Crystal structure of 2(*R*),3(*S*),4(*R*),4a(*R*),4b(*R*),5(*R*),8a(*S*),9a(*S*)-2-acetoxymethyl-5-tri-methylsilyl-7-iodo-3,4,4a,4b,5,8,8a,9a-octahydro-2*H*-pyrano[2,3-b]-benzofuran-3,4-diol diacetate, $C_{21}H_{31}IO_8Si$

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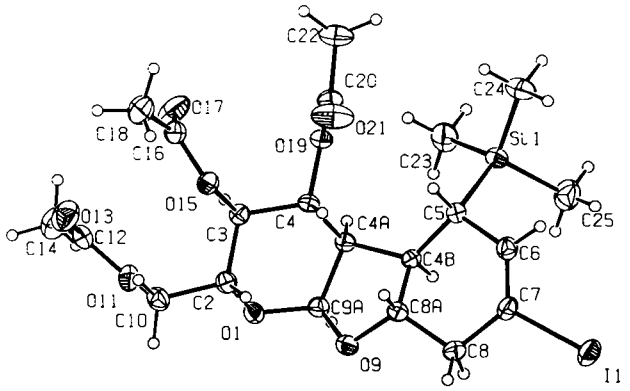
Received May 31, 1996, CSD-No. 402547



Source of material: see ref. 2.
The compound is called (*S*)Et in ref. 1.
Programs used : SHELXS-86, SHELXL-93, STRUX, PLATON.

Table 1. Parameters used for the X-ray data collection

Crystal:	average diameter 0.75 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	12.20 cm^{-1}
Diffractometer:	Siemens-Stoe
Scan mode:	ω/2θ
$T_{measurement}$:	298 K
$2\theta_{max}$:	50°
$N(hkl)_{unique}$:	4425
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	312
Program:	SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in $Å^2$)

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1)	4*a*	0.7430(3)	0.4977(3)	0.4010(1)	0.036(8)
H(2)	4*a*	0.5624(3)	0.4075(3)	0.4872(1)	0.025(7)
H(3)	4*a*	0.5989(3)	0.3444(2)	0.3603(1)	0.033(8)
H(4)	4*a*	0.6609(3)	0.1836(2)	0.4563(1)	0.028(7)
H(5)	4*a*	0.7961(3)	0.0956(3)	0.3884(1)	0.030(8)
H(6)	4*a*	0.5908(3)	0.1511(3)	0.3092(1)	0.06(1)
H(7)	4*a*	0.6990(3)	0.0180(3)	0.2353(1)	0.048(9)
H(8)	4*a*	0.9747(3)	0.2349(3)	0.2731(2)	0.05(1)
H(9)	4*a*	0.9883(3)	0.1380(3)	0.3247(2)	0.07(1)
H(10)	4*a*	0.7821(3)	0.2969(3)	0.3114(1)	0.042(8)
H(11)	4*a*	0.8624(3)	0.2418(3)	0.4688(1)	0.035(8)
H(12)	4*a*	0.8129(4)	0.6301(3)	0.4768(2)	0.041(9)
H(13)	4*a*	0.6709(4)	0.6585(3)	0.4596(2)	0.036(8)
H(14)	4*a*	0.6303(5)	0.5680(4)	0.6462(2)	0.11(2)
H(15)	4*a*	0.4846(5)	0.5931(4)	0.6381(2)	0.16(3)
H(16)	4*a*	0.5781(5)	0.6967(4)	0.6537(2)	0.16(3)
H(17)	4*a*	0.3602(5)	0.6605(4)	0.3871(3)	0.18(4)
H(18)	4*a*	0.3021(5)	0.6926(4)	0.4517(3)	0.21(4)
H(19)	4*a*	0.2324(5)	0.6022(4)	0.4086(3)	0.14(2)
H(20)	4*a*	0.2630(4)	0.1808(4)	0.4228(2)	0.12(2)
H(21)	4*a*	0.2320(4)	0.1616(4)	0.3527(2)	0.14(3)
H(22)	4*a*	0.1882(4)	0.2776(4)	0.3859(2)	0.13(2)
H(23)	4*a*	0.4784(4)	0.0287(3)	0.4407(2)	0.06(1)
H(24)	4*a*	0.6111(4)	−0.0254(3)	0.4578(2)	0.09(2)
H(25)	4*a*	0.4940(4)	−0.1084(3)	0.4467(2)	0.05(1)
H(26)	4*a*	0.3752(4)	−0.0035(5)	0.3074(2)	0.10(2)
H(27)	4*a*	0.3903(4)	−0.1404(5)	0.3146(2)	0.18(3)
H(28)	4*a*	0.4567(4)	−0.0748(5)	0.2596(2)	0.15(3)
H(29)	4*a*	0.7078(5)	−0.1800(4)	0.2972(2)	0.13(2)
H(30)	4*a*	0.6435(5)	−0.2444(4)	0.3532(2)	0.14(2)
H(31)	4*a*	0.7606(5)	−0.1614(4)	0.3643(2)	0.10(2)

$C_{21}H_{31}IO_8Si$, orthorhombic, $P2_12_12_1$ (No. 19), a =10.512(1) Å, b =11.333(1) Å, c =21.640(2) Å, V =2578.0 $Å^3$, Z =4, $R(F)$ =0.024, $R_w(F^2)$ =0.064, Flack x parameter = −0.01(2).

Table 3. Final atomic coordinates and displacement parameters (in $Å^2$)

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
I(1)	4*a*	0.96542(2)	0.01479(2)	0.18758(1)	0.0546(1)	0.0540(1)	0.0518(1)	0.0100(1)	0.0181(1)	−0.0077(1)
Si(1)	4*a*	0.57606(8)	−0.04603(8)	0.35066(4)	0.0386(5)	0.0390(5)	0.0525(5)	−0.0096(3)	0.0082(4)	−0.0056(4)
O(1)	4*a*	0.8033(2)	0.4042(2)	0.47214(9)	0.037(1)	0.036(1)	0.041(1)	−0.0003(9)	−0.0066(9)	−0.0078(9)
C(2)	4*a*	0.7172(3)	0.4849(3)	0.4440(1)	0.039(2)	0.034(1)	0.035(1)	−0.001(1)	−0.000(1)	0.001(1)
C(3)	4*a*	0.5863(3)	0.4291(3)	0.4449(1)	0.035(2)	0.030(1)	0.034(1)	0.001(1)	0.001(1)	0.003(1)
C(4)	4*a*	0.5868(3)	0.3206(2)	0.4035(1)	0.028(1)	0.033(1)	0.031(1)	−0.005(1)	0.001(1)	0.004(1)
C(4A)	4*a*	0.6912(3)	0.2338(2)	0.4225(1)	0.030(1)	0.030(1)	0.032(1)	−0.001(1)	−0.001(1)	0.003(1)

Table 3. (Continued)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(4b)	4*a*	0.7428(3)	0.1568(3)	0.3696(1)	0.027(1)	0.030(1)	0.036(1)	0.001(1)	0.003(1)	–0.001(1)
C(5)	4*a*	0.6568(3)	0.0954(3)	0.3223(1)	0.033(1)	0.033(1)	0.036(2)	–0.000(1)	0.000(1)	–0.003(1)
C(6)	4*a*	0.7371(3)	0.0627(3)	0.2663(1)	0.044(2)	0.039(2)	0.035(2)	–0.000(1)	0.004(1)	–0.004(1)
C(7)	4*a*	0.8567(3)	0.0934(3)	0.2588(1)	0.042(2)	0.036(2)	0.038(2)	0.005(1)	0.011(1)	–0.002(1)
C(8)	4*a*	0.9281(3)	0.1795(3)	0.2986(2)	0.035(2)	0.043(2)	0.050(2)	–0.004(1)	0.011(1)	–0.003(1)
C(8A)	4*a*	0.8320(3)	0.2438(3)	0.3377(1)	0.033(2)	0.033(1)	0.041(1)	–0.005(1)	0.004(1)	0.000(1)
O(9)	4*a*	0.8896(2)	0.3106(2)	0.3867(1)	0.037(1)	0.051(1)	0.051(1)	–0.012(1)	0.008(1)	–0.014(1)
C(9A)	4*a*	0.8158(3)	0.2954(3)	0.4414(1)	0.032(2)	0.035(1)	0.040(2)	0.000(1)	–0.003(1)	–0.001(1)
C(10)	4*a*	0.7263(4)	0.6006(3)	0.4787(2)	0.049(2)	0.034(2)	0.051(2)	–0.004(1)	–0.002(2)	0.001(1)
O(11)	4*a*	0.6897(2)	0.5838(2)	0.5426(1)	0.054(1)	0.039(1)	0.047(1)	0.007(1)	–0.002(1)	–0.007(1)
C(12)	4*a*	0.5888(4)	0.6453(3)	0.5635(2)	0.049(2)	0.034(2)	0.063(2)	–0.007(1)	0.000(2)	–0.011(1)
O(13)	4*a*	0.5267(3)	0.7104(3)	0.5327(1)	0.068(2)	0.069(2)	0.081(2)	0.024(2)	–0.004(2)	–0.004(1)
C(14)	4*a*	0.5686(5)	0.6238(4)	0.6316(2)	0.081(3)	0.075(3)	0.063(2)	0.009(2)	0.019(2)	–0.005(2)
O(15)	4*a*	0.4979(2)	0.5143(2)	0.41997(9)	0.038(1)	0.036(1)	0.047(1)	0.0065(8)	–0.0018(8)	0.0004(9)
C(16)	4*a*	0.3877(3)	0.5307(3)	0.4514(2)	0.041(2)	0.033(2)	0.079(2)	0.002(1)	0.001(2)	–0.007(2)
O(17)	4*a*	0.3577(3)	0.4746(3)	0.4951(2)	0.067(2)	0.062(2)	0.114(2)	0.017(2)	0.045(2)	0.023(2)
C(18)	4*a*	0.3138(5)	0.6306(4)	0.4220(3)	0.057(3)	0.053(2)	0.105(4)	0.023(2)	–0.011(3)	–0.009(2)
O(19)	4*a*	0.4655(2)	0.2602(2)	0.41038(8)	0.028(1)	0.037(1)	0.0356(9)	–0.0031(9)	–0.0031(9)	0.0025(8)
C(20)	4*a*	0.3768(3)	0.2768(3)	0.3664(2)	0.035(2)	0.051(2)	0.045(2)	0.000(1)	–0.006(1)	0.002(1)
O(21)	4*a*	0.3947(3)	0.3310(3)	0.3201(1)	0.053(2)	0.122(2)	0.057(2)	–0.017(2)	–0.020(1)	0.040(2)
C(22)	4*a*	0.2540(4)	0.2190(4)	0.3835(2)	0.036(2)	0.082(3)	0.076(3)	–0.010(2)	–0.013(2)	0.013(2)
C(23)	4*a*	0.5349(4)	–0.0367(3)	0.4341(2)	0.078(3)	0.047(2)	0.062(2)	–0.015(2)	0.023(2)	0.004(2)
C(24)	4*a*	0.4322(4)	–0.0690(5)	0.3022(2)	0.044(2)	0.093(3)	0.097(4)	–0.021(2)	–0.002(2)	–0.029(3)
C(25)	4*a*	0.6852(5)	–0.1734(4)	0.3401(2)	0.077(3)	0.046(2)	0.085(3)	0.008(2)	0.014(3)	–0.001(2)

Acknowledgment. This work was supported by Prof. Dr. M. Binnewies.

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