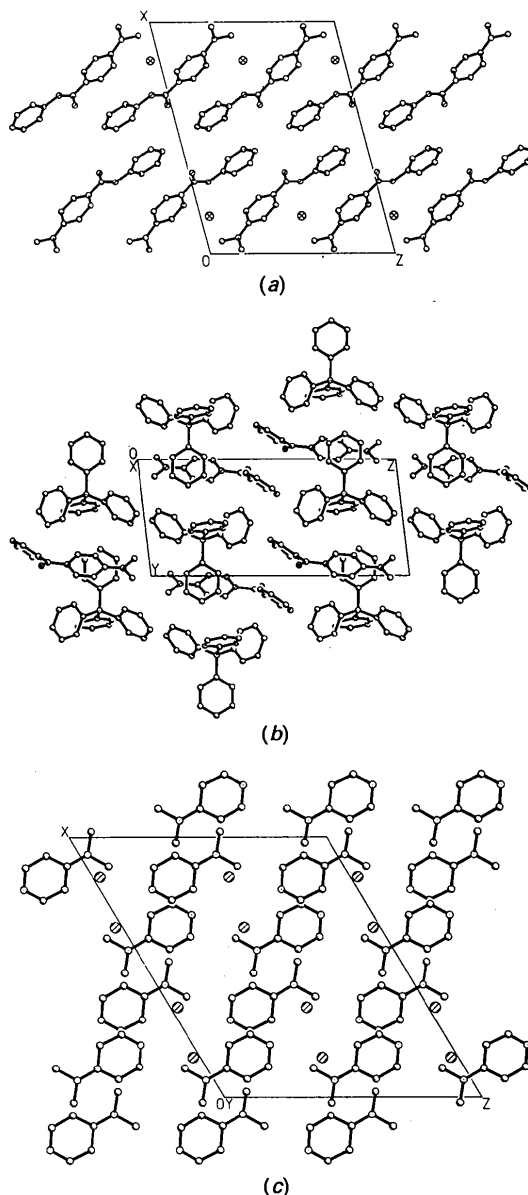


Fig. 1. Thermal-ellipsoid (50% probability) plots of (a) compound (I), (b) the cation of compound (II) and (c) compound (III).

atom in the compound. The Cl ions are situated in the crystal lattice such that they are disposed 0.4 Å closer to N(1) than to N(2): N(1)—Cl(1) = 3.065 versus N(2)—Cl(1) = 3.469 Å.

Experimental. Compound (I) was obtained by reaction of 4-dimethylaminopyridine and phenylchloroformate in an acetonitrile solution. Compound (I) was concentrated and crystallized by the addition of ether at 253 K. Compound (II) was obtained by reaction of 4-dimethylaminopyridine, benzoyl chloride and sodium tetraphenylborate in acetonitrile. A solution of compound (II) was filtered, the solvent removed by rotary evaporation, and then (II) recrystallized from a CH₂Cl₂/ether solution at 253 K. Compound (III) was obtained by reaction of H₂O on (I) in acetonitrile. Compound (III) recrystallized from CH₂Cl₂/ether at 253 K. Compounds (I), (II)

and (III) were sealed in glass capillaries under dry nitrogen owing to their moisture sensitivity. Data were collected on a Siemens R3m/V upgrade of a Nicolet P3F automated diffractometer, using 2θ-θ scans for (I) and (III), and Wyckoff scans for (II), all with variable scan speeds. Both structures were solved by direct methods and refined on *F* using the *SHELX-Plus* (MicroVAX II) program package (Sheldrick, 1988). H atoms were placed in idealized positions and constrained to have C—H = 0.96 Å and isotropic thermal parameters, *U* = 0.08 Å². All non-H atoms were treated as anisotropic. No

Fig. 2. Projected packing plots of (a) (I) viewed down the *b* axis, (b) (II) viewed down the *a* axis, and (c) (III) viewed down the *b* axis.

absorption correction was necessary for any of the structures. Details of the data collection are given in Table 1. Scattering factors were obtained from *International Tables for X-ray Crystallography* (1974, Vol. IV). Atomic coordinates for (I), (II) and (III) are contained in Table 2.* Important bond lengths and angles are given in Table 3. Fig. 1 illustrates the molecules with the numbering scheme employed. Fig. 2 illustrates the projected packing of the molecules.

Related literature. For additional information on related *N*-acylpyridinium salt reactions and chemistry see Battye, Ihsan & Moodie (1980), Hassner, Krepski & Alexanian (1978), Sheinkman, Suminov &

* Lists of structure factors, anisotropic thermal parameters, bond lengths and angles, and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55216 (56 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CR0409]

Kost (1973), Titov, Rydachenko & Chotiy (1990), Castro & Ureta (1987), Höfle, Steglich & Vorbrüggen (1978), and King & Bryant (1991).

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anti-2-Methyl-1,3-dithiane 1,1,3-Trioxide

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Abstract. $C_5H_{10}O_3S_2$, $M_r = 182.25$, orthorhombic, $P2_12_12_1$, $a = 9.019$ (1), $b = 14.522$ (1), $c = 6.059$ (1) Å, $V = 793.7$ Å³, $Z = 4$, $D_x = 1.525$ g cm⁻³, Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å, $\mu = 5.93$ cm⁻¹, $F(000) = 384$, room temperature, $R = 0.031$ for 753 reflections with $I > 3\sigma(I)$. The S=O bond lengths in —SO₂⁻ are 1.426 (3) and 1.432 (3) Å while in the —SO— group the S=O bond is substantially longer, 1.497 (3) Å.

Experimental. Colourless crystal, prepared by sequential asymmetric oxidation and deacylation of 2-acetyl-2-methyl-1,3-dithiane (Page & Namwindwa, 1991).

Crystal $0.38 \times 0.38 \times 0.28$ mm, Rigaku AFC-6S diffractometer, $\omega/2\theta$ scans, unit cell from 25 reflections with $15 < 2\theta < 27^\circ$, Lp corrections, no absorption correction, $2\theta_{\max} = 50^\circ$, $0 < h < 10$, $0 < k < 16$, $0 < l < 7$ and Friedel equivalents, three standard reflections showed no significant change, 1710 reflections measured, 1410 unique, $R_{\text{int}} = 0.009$, 753

with $I > 3\sigma(I)$ used for refinement. Structure solution by direct methods (*SHELXS86*; Sheldrick, 1986) and refinement on F , all within *TEXSAN* (Molecular Structure Corporation, 1985); anisotropic vibration parameters for non-H atoms, H atoms located in difference map and their isotropic U values, but not their coordinates, refined; 91 parameters, $w^{-1} = [\sigma^2(F) + 0.0009F^2]$, $R = 0.031$, $wR = 0.040$, $S = 1.67$, max. shift/e.s.d. 0.003, max. and min. peaks in final difference map 0.14, -0.11 e Å⁻³. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). Table 1* gives the atomic coordinates and Table 2 selected bond lengths and angles. Fig. 1 shows the atom numbering.

* 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 55267 (11 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: LI0123]