chemistry of parent acid and its derivatives: Oliver (1986); structure of dibenzyl: Robertson (1935), Jeffrey (1947), Cruickshank (1949); structures of some dibenzyl derivatives: Brown (1954), Sato, Yamato, Hashigaki & Koyama (1978), Corey (1979).

References

BAKER, W., OLLIS, W. D. & ZEALLEY, T. S. (1952). *J. Chem. Soc.* pp. 1447–1451.

BROWN, C. J. (1954). *Acta Cryst.* **7**, 97–100.

CHATTEYEA, J. N., PRASAD, N. & BANERJI, K. D. (1964). *J. Indian Chem. Soc.* **41**, 93–102.

COREY, E. R. (1979). *Acta Cryst.* B**35**, 201–202.

CRUICKSHANK, D. W. J. (1949). *Acta Cryst.* **2**, 65–82.

FRENZ, B. A. (1978). In *Computing in Crystallography*, edited by H. SCHENK, R. OLTHOF-HAZEKAMP, H. VAN KONINGSVELD & G. C. BASSI, pp. 64–71. Delft Univ. Press.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

JEFFREY, G. A. (1947). *Proc. R. Soc. London Ser. A*, **188**, 222–236.

JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). *MULTAN*80. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain, Belgium.

OLIVER, M. A. (1986). PhD Thesis. Louisiana State Univ., Baton Rouge, Louisiana, USA.

ROBERTSON, J. M. (1935). *Proc. R. Soc. London*, **150**, 348–362.

SATO, K., YAMATO, M., HASHIGAKI, K. & KOYAMA, T. (1978). *Yakugaku Zasshi*, **97**, 1180–1193.

VEJDELEK, Z. J., NEMECEK, O., MUSIL, V. & SIMEK, A. (1964). *Coll. Czech. Chem. Commun.* **29**, 776–794.

Acta Cryst. (1988). C**44**, 1143–1144

Structure of 2-Chloro-1-(2,4-dihydroxyphenyl)ethanone

BY P. H. VAN ROOYEN*

National Chemical Research Laboratory, Council for Scientific and Industrial Research, PO Box 395, *Pretoria* 0001, *Republic of South Africa*

AND J. C. BREYTENBACH

Department of Pharmaceutical Chemistry, Potchefstroom University for CHE, Potchefstroom 2520, *Republic of South Africa*

(*Received* 3 *September* 1987; *accepted* 18 *February* 1988)

Abstract. ω-Chlororesacetophenone, $C_8H_7ClO_3$, M_r = 186·8, monoclinic, $P2_1/a$, $a = 7{\cdot}335\ (1)$, $b = 15{\cdot}457\ (10)$, $c = 6{\cdot}818\ (1)$ Å, $\beta = 92{\cdot}29\ (1)°$, $U = 772\ (1)$ Å^3, $Z = 4$, $D_x = 1{\cdot}61$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 0{\cdot}783$ mm^{-1}, $F(000) = 768$, $T = 298$ K. Final $R = 0{\cdot}077$ for 1275 observed reflections with $F_o > 4\sigma(F_o)$ and 131 variable parameters. The molecule is planar with normal bond lengths and angles. There is strong intramolecular hydrogen bonding through a hydroxyl H atom and the ketone O atom, with an H···O distance of 1·63 (1) Å.

Experimental. The title compound was formed by the Hoesch condensation of resorcinol with chloroacetonitrile (Dawkins & Mulholland, 1959) and yielded almost colourless needles (toluene, m.p. 404 K). Crystal 0·26 × 0·23 × 0·16 mm; Enraf–Nonius CAD-4 diffractometer, graphite-monochromatized radiation; unit cell from 25 reflections ($7 \le \theta \le 20°$); 1759 reflections for $3 \le \theta \le 27°$ in the range ($0 \le h \le 9$, $0 \le k \le 19$ and $-9 \le l \le 9$) using $\omega/2\theta$ scans where ω changed as $0{\cdot}59 + 0{\cdot}35\tan\theta°$ with a variable but maximum speed that corresponds to 5·49° min^{-1}. Three standard reflections varied less than 1%, measured every hour; Lorentz–polarization; no absorption correction. 1759 unique reflections, 484 rejected with $F_o \le 4\sigma(F_o)$; structure solved using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980); all H atoms from difference Fourier synthesis; least-squares refinement using *SHELX*76 (Sheldrick, 1976), F magnitudes, $\sigma^{-2}(F)$ weights, all non-H atoms anisotropic, H atoms isotropic with a common thermal parameter [U_{iso} (H) 0·092 (10) Å^2], 131 variables refined. Final $wR = 0{\cdot}066$, $R = 0{\cdot}077$, $(\Delta/\sigma)_{max} = 0{\cdot}07$, residual electron density = 0·56 e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974). Table 1 gives the atom parameters, Fig. 1 shows the molecular structure and the atomic numbering scheme drawn by *ORTEP* (Johnson, 1965).†

* To whom all correspondence should be addressed.

† Lists of structure factors, anisotropic thermal parameters and bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44792 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

0108-2701/88/061143-02$03.00

Table 1. *Fractional coordinates* ($\times 10^4$; *for* H $\times 10^3$) *and equivalent isotropic thermal parameters* ($Å^2 \times 10^3$) *for* 2-*chloro*-1-(2,4-*dihydroxyphenyl*)*ethanone*

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

	x	y	z	U_{eq}
C(1)	5424 (8)	−2169 (4)	1567 (8)	29 (1)
C(2)	4654 (9)	−1996 (4)	−320 (9)	33 (2)
C(3)	4086 (8)	−2634 (4)	−1607 (9)	34 (2)
C(4)	4206 (8)	−3499 (4)	−1004 (9)	34 (1)
C(5)	4993 (9)	−3705 (4)	830 (9)	35 (2)
C(6)	5562 (8)	−3073 (4)	2107 (9)	33 (1)
C(7)	6038 (8)	−1514 (4)	2911 (9)	30 (1)
C(8)	5813 (10)	−572 (4)	2213 (10)	40 (2)
O(9)	3551 (6)	−4145 (3)	−2122 (7)	45 (1)
O(10)	6297 (6)	−3293 (3)	3872 (6)	46 (1)
O(11)	6695 (6)	−1667 (3)	4576 (6)	39 (1)
Cl	7092 (3)	157 (1)	3742 (3)	48 (1)
H(2)	462 (9)	−149 (5)	−110 (10)	92 (10)*
H(3)	366 (9)	−252 (5)	−315 (10)	92 (10)*
H(5)	519 (10)	−430 (4)	111 (10)	92 (10)*
H(8*A*)	636 (9)	−22 (4)	77 (10)	92 (10)*
H(8*B*)	443 (10)	−22 (4)	195 (10)	92 (10)*
H(9)	298 (9)	−373 (5)	−324 (10)	92 (10)*
H(10)	606 (9)	−267 (5)	485 (10)	92 (10)*

* Isotropic temperature factor.

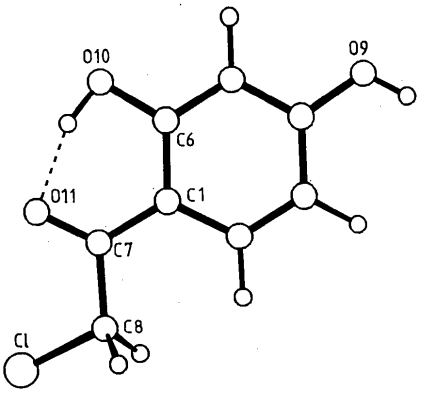

Fig. 1. Drawing of a molecule of 2-chloro-1-(2,4-dihydroxyphenyl)ethanone with the atom numbering.

Related literature. ω-Chlororesacetophenone showed a strong inhibition of the growth of the gram-positive micro organisms *Staphylococcus aureus, Bacillus licheniformis, B. cereus* and *Micrococcus luteus,* the gram-negative organisms *Escherichia coli* and *Pseudomonas aeruginosa,* the yeast *Candida albicans* and certain *Aspergillus* moulds when tested by the direct plate method (van der Vyver & Lötter, 1971). It did not seem to possess any phototoxic activity (Weimarck & Nilsson, 1980). The molecule is planar; the distance of the Cl atom from the least-squares plane of all non-H atoms is 0·21 (9) Å. The packing is unexceptional. Related structures: 2-hydroxy-4-ω,ω-dichloroacetophenone (Chattopadhyay & Mazumdar, 1984) and 2,2-dichloro-2′-hydroxy-4′-methoxyacetophenone (Chattopadhyay, Banerjee, Mazumdar & Podder, 1985).

References

CHATTOPADHYAY, D., BANERJEE, T., MAZUMDAR, S. K. & PODDER, G. (1985). *Acta Cryst.* C**41**, 287–289.

CHATTOPADHYAY, D. & MAZUMDAR, S. K. (1984). *Acta Cryst.* A**40**, C274.

DAWKINS, A. W. & MULHOLLAND, T. P. C. (1959). *J. Chem. Soc.* *C*, pp. 2203–2210.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

JOHNSON, C. K. (1965). *ORTEP.* Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

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

VYVER, L. M. VAN DER & LÖTTER, A. P. (1971). *Planta Med.* **20**, 8–13.

WEIMARCK, G. & NILSSON, E. (1980). *Planta Med.* **38**, 97–111.

Acta Cryst. (1988). C**44**, 1144–1147

The Structure of the Ethylenediammonium Salt of 3-Nitro-1,2,4-triazol-5-one, $C_2H_4(NH_3)_2.2C_2N_4O_3H$*

BY DON T. CROMER,† JOHN H. HALL, KIEN-YIN LEE AND ROBERT R. RYAN

Los Alamos National Laboratory, University of California, Los Alamos, New Mexico 87545, *USA*

(*Received* 22 *September* 1987; *accepted* 5 *February* 1988)

Abstract. $C_6H_{12}N_{10}O_6$, $M_r = 320{\cdot}22$, triclinic, $P\bar{1}$, $a = 6{\cdot}528$ (3), $b = 10{\cdot}780$ (2), $c = 14{\cdot}236$ (3) Å, $\alpha = 81{\cdot}11$ (2), $\beta = 87{\cdot}13$ (3), $\gamma = 74{\cdot}05$ (3)°, $V = 951{\cdot}73$ Å^3, $Z = 3$, $D_x = 1{\cdot}676$ Mg m^{-3}, λ(Mo $K\alpha_1$) = 0·70926 Å, $\mu = 0{\cdot}14$ mm^{-1}, $F(000) = 498$, room temperature, final $R = 0{\cdot}030$ for 1693 observed reflections [$I > 2\sigma(I)$] out of 2469 independent reflections. There are 1·5 formula units in the asymmetric unit.

* This work was performed under the auspices of the US Department of Energy.

† Author to whom correspondence should be addressed.

0108-2701/88/061144-04$03.00