## References

CREMER, D. & POPLE, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.

HOLZAPFEL, C. W., KOEKEMOER, J. M. & VAN DYK, M. S. (1985). Abstr. Papers 10th International Congress of Heterocyclic Chemistry, Waterloo, Ontario, P1–11.

HOLZAPFEL, C. W., KRUGER, G. J. & VAN DYK, M. S. (1987). *Acta Cryst.* C43, 514–517.

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

PETRZILKA, M., FELIX, D. & ESCHENMOSER, A. (1973). *Helv. Chim. Acta*, **56**, 2950–2960.

RIEDIKER, M. & GRAF, W. (1979). *Helv. Chim. Acta*, **62**, 2053–2061.

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

VAN DYK, M. S. (1986). PhD Thesis. Rand Afrikaans Univ., South Africa.

---

# 2-Ethyl-1,3-diphenyl-1,3-propanedione

BY D. F. MULLICA, J. W. KARBAN AND DAVID A. GROSSIE

*Departments of Chemistry and Physics, Baylor University, Waco, Texas 76798, USA*

**Abstract.** $C_{17}H_{16}O_2$, $M_r = 252\cdot31$, monoclinic, $P2_1/a$, $a = 10\cdot260$ (4), $b = 9\cdot998$ (4), $c = 13\cdot739$ (3) Å, $\beta = 92\cdot15$ (3)°, $V = 1408\cdot3$ Å$^3$, $Z = 4$, $D_x = 1\cdot19$ Mg m$^{-3}$, $\lambda$ (Mo $K\alpha$) $= 0\cdot71073$ Å, $\mu = 0\cdot072$ mm$^{-1}$, $F(000) = 536$, $T = 288$K, final $R = 0\cdot037$ for 926 unique observed reflections with $I > 3\sigma(I)$. The carbonyl functions which are oriented in a *cis* arrangement are non-coplanar (89·3°), indicating a lack of hydrogen-bonded enol formation. Details of the structural content and important bond distances and angles are reported. The bond lengths and angles are internally consistent.

**Experimental.** Crystals of the title compound (I) synthesized by a previously reported method (Kalyanam, Karban & McAtee, 1979); colorless rectangular crystal, $0\cdot32 \times 0\cdot35 \times 0\cdot84$ mm, glass fiber mount, Enraf–Nonius CAD-4F four-circle diffractometer, graphite-monochromatized Mo $K\alpha$ radiation; cell constants from setting angles of 22 reflections ($4\cdot0 \le \theta \le 13\cdot0°$); correction for Lorentz, polarization effects, no absorption correction; 288K; intensity data collected by $\omega–2\theta$ scan technique, variable scan rate of

Table 1. *Atomic positional parameters* (× 10$^4$) *and equivalent isotropic thermal parameters* (Å$^2$ × 10$^3$)

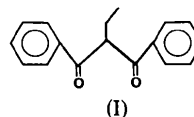|     | $x$ | $y$ | $z$ | $U_{eq}$* |
|-----|-----|-----|-----|-----|
| O1  | 9811 (2) | 3188 (2) | 1700 (2) | 779 (8) |
| O3  | 10237 (2) | 2178 (2) | 3875 (2) | 971 (9) |
| C1  | 8808 (3) | 3612 (3) | 2039 (2) | 55 (1) |
| C2  | 8449 (3) | 3266 (3) | 3072 (2) | 51 (1) |
| C3  | 9214 (3) | 2037 (3) | 3407 (2) | 62 (1) |
| C11 | 7980 (3) | 4578 (3) | 1473 (2) | 53 (1) |
| C12 | 6660 (3) | 4708 (4) | 1605 (2) | 64 (1) |
| C13 | 5931 (3) | 5618 (4) | 1049 (3) | 79 (1) |
| C14 | 6519 (4) | 6395 (4) | 372 (3) | 87 (1) |
| C15 | 7834 (4) | 6277 (4) | 243 (3) | 91 (1) |
| C16 | 8555 (3) | 5368 (4) | 784 (2) | 75 (1) |
| C21 | 8718 (3) | 4477 (4) | 3724 (2) | 69 (1) |
| C22 | 8247 (4) | 4311 (5) | 4742 (3) | 101 (2) |
| C31 | 8742 (3) | 680 (3) | 3146 (2) | 55 (1) |
| C32 | 7641 (3) | 478 (3) | 2539 (2) | 72 (1) |
| C33 | 7260 (4) | −802 (4) | 2311 (3) | 88 (1) |
| C34 | 7920 (4) | −1878 (4) | 2675 (3) | 96 (1) |
| C35 | 9001 (4) | −1682 (4) | 3287 (3) | 88 (1) |
| C36 | 9398 (3) | −419 (4) | 3519 (2) | 70 (1) |

* Equivalent isotropic thermal parameter ($U_{eq}$) defined as $\frac{1}{3}$ the trace of the orthogonalized $U_{ij}$ tensor.

Table 2. *Bond distances* (Å) *and angles* (°)

| | | | |
|---|---|---|---|
| O1—C1 | 1·221 (4) | O1—C1—C2 | 120·9 (3) |
| O3—C3 | 1·218 (4) | O1—C1—C11 | 120·0 (3) |
| C1—C2 | 1·519 (4) | C2—C1—C11 | 118·9 (3) |
| C1—C11 | 1·486 (4) | C1—C2—C3 | 109·1 (2) |
| C2—C3 | 1·520 (4) | C1—C2—C21 | 108·9 (3) |
| C2—C21 | 1·526 (5) | C3—C2—C21 | 112·5 (3) |
| C3—C31 | 1·480 (5) | O3—C3—C2 | 119·4 (3) |
| C11—C12 | 1·379 (4) | O3—C3—C31 | 120·1 (3) |
| C11—C16 | 1·382 (5) | C2—C3—C31 | 120·4 (3) |
| C12—C13 | 1·388 (5) | C1—C11—C12 | 122·5 (3) |
| C13—C14 | 1·370 (5) | C1—C11—C16 | 118·6 (3) |
| C14—C15 | 1·372 (5) | C12—C11—C16 | 118·9 (3) |
| C15—C16 | 1·373 (5) | C11—C12—C13 | 120·1 (3) |
| C21—C22 | 1·505 (5) | C12—C13—C14 | 120·2 (3) |
| C31—C32 | 1·393 (4) | C13—C14—C15 | 120·0 (3) |
| C31—C36 | 1·377 (5) | C14—C15—C16 | 119·9 (3) |
| C32—C33 | 1·371 (5) | C11—C16—C15 | 120·9 (3) |
| C33—C34 | 1·357 (5) | C2—C21—C22 | 113·7 (3) |
| C34—C35 | 1·380 (5) | C3—C31—C32 | 121·9 (3) |
| C35—C36 | 1·361 (5) | C3—C31—C36 | 119·3 (3) |
| | | C32—C31—C36 | 118·8 (3) |
| | | C31—C32—C33 | 119·3 (3) |
| | | C32—C33—C34 | 121·4 (3) |
| | | C33—C34—C35 | 119·4 (3) |
| | | C34—C35—C36 | 120·1 (3) |
| | | C31—C36—C35 | 121·0 (3) |

$0{\cdot}38{-}3{\cdot}35°\text{min}^{-1}$, intensities of two check reflections ($3\bar{1}0$ and 143) measured every 2 h revealed only random deviations ( < 1%) from mean intensities; 2910 reflections collected ($3 < 2\theta < 50°$, $h: 0{\rightarrow}12$, $k: 0{\rightarrow}11$, $l: -16{\rightarrow}16$), averaged to 926 unique reflections with $I > 3\sigma(I)$ used in solution and refinement of the structure using *SDP/VAX* (Enraf–Nonius, 1983); $R_{int} = 0{\cdot}014$; all 19 nonhydrogen atoms located by *MULTAN*11/82 (Main, 1982); H atoms calculated and included at fixed positions with $B = 5{\cdot}0$ Å$^2$; full-matrix least-squares refinement on $F$ yielded $R = 0{\cdot}037$, $wR = 0{\cdot}038$, $w = \sigma^{-2}(F_o)$ with $\sigma(F_o) = \{I_p + I_b + [0{\cdot}03(I_p - I_b)]^2\}^{1/2}$, where $I_p$ and $I_b$ are the peak and background counts respectively, $S = 1{\cdot}23$, maximum shift-to-e.s.d. ratio of a parameter in final least-squares cycle was $0{\cdot}002$; maximum and minimum residual density on final difference Fourier map, $0{\cdot}12$ (3) and $-0{\cdot}19$ (3) e Å$^{-3}$; secondary-extinction factor $g$, $5{\cdot}9$ (9) $\times 10^{-7}$, refined using the equation $|F_o| = |F_c|/(1 + gI_c)$, where $I_c$ is the calculated intensity; scattering factors and anomalous-dispersion terms taken from *International Tables for X-ray Crystallography* (1974). Table 1 presents the final atomic coordinates and

equivalent isotropic thermal parameters for the 19 nonhydrogen atoms; interatomic distances and angles are shown in Table 2.* Fig. 1 gives a steroview of the title compound.



(I)

**Related literature.** The two carbonyl groups are non-coplanar (angle = $89{\cdot}3°$), unlike the carbonyl groups of the parent compound, dibenzoylmethane (Jones, 1976).
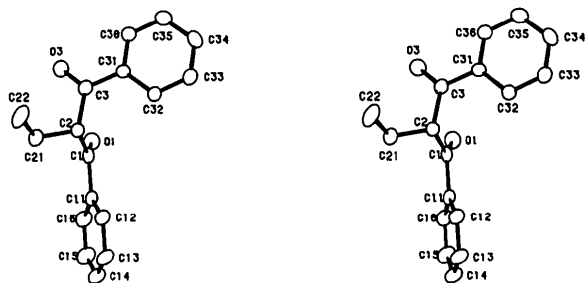
Fig. 1. A steroview of the title compound displaying ellipsoids of 20% thermal probability. Hydrogen atoms have been omitted for clarity.

**References**

Enraf–Nonius (1983). *VAX Structure Determination Package.* Enraf–Nonius, Delft.
*International Tables for X-ray Crystallography* (1974). Vol. IV, pp. 72–151. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht).
Jones, R. D. G. (1976). *Acta Cryst.* **B32**, 1807–1811.
Kalyanam, N., Karban, J. W. & McAtee, J. L. (1979). *Organic Preparation and Procedures International*, Vol. II, pp. 100–101.
Main, P. (1982). Editor. *MULTAN*11/82. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univ. of York, England.