labeling; Fig. 2 illustrates the intermolecular hydrogen bonding which is detailed in Table 4.

Related literature. A single imidazoline structure has been reported (Ellestad *et al.*, 1978). Sugar conformations in nucleosides and nucleotides were discussed by Altona & Sundaralingam (1972). A recent summary of nucleoside and nucleotide structures has been given by Jeffrey & Sundaralingam (1985).

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Acta Cryst. (1988). C**44**, 944–946

Structure of 5,5-Dimethyl-1,3,4-triphenylhexane-1,2-dione

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(*Received* 18 *June* 1987; *accepted* 21 *January* 1988)

Abstract. $C_{26}H_{26}O_2$, $M_r = 370{\cdot}490$, triclinic, $P\bar{1}$, $a = 8{\cdot}716\,(3)$, $b = 11{\cdot}077\,(8)$, $c = 12{\cdot}182\,(4)$ Å, $\alpha = 109{\cdot}17\,(4)$, $\beta = 105{\cdot}88\,(3)$, $\gamma = 91{\cdot}39\,(4)°$, $V = 1060{\cdot}1\,(9)$ Å^3, $D_x = 1{\cdot}1607$ g cm^{-3}, $\lambda(\text{Mo}\ K\alpha) = 0{\cdot}7107$ Å, $\mu = 0{\cdot}669$ cm^{-1}, $F(000) = 396$, $T = 293$ K, $R = 0{\cdot}055$ for 2321 observed diffractometer data and 357 refined parameters. The existence of the 1,2-dione group is verified. The molecule displays a steric interaction between the different groups attached to the central chain.

Experimental. Crystal 0·4 × 0·4 × 0·5 mm. Automated Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ radiation. 25 centered reflections within $5 < \theta \leq 20°$ used for determining lattice parameters. Data corrected for Lorentz and polarization effects, absorption ignored. $2\theta_{\text{max}} = 52°$, range of *hkl*: $0 \leq h \leq 10$, $-13 \leq k \leq 13$, $-15 \leq l \leq 15$. Two check reflections measured every 100 reflections showed no significant variation over data collection. $\omega/2\theta$ scans, 4139 reflections measured, 2678 independent and 2321 observed with $I > 2\sigma(I)$. $R_{\text{int}} = 0{\cdot}007$.

Structure solved by direct methods with *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980); refined by full-matrix least squares minimizing $\sum w(|F_o| - |F_c|)^2$; anisotropic thermal parameters for all non-H atoms and isotropic thermal parameters for H atoms, located from difference Fourier maps. *w* from an empirical weighting scheme so as to give no trends in $\langle w\Delta^2F\rangle$ *vs* $\langle |F_o| \rangle$ and $\langle(\sin\theta)/\lambda\rangle$. $(\Delta/\sigma)_{\text{max}} = 0{\cdot}01$, $R = 0{\cdot}055$, $wR = 0{\cdot}052$, $S = 3{\cdot}97$. Final difference Fourier excursions 0·17 and −0·22 e Å^{-3}. Atomic scattering factors and anomalous-dispersion coefficients were taken from *International Tables for X-ray Crystallography* (1974). Calculations performed with *XRAY*76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976), *PARST* (Nardelli, 1983) and *PESOS* (Martinez-Ripoll & Cano, 1975) on a VAX11/750 computer.

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The atomic parameters are listed in Table 1.* Fig. 1 shows a view of the molecule with the numbering scheme used and Fig. 2 shows a stereoview of the structure. Bond lengths and angles are given in Table 2.

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

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

	x	y	z	U_{eq}
O1	0·8209 (3)	0·0294 (2)	0·3634 (2)	782 (10)
O31	0·8929 (2)	0·3357 (2)	0·4071 (2)	643 (8)
C2	0·8655 (3)	0·1093 (2)	0·3270 (2)	547 (11)
C21	0·8378 (3)	0·0894 (2)	0·1968 (2)	606 (11)
C22	0·7319 (5)	−0·0145 (3)	0·1091 (3)	896 (17)
C23	0·7064 (6)	−0·0343 (4)	−0·0133 (3)	1148 (22)
C24	0·7874 (6)	0·0475 (5)	−0·0473 (3)	1160 (24)
C25	0·8938 (6)	0·1484 (4)	0·0378 (3)	1099 (22)
C26	0·9194 (5)	0·1701 (3)	0·1603 (3)	835 (16)
C3	0·9446 (3)	0·2403 (2)	0·4226 (2)	486 (10)
C4	1·0851 (3)	0·2415 (2)	0·5288 (2)	483 (10)
C41	1·2244 (3)	0·2335 (2)	0·4742 (2)	516 (10)
C42	1·2942 (3)	0·1216 (3)	0·4437 (2)	676 (13)
C43	1·4163 (4)	0·1152 (5)	0·3883 (3)	893 (18)
C44	1·4651 (4)	0·2188 (5)	0·3633 (3)	940 (20)
C45	1·3965 (4)	0·3301 (4)	0·3929 (3)	854 (17)
C46	1·2768 (3)	0·3379 (3)	0·4485 (2)	669 (13)
C5	1·1057 (3)	0·3592 (2)	0·6453 (2)	493 (10)
C51	1·2784 (3)	0·3905 (2)	0·7271 (2)	531 (11)
C52	1·3647 (3)	0·2964 (3)	0·7575 (2)	656 (13)
C53	1·5197 (4)	0·3284 (5)	0·8360 (3)	851 (18)
C54	1·5906 (4)	0·4539 (5)	0·8836 (3)	960 (21)
C55	1·5092 (4)	0·5475 (4)	0·8525 (3)	900 (18)
C56	1·3535 (4)	0·5159 (3)	0·7744 (2)	686 (14)
C6	0·9823 (3)	0·3496 (2)	0·7161 (2)	563 (11)
C61	0·9917 (5)	0·4832 (4)	0·8115 (3)	855 (17)
C62	0·8097 (4)	0·3137 (4)	0·6318 (3)	757 (16)
C63	1·0171 (5)	0·2525 (4)	0·7806 (4)	871 (21)

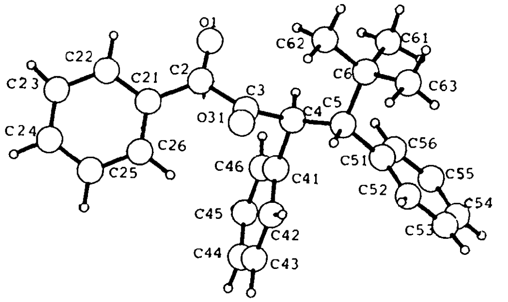

Fig. 1. A view of the molecule with the atomic labeling.

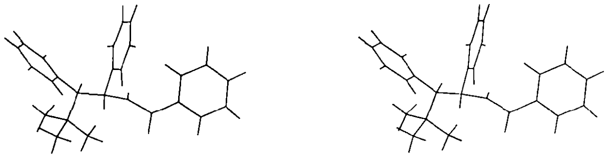

Fig. 2. A stereoscopic view of the molecule.

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

O1–C2	1·211 (4)	O31–C3	1·210 (3)
C2–C21	1·478 (4)	C2–C3	1·529 (3)
C21–C22	1·385 (4)	C21–C26	1·380 (5)
C22–C23	1·386 (6)	C23–C24	1·366 (8)
C24–C25	1·358 (6)	C25–C26	1·384 (5)
C3–C4	1·515 (3)	C4–C41	1·528 (4)
C4–C5	1·542 (3)	C41–C42	1·379 (4)
C41–C46	1·391 (5)	C42–C43	1·399 (5)
C43–C44	1·367 (8)	C44–C45	1·367 (7)
C45–C46	1·381 (5)	C5–C51	1·518 (3)
C5–C6	1·573 (4)	C51–C52	1·391 (5)
C51–C56	1·383 (4)	C52–C53	1·383 (4)
C53–C54	1·372 (7)	C54–C55	1·367 (7)
C55–C56	1·386 (4)	C6–C61	1·536 (4)
C6–C62	1·528 (4)	C6–C63	1·519 (6)

O1–C2–C3	117·0 (3)	O1–C2–C21	123·6 (3)
C21–C2–C3	119·3 (3)	C2–C21–C26	121·3 (3)
C2–C21–C22	119·6 (3)	C22–C21–C26	119·1 (3)
C21–C22–C23	119·9 (4)	C22–C23–C24	120·0 (4)
C23–C24–C25	120·7 (4)	C24–C25–C26	120·0 (5)
C21–C26–C25	120·3 (4)	O31–C3–C2	117·9 (3)
C2–C3–C4	117·5 (3)	O31–C3–C4	124·6 (3)
C3–C4–C5	113·6 (3)	C3–C4–C41	101·5 (2)
C41–C4–C5	114·9 (3)	C4–C41–C46	119·9 (3)
C4–C41–C42	121·1 (3)	C42–C41–C46	119·0 (3)
C41–C42–C43	119·8 (4)	C42–C43–C44	120·2 (4)
C43–C44–C45	120·6 (4)	C44–C45–C46	119·7 (5)
C41–C46–C45	120·8 (4)	C4–C5–C6	113·9 (3)
C4–C5–C51	111·7 (3)	C51–C5–C6	112·4 (2)
C5–C51–C56	120·0 (3)	C5–C51–C52	121·8 (3)
C52–C51–C56	118·2 (3)	C51–C52–C53	120·6 (4)
C52–C53–C54	120·1 (4)	C53–C54–C55	120·2 (4)
C54–C55–C56	119·9 (5)	C51–C56–C55	121·0 (4)
C5–C6–C63	112·9 (3)	C5–C6–C62	111·8 (3)
C5–C6–C61	107·9 (3)	C62–C6–C63	108·1 (3)
C61–C6–C63	108·7 (3)	C61–C6–C62	107·3 (3)

O1–C2–C3–O31	−127·8 (4)	C21–C2–C3–O31	48·2 (4)
O1–C2–C3–C4	53·6 (4)	C21–C2–C3–C4	−130·4 (3)
C2–C3–C4–C41	83·4 (3)	O31–C3–C4–C41	−95·1 (4)
C2–C3–C4–C5	−152·8 (3)	O31–C3–C4–C5	28·8 (5)
C3–C4–C5–C51	−154· 5 (3)	C3–C4–C5–C6	76·9 (3)
C41–C4–C5–C51	−38·2 (4)	C41–C4–C5–C6	−166·8 (3)
C4–C5–C6–C61	−167·5 (3)	C4–C5–C6–C62	−49·8 (4)
C4–C5–C6–C63	72·4 (4)	C51–C5–C6–C61	64·2 (4)
C51–C5–C6–C62	−178·1 (3)	C51–C5–C6–C63	−55·9 (4)

Related literature. Examples of structurally similar ketones that may be used as comparisons are 3,3-dihydroxy-1,4-diphenylbutane-1,2,4-trione and 1,4-diphenylbutane-1,2,3,4-tetraone (Beddoes, Cannon, Heller, Mills, Patrick, Rubin & White, 1982) and dimesityl tetraketone (Kaftory & Rubin, 1983), which point out the dependence of the steric interaction on the torsion angle O=C–C=O.

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44709 (20 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1988). C**44**, 946–947

(5Z,14Z)-1,10-Dioxa-4,7,13,15-tetrathiaoctadeca-5,14-diene

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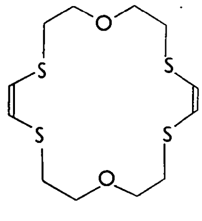
(*Received* 19 *October* 1987; *accepted* 18 *January* 1988)

Abstract. $C_{12}H_{20}O_2S_4$, $M_r = 324{\cdot}52$, monoclinic, $P2_1/a$, $a = 9{\cdot}106\,(2)$, $b = 10{\cdot}033\,(1)$, $c = 17{\cdot}307\,(3)$ Å, $\beta = 97{\cdot}51\,(2)^\circ$, $V = 1567{\cdot}6$ Å^3, $Z = 4$, $D_x = 1{\cdot}38$ Mg m^{-3}, $\lambda(\mathrm{Cu}\,K\alpha) = 1{\cdot}5418$ Å, $\mu = 53{\cdot}2$ cm^{-1}, $F(000) = 688$, $T = 293$ K, $R = 0{\cdot}034$ for 2460 reflexions ($F_o > 2\sigma_F$). The conformation at each C—S—C=C group is *anti* whereas each C—S—C—C group is *gauche*. Each of the O—C—C—S groups is *gauche*. There is not even approximate symmetry within the molecule in any direction. The angle between the normals to the S—C=C—S mean planes is 81·4 (2)°.

Experimental. The preparation and characterization of the title compound (I) will be reported separately. After preliminary photographs, unit-cell dimensions were refined from 25 accurately centred reflections with $\theta \simeq 30^\circ$ using an Enraf–Nonius CAD-4F diffractometer. Data were collected on one quadrant of a colourless crystal 0·3 × 0·5 × 0·1 mm for $\theta \leq 75^\circ$. 4492 measured reflexions gave 3212 unique reflexions (R_{int} 0·051) of which 2460 with $F > 2\sigma(F)$ were used in the refinement. Ranges of indices $-11 \leq h \leq 11$, $0 \leq k \leq 12$, $0 \leq l \leq 21$. The intensities of two standard reflexions were checked every hour and the orientation of the crystal was verified every 200 reflexions. Data were corrected for the Lorentz and polarization terms and for absorption using a ψ-scan routine. Correction factors ranged from 1·00 to 1·48.

The structure was solved using *MULTAN* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). Refinement was carried out using *SHELX76* (Sheldrick, 1976), *XANADU* (Roberts & Sheldrick, 1975) and *PLUTO* (Motherwell & Clegg, 1978). Atomic scattering factors from *SHELX76*. In the final refinement in two blocks all non-hydrogen atoms had



(I)

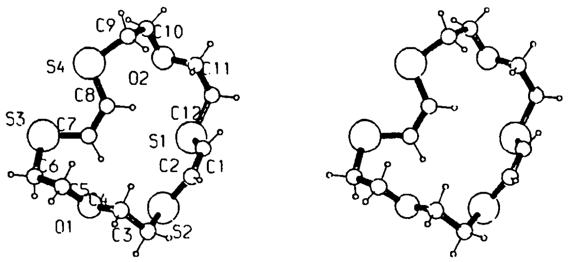


Fig. 1. Stereoview of the title compound normal to the plane S1, S3, S4, showing atomic numbering.

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