Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and equivalent isotropic displacement parameters* ($Å^2 \times 10^4$) *for non-H atoms*

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

	x	y	z	U_{eq}
C(1)	−2706 (3)	−461 (2)	1243 (1)	532 (5)
C(2)	−537 (3)	−775 (1)	1779 (1)	518 (5)
C(3)	1092 (3)	485 (2)	1847 (1)	485 (5)
C(4)	−217 (2)	1475 (1)	1343 (1)	385 (4)
C(5)	481 (3)	2947 (1)	1054 (1)	460 (5)
C(6)	−1078 (2)	4589 (1)	2534 (1)	379 (4)
C(7)	−3022 (2)	5623 (1)	2818 (1)	364 (4)
C(8)	−4732 (2)	5982 (1)	1884 (1)	395 (4)
C(9)	−3092 (2)	6136 (1)	3950 (1)	402 (21)
C(10)	−4738 (2)	7092 (1)	4461 (1)	402 (5)
C(11)	−4888 (3)	7515 (2)	5618 (1)	519 (5)
C(12)	−6875 (3)	8448 (2)	5668 (1)	581 (6)
C(13)	−7792 (3)	8518 (2)	4552 (1)	568 (6)
O(1)	−2579 (2)	916 (1)	965 (1)	513 (4)
O(2)	561 (2)	4325 (1)	3273 (1)	532 (4)
O(3)	−6515 (2)	7717 (1)	3787 (1)	506 (4)
N(1)	−1277 (2)	3975 (1)	1428 (1)	429 (4)
N(2)	−5982 (3)	6201 (1)	1071 (1)	539 (5)

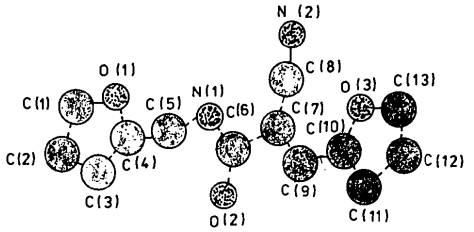

Fig. 1. A perspective view of the title compound, with the numbering scheme.

ties. The molecular structure described here should aid the interpretation of spectroscopic investigations and the elucidation of the bioactivity data.

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

C(1)—C(2)	1.328 (3)	C(7)—C(8)	1.429 (2)
C(1)—O(1)	1.365 (2)	C(8)—N(2)	1.145 (2)
C(2)—C(3)	1.422 (3)	C(7)—C(9)	1.354 (2)
C(3)—C(4)	1.343 (3)	C(9)—C(10)	1.421 (3)
C(4)—C(5)	1.488 (3)	C(10)—C(11)	1.364 (2)
C(4)—O(1)	1.360 (2)	C(10)—O(3)	1.369 (2)
C(5)—N(1)	1.453 (3)	C(11)—C(12)	1.420 (3)
C(6)—N(1)	1.350 (2)	C(12)—C(13)	1.343 (3)
C(6)—O(2)	1.221 (2)	C(13)—O(3)	1.360 (3)
C(6)—C(7)	1.502 (2)		

C(2)—C(1)—O(1)	110.7 (2)	C(8)—C(7)—C(9)	123.7 (1)
C(1)—C(2)—C(3)	106.1 (1)	C(7)—C(8)—N(2)	174.0 (1)
C(2)—C(3)—C(4)	107.0 (1)	C(7)—C(9)—C(10)	129.8 (1)
C(3)—C(4)—O(1)	109.6 (1)	C(9)—C(10)—O(3)	121.4 (1)
C(3)—C(4)—C(5)	132.9 (1)	C(9)—C(10)—C(11)	128.6 (1)
C(5)—C(4)—O(1)	117.2 (1)	C(11)—C(10)—O(3)	109.9 (1)
C(4)—C(5)—N(1)	114.1 (1)	C(10)—C(11)—C(12)	106.6 (1)
O(2)—C(6)—N(1)	122.8 (1)	C(11)—C(12)—C(13)	105.9 (2)
C(7)—C(6)—N(1)	115.9 (1)	C(12)—C(13)—O(3)	111.7 (2)
C(7)—C(6)—O(2)	121.3 (1)	C(1)—O(1)—C(4)	106.6 (1)
C(6)—C(7)—C(9)	118.0 (1)	C(10)—O(3)—C(13)	105.9 (1)
C(6)—C(7)—C(8)	118.2 (1)	C(5)—N(1)—C(6)	120.9 (1)

C(2)—C(3)—C(4)—C(5)	−174.1 (1)	C(8)—C(7)—C(9)—C(10)	−0.3 (2)
C(3)—C(4)—C(5)—N(1)	−131.7 (2)	C(7)—C(9)—C(10)—C(11)	174.8 (2)
C(6)—C(7)—C(9)—C(10)	−178.7 (1)	C(9)—C(10)—C(11)—C(12)	−178.6 (2)

We thank Dr Ralf-Jürgen Kuban (Central Laboratory of Physical Chemistry, Berlin) for the data collection on their Enraf–Nonius CAD-4 diffractometer.

References

BARTROLI, R., LAMÍ, L. & DÍAZ, M. (1984). Cuban patent 21789.
BERMELLO, A. (1990). Private communication.
GOLENDER, V. E. & REZENBLIT, A. B. (1983). *Logical and Combinatorial Algorithms for Drug Design.* Research Studies Press Ltd, England.
SHELDRICK, G. M. (1976). *SHELX76.* Program for crystal structure determination. Univ. of Cambridge, England.

Acta Cryst. (1993). C**49**, 559–560

Structure of Ethyl 5-(2,2,2-Trichloro-1-hydroxyethyl)furan-2-carboxylate

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(*Received* 19 *December* 1991; *accepted* 29 *June* 1992)

Abstract. $C_9H_9Cl_3O_4$, $M_r = 287.5$, orthorhombic, *Pbca*, $a = 23.01$ (4), $b = 13.91$ (1), $c = 7.58$ (4) Å, $V = 2426$ (14) Å^3, $Z = 8$, $D_x = 1.57$ (1) g cm^{-3}, graphite-monochromated Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å, $\mu = 7.516$ cm^{-1}, $F(000) = 1168$, room temperature, $R = 0.034$ for 460 observed reflections

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0108-2701/93/030559-02$06.00

Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and equivalent isotropic displacement parameters* ($Å^2 \times 10^4$) *for non-H atoms*

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

	x	y	z	U_{eq}
C(1)	3562 (7)	4328 (10)	3651 (20)	548 (119)
C(2)	3133 (8)	5038 (11)	4522 (25)	429 (121)
C(3)	3171 (8)	6045 (11)	3853 (18)	328 (112)
C(4)	2791 (9)	6609 (15)	3007 (21)	480 (152)
C(5)	3038 (8)	7545 (16)	2817 (21)	474 (128)
C(6)	3555 (8)	7482 (12)	3657 (20)	401 (117)
C(7)	3988 (8)	8222 (15)	3907 (20)	478 (135)
C(8)	4851 (11)	8692 (18)	5246 (39)	867 (220)
C(9)	5206 (13)	8327 (21)	6726 (41)	1198 (235)
Cl(1)	3414 (2)	3164 (3)	4433 (7)	828 (35)
Cl(2)	4285 (2)	4617 (3)	4178 (6)	709 (34)
Cl(3)	3459 (2)	4370 (3)	1379 (5)	825 (41)
O(1)	3184 (5)	5013 (8)	6347 (22)	670 (104)
O(2)	3643 (5)	6568 (8)	4320 (12)	456 (81)
O(3)	4410 (5)	7948 (7)	4972 (13)	553 (77)
O(4)	3965 (6)	9014 (9)	3270 (14)	729 (27)

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

Cl(1)—C(1)	1.757 (15)	C(5)—C(6)	1.352 (25)
Cl(2)—C(1)	1.757 (17)	C(6)—C(7)	1.446 (26)
Cl(3)—C(1)	1.739 (18)	C(8)—C(9)	1.478 (41)
O(1)—C(2)	1.389 (26)	O(4)—C(7)	1.204 (23)
O(2)—C(3)	1.354 (21)	C(1)—C(2)	1.545 (23)
O(2)—C(6)	1.382 (20)	C(2)—C(3)	1.492 (22)
O(3)—C(7)	1.314 (21)	C(3)—C(4)	1.338 (25)
O(3)—C(8)	1.464 (27)	C(4)—C(5)	1.428 (30)

C(3)—O(2)—C(6)	106 (1)	C(2)—C(3)—C(4)	132 (2)
C(7)—O(3)—C(8)	113 (1)	O(2)—C(3)—C(4)	109 (1)
Cl(2)—C(1)—Cl(3)	110 (1)	C(3)—C(4)—C(5)	109 (2)
Cl(1)—C(1)—Cl(3)	110 (1)	C(4)—C(5)—C(6)	104 (2)
Cl(1)—C(1)—Cl(2)	108 (1)	O(2)—C(6)—C(5)	111 (1)
Cl(3)—C(1)—C(2)	108 (1)	C(5)—C(6)—C(7)	129 (2)
Cl(2)—C(1)—C(2)	111 (1)	O(2)—C(6)—C(7)	120 (1)
Cl(1)—C(1)—C(2)	109 (1)	O(4)—C(7)—C(6)	124 (2)
O(1)—C(2)—C(1)	111 (1)	O(3)—C(7)—C(6)	113 (1)
C(1)—C(2)—C(3)	115 (1)	O(3)—C(7)—O(4)	123 (2)
O(1)—C(2)—C(3)	111 (1)	O(3)—C(8)—C(9)	104 (2)
O(2)—C(3)—C(2)	117 (1)		

C(4)—C(5)—C(6)—C(7)	−179 (2)	C(5)—C(6)—C(7)—O(4)	−6 (3)
C(5)—C(6)—C(7)—O(3)	172 (2)	C(8)—O(3)—C(7)—C(6)	−180 (2)

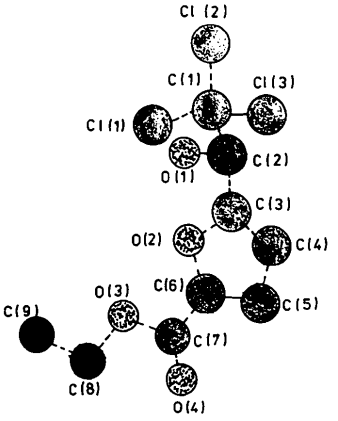

Fig. 1. A perspective view of the molecule, showing atom numbering.

with $I \geq 2\sigma(I)$. The structure consists of discrete molecules; there are no unusual intramolecular distances or angles.

Experimental. A white prismatic crystal, 0.2 × 0.2 × 0.4 mm, recrystallized from an ethanol solution, was used for data collection on a URS-50IM semi-automatic diffractometer in the ω–2θ scan mode ($0 \leq h \leq 20$, $0 \leq k \leq 15$, $0 \leq l \leq 6$; $\sin\theta_{max}/\lambda = 0.595$ Å^{-1}). Unit-cell parameters were determined from least-squares refinement of 25 reflections in the range $12 \leq \theta \leq 33°$. 498 unique reflections were collected of which 460 were considered observed [$I \geq 2\sigma(I)$]. Seven standard reflections (400, 021, 122, 123, 064, 045, 066), measured after every 25 reflections, did not show any significant change in intensity during data collection. Lorentz–polarization corrections were made, but absorption was ignored. The structure was solved by direct methods (Sheldrick, 1976). Full-matrix least-squares refinement was based on F using *SHELX*76 (Sheldrick, 1976). Non-H atoms were refined with anisotropic displacement parameters; all H atoms were located from a $\Delta\rho$ map and refined isotropically. 181 parameters were refined. Final $R = 0.034$, $wR = 0.038$ $\{w = [\sigma^2(F) + 0.001F^2]^{-1}\}$; $\Delta\rho_{max} = 0.20$, $\Delta\rho_{min} = -0.19$ e Å^{-3}; $(\Delta/\sigma)_{max} = 0.36$. Atomic scattering factors were those stored in *SHELX*76. Fractional coordinates and equivalent values of the anisotropic displacement parameters are given in Table 1.* Bond lengths, bond angles and selected torsion angles are listed in Table 2. The numbering system for the molecule can be found in Fig. 1.

Related literature. The title compound was synthesized by Bartroli, Lamí & Díaz (1982) and interesting bioactivity has been investigated by Bermello (1990) using Golender & Rezenblit (1983) algorithms.

* Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, and bond distances, bond angles and torsion angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55538 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AB0277]

References

BARTROLI, R., LAMÍ, L. & DÍAZ, M. (1982). *Rev. ICIDCA (Inst. Cubana Invest. Deriv. Cana Azucar)*, **16**(2), pp. 35–40.

BERMELLO, A. (1990). Private communication.

GOLENDER, V. E. & REZENBLIT, A. B. (1983). *Logical and Combinatorial Algorithms for Drug Design*. Research Studies Press Ltd, England.

SHELDRICK, G. M. (1976). *SHELX*76. Program for crystal structure determination. Univ. of Cambridge, England.