DRIJVER, L. DEN (1985). PhD Thesis. Rand Afrikaans Univ.
HAAS, H. J. & SCHLIMMER, P. (1972). *Justus Liebigs Ann. Chem.* **759**, 208–210.
International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)
LIU, T. E., WOLF, B., GEIGERT, J., NIEDLEMAN, S. L., CHIN, J. D. & SHIRANG, D. (1983). *Carbohydr. Res.* **113**, 151–157.
NIEMAND, J. G., DEN DRIJVER, L., PRETORIUS, C. J., HOLZAPFEL, C. W. & VAN DER LINDE, H. J. (1983). *J. Agric. Food Chem.* **31**, 1016–1020.
SHELDRICK, G. M. (1976). *SHELX*76. Program for crystal structure determination. Univ. of Cambridge, England.
SHELDRICK, G. M. (1983). *SHELXS*84. Direct methods program (preliminary version). Univ. of Göttingen.
WALTON, D. J. (1969). *Can. J. Chem.* **47**, 3483–3487.

Acta Cryst. (1987). C**43**, 374–375

Diphenyl(2,2-diphenylvinyloxy)acetaldehyde

BY HANS PREUT, RALF STAPEL AND WILHELM P. NEUMANN

Fachbereich Chemie, Universität Dortmund, D-4600 *Dortmund* 50, *Postfach* 50 05 00, *Federal Republic of Germany*

(*Received* 27 *June* 1986; *accepted* 8 *September* 1986)

Abstract. $C_{28}H_{22}O_2$, $M_r = 390{\cdot}49$, triclinic, $P\bar{1}$, $a = 9{\cdot}604$ (5), $b = 10{\cdot}567$ (8), $c = 11{\cdot}346$ (9) Å, $\alpha = 79{\cdot}89$ (6), $\beta = 72{\cdot}79$ (6), $\gamma = 78{\cdot}54$ (6)°, $V = 1070$ (1) Å^3, $Z = 2$, $D_x = 1{\cdot}212$ Mg m^{-3}, $F(000) = 412$, λ(Ag $K\alpha$) $= 0{\cdot}5608$ Å, $\mu = 0{\cdot}05$ mm^{-1}, $T = 291$ (1) K, final $R = 0{\cdot}038$, for 1865 unique observed X-ray diffractometer data and 272 variables. The compound is the first and unexpected example of a reversible dimerization of diphenylmethyl radicals of the kind $Ph_2C^{\cdot}$—CO—R using their enoxyl form, and yielding a strainless new type of enol ether.

Experimental. The substance (Neumann & Stapel, 1986) was crystallized from a boiling mixture of benzene/petroleum ether (333–363 K) (1:1) by slow cooling to 277 K.

Crystal size $0{\cdot}22 \times 0{\cdot}42 \times 0{\cdot}42$ mm, $\omega/2\theta$ scan, scan speed 2·9–6·7° min^{-1} in θ, Nonius CAD-4 diffractometer, graphite-monochromated Ag $K\alpha$; lattice parameters from least-squares fit with 25 reflections up to $2\theta = 25{\cdot}6°$; five standard reflections recorded every 2·5 h, only random deviations; 8232 reflections measured; $1 \le \theta \le 20°$, $-11 \le h \le 11$, $-12 \le k \le 12$, $-13 \le l \le 13$; after averaging ($R_{int} = 0{\cdot}023$): 4044 unique reflections, 1865 with $I > 1{\cdot}96\sigma(I)$; Lorentz–polarization correction, no absorption correction; space group $P\bar{1}$; structure solution *via* direct methods, ΔF syntheses and full-matrix least-squares refinement with anisotropic temperature factors for all non-H atoms and a common isotropic temperature factor for H atoms, which were placed in geometrically calculated positions (C—H 0·95 Å); refinement on F with 1865 reflections and 272 refined parameters; $w = 4F_o^2/[\sigma^2(F_o^2) + 0{\cdot}06F_o^2]^2$; $S = 0{\cdot}95$, $R = 0{\cdot}038$, $wR = 0{\cdot}046$, $(\Delta/\sigma)_{max} = 0{\cdot}01$; no extinction correction; largest peak in final ΔF map $\pm 0{\cdot}13$ (7) e Å^{-3}; complex neutral-atom scattering factors from *International Tables for X-ray Crystallography* (1974); programs: *Enraf–Nonius Structure Determination Package* (Frenz, 1981), *ORTEP*II (Johnson, 1976), *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), *POP*1 (van de Waal, 1976).

Table 1 contains final atom coordinates and equivalent isotropic thermal parameters for non-hydrogen

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* (Å$^2 \times 10^3$)

$U_{eq} = (1/24\pi^2)\sum_i\sum_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
O(1)	0·7334 (2)	0·1757 (1)	0·3689 (1)	50
O(2)	0·4390 (2)	0·1821 (2)	0·4381 (2)	65
C(1)	0·6686 (2)	0·1454 (2)	0·2804 (2)	44
C(2)	0·7395 (3)	0·0857 (2)	0·4708 (2)	46
C(3)	0·7602 (2)	0·1171 (2)	0·5720 (2)	43
C(4)	0·5020 (3)	0·1567 (2)	0·3357 (2)	51
C(11)	0·6901 (3)	0·2543 (2)	0·1719 (2)	45
C(12)	0·6489 (3)	0·2465 (2)	0·0668 (2)	59
C(13)	0·6620 (3)	0·3462 (3)	−0·0302 (2)	70
C(14)	0·7172 (4)	0·4523 (3)	−0·0253 (3)	83
C(15)	0·7588 (4)	0·4600 (3)	0·0779 (3)	100
C(16)	0·7449 (3)	0·3631 (3)	0·1765 (2)	74
C(21)	0·7376 (2)	0·0122 (2)	0·2393 (2)	41
C(22)	0·6610 (3)	−0·0921 (2)	0·2689 (2)	55
C(23)	0·7309 (3)	−0·2123 (2)	0·2334 (3)	67
C(24)	0·8765 (3)	−0·2299 (3)	0·1696 (2)	66
C(25)	0·9534 (3)	−0·1281 (3)	0·1400 (2)	63
C(26)	0·8848 (3)	−0·0076 (2)	0·1744 (2)	54
C(31)	0·7634 (3)	0·2531 (2)	0·5873 (2)	46
C(32)	0·6498 (3)	0·3510 (3)	0·5708 (3)	79
C(33)	0·6522 (4)	0·4772 (3)	0·5853 (3)	106
C(34)	0·7692 (4)	0·5079 (3)	0·6139 (3)	87
C(35)	0·8804 (3)	0·4123 (3)	0·6324 (2)	68
C(36)	0·8777 (3)	0·2852 (2)	0·6203 (2)	54
C(41)	0·7802 (2)	0·0117 (2)	0·6738 (2)	44
C(42)	0·7131 (3)	0·0298 (2)	0·7975 (2)	55
C(43)	0·7251 (3)	−0·0701 (3)	0·8914 (2)	71
C(44)	0·8035 (3)	−0·1889 (3)	0·8654 (2)	75
C(45)	0·8732 (3)	−0·2087 (3)	0·7439 (3)	69
C(46)	0·8623 (3)	−0·1092 (2)	0·6492 (2)	54

0108-2701/87/020374-02$01.50

Table 2. *Bond distances* (Å), *angles* (°), *least-squares planes and dihedral angles* (°)

1	2	3	1–2	1–2–3
O(1)	C(1)	C(4)	1·435 (3)	109·2 (2)
C(21)	C(1)	O(1)	1·521 (3)	111·5 (2)
C(4)	C(1)	C(21)		112·2 (2)
C(2)	O(1)	C(1)	1·370 (3)	117·5 (2)
C(31)	C(3)	C(2)	1·485 (4)	122·6 (2)
C(31)	C(3)	C(41)		119·0 (2)

1	2	3	1–2	1–2–3
C(11)	C(1)	O(1)	1·526 (3)	106·4 (2)
C(4)	C(1)	C(11)	1·525 (5)	105·1 (2)
C(11)	C(1)	C(21)		112·2 (2)
C(3)	C(2)	O(1)	1·328 (4)	121·6 (2)
C(41)	C(3)	C(2)	1·485 (3)	118·4 (2)
O(2)	C(4)	C(1)	1·190 (3)	124·2 (3)

No.	Plane through atoms	Equation of the plane (x along **a**; y in plane ab; z along **c***)	χ^2
1	C(11), C(12), C(13), C(14), C(15), C(16)	$0{\cdot}758x - 0{\cdot}502y - 0{\cdot}417z = -3{\cdot}653$ Å	10
2	C(21), C(22), C(23), C(24), C(25), C(26)	$-0{\cdot}486x + 0{\cdot}139y - 0{\cdot}863z = 6{\cdot}007$ Å	2
3	C(31), C(32), C(33), C(34), C(35), C(36)	$0{\cdot}240x + 0{\cdot}043y - 0{\cdot}970z = 3{\cdot}634$ Å	80
4	C(41), C(42), C(43), C(44), C(45), C(46)	$-0{\cdot}950x - 0{\cdot}306y - 0{\cdot}066z = 10{\cdot}095$ Å	37
5	C(2), C(3), C(31), C(41)	$0{\cdot}891x - 0{\cdot}183y - 0{\cdot}415z = -5{\cdot}517$ Å	1

Dihedral angles: 1,2: 94·5°; 1,3: 55·6°; 1,4: 122·6°; 1,5: 19·9°; 2,3: 43·4°; 2,4: 61·5°; 2,5: 95·8°; 3,4: 100·2°; 3,5: 52·5°; 4,5: 139·7°; ($\sigma \sim 0{\cdot}2°$).

The C–C bond lengths and C–C–C angles in the phenyl groups range from 1·348 (5) to 1·390 (3) Å [mean: 1·374 (4) Å] and from 117·7 (2) to 121·6 (4)° [mean: 120·0 (3)°].

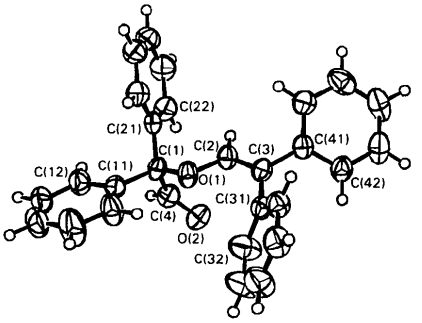

Fig. 1. General view of the molecule.

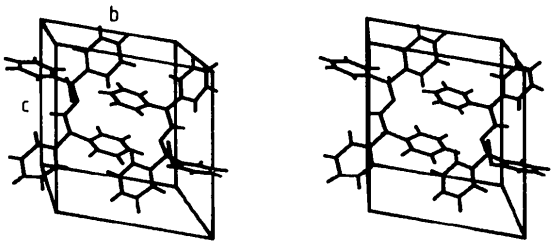

Fig. 2. Stereoscopic view of the unit cell.

atoms;* Table 2 lists bond distances and angles. Fig. 1 shows a general view of the molecule (*ORTEP*II) and Fig. 2 a stereoscopic view of the unit cell (*POP*1).

* Lists of H-atom coordinates, anisotropic thermal parameters, a complete list of bond distances and angles, and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43387 (35 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

FRENZ, B. A. (1981). *Enraf–Nonius Structure Determination Package,* 4th ed. Version 18. Enraf–Nonius, Delft, The Netherlands.

International Tables for X-ray Crystallography (1974). Vol. IV, Tables 2.2B and 2.3.1. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

JOHNSON, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee.

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.

NEUMANN, W. P. & STAPEL, R. (1986). *Chem. Ber.* **119**, 3422–3431.

WAAL, B. W. VAN DE (1976). *POP*1. *Plot of Packing Program.* Twente Univ. of Technology, The Netherlands.

Acta Cryst. (1987). C**43**, 375–376

Structure of *S*-Benzyl-L-cysteine Methyl Ester Hydrochloride

BY V. NASTOPOULOS AND G. GERMAIN

Laboratoire de Chimie Quantique, Université de Louvain, 1348 *Louvain-la-Neuve, Belgium*

AND P. CORDOPATIS AND S. VOLIOTIS

*Chemistry Department, University of Patras, Gr-*26110 *Patras, Greece*

(*Received* 29 *July* 1986; *accepted* 8 *September* 1986)

Abstract. $C_{11}H_{16}NO_2S^+.Cl^-$, $M_r = 261{\cdot}7$, monoclinic, $P2_1$, $a = 15{\cdot}327$ (11), $b = 8{\cdot}741$ (3), $c = 5{\cdot}211$ (2) Å, $\beta = 100{\cdot}01$ (5)°, $V = 687{\cdot}5$ (6) Å^3, $Z = 2$, $D_x = 1{\cdot}26$ g cm^{-3}, $F(000) = 276$, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 4{\cdot}12$ cm^{-1}, room temperature, $R = 0{\cdot}0374$ for 977 unique reflections. Cl^- ions link the organic cations

0108-2701/87/020375-02$01.50