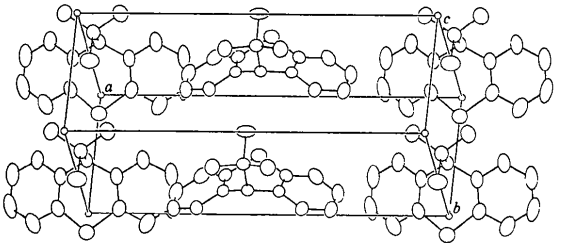

Fig. 3. The molecular packing of 9-*tert*-butylthioxanthene, excluding hydrogen atoms, in a unit cell.

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References

BRENNAN, T., PUTKEY, E. F. & SUNDARALINGAM, M. (1971). *J. Chem. Soc. D*, pp. 1490–1491.

BUSING, W. R., MARTIN, K. O. & LEVY, H. A. (1962). *ORFLS*. Report ORNL-TM-305. Oak Ridge National Laboratory, Tennessee.

CHU, S. S. C. (1972). *Acta Cryst.* B**28**, 3625–3632.

CHU, S. S. C. (1973). *Acta Cryst.* B**29**, 1690–1696.

CHU, S. S. C. & MANGION, M. (1975). *Acta Cryst.* B**31**, 2131–2134.

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

International Tables for X-ray Crystallography (1962). Vol. III, pp. 201–207. Birmingham: Kynoch Press.

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

SHIONO, R. (1971). Tech. Rep. 49. Crystallography Department, Univ. of Pittsburgh.

STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

Acta Cryst. (1978). B**34**, 2350–2351

2,6-Naphthalenediacrylic Acid Bis(2,4-dichlorophenyl) Ester

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Abstract. $C_{28}H_{16}Cl_4O_4$, triclinic, $P\bar{1}$, $a = 5{\cdot}897\ (2)$, $b = 8{\cdot}799\ (4)$, $c = 12{\cdot}784\ (4)$ Å, $\alpha = 69{\cdot}42\ (3)$, $\beta = 97{\cdot}14\ (3)$, $\gamma = 99{\cdot}98\ (3)°$, $Z = 1$, $D_x = 1{\cdot}52$ g cm^{-3}. The distance between the double bonds in adjacent molecules is 3·76 Å.

Introduction. The title substance is of interest because it is known to polymerize in the solid state (Meyer & Wegner, 1978). This study was undertaken to assist investigation of the mechanism of this topochemical reaction. It was of special interest to know whether the molecular packing allows reaction of neighbouring molecules without large molecular motions.

Single crystals suitable for data collection were obtained by slow cooling (3° h^{-1}) of a solution in γ-butyrolactone. A crystal, 0·6 × 0·2 × 0·1 mm, was used for data collection on a Nonius automatic four-circle diffractometer with Mo $K\alpha$ radiation. The θ–2θ scan mode was used. Of the 3241 accessible unique reflexions significant counts were recorded for 2974 ($2\theta < 60°$). The structure was solved with *MULTAN* (Declercq, Germain, Main & Woolfson, 1973). Refinement was by full-matrix least squares with unit weights. The coordinates of the H atoms were found in a

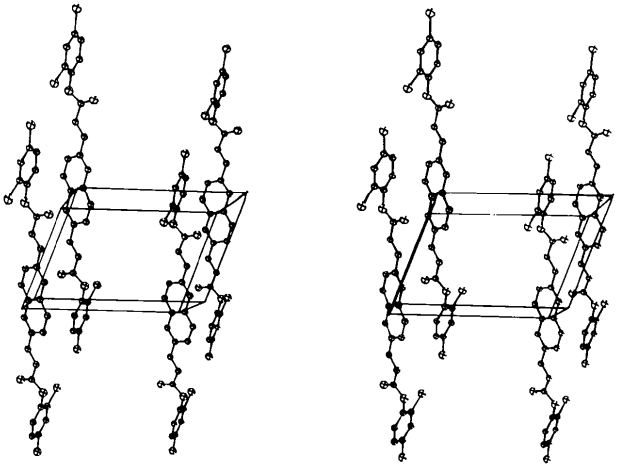

Fig. 1. Stereoscopic diagram of the packing arrangement (Johnson, 1965). The *c* axis is horizontal and *b* vertical.

Table 1. *Final atomic parameters* ($\times 10^4$)

	x	y	z	B (Å^2)
C(1)	1005 (4)	42 (2)	−266 (2)	
C(2)	1955 (4)	−1423 (3)	−68 (2)	
C(3)	991 (4)	−2897 (3)	651 (2)	
C(4)	−1045 (4)	−2977 (3)	1164 (2)	
C(5)	−2020 (4)	−1584 (3)	976 (2)	
C(6)	2163 (4)	−4340 (3)	888 (2)	
C(7)	1725 (5)	−5765 (3)	1696 (2)	
C(8)	3166 (5)	−7068 (3)	1872 (2)	
C(9)	3870 (4)	−9649 (3)	3112 (2)	
C(10)	6040 (4)	−9531 (3)	3650 (2)	
C(11)	7273 (4)	−10849 (3)	4013 (2)	
C(12)	6270 (4)	−12281 (3)	3828 (2)	
C(13)	4122 (5)	−12428 (3)	3298 (2)	
C(14)	2916 (4)	−11090 (3)	2928 (2)	
O(1)	2554 (3)	−8370 (2)	2807 (2)	
O(2)	4653 (4)	−7040 (2)	1318 (2)	
Cl(1)	7207 (1)	−7745 (1)	3913 (1)	
Cl(2)	7806 (1)	−13944 (1)	4298 (1)	
H(1)	3342 (45)	−1317 (32)	−463 (22)	3·19 (56)
H(2)	−1776 (45)	−4032 (32)	1683 (21)	3·25 (57)
H(3)	−3457 (46)	−1681 (32)	1372 (22)	3·20 (56)
H(4)	3401 (50)	−4172 (32)	396 (20)	3·26 (57)
H(5)	527 (50)	−6044 (35)	2246 (24)	4·12 (65)
H(6)	8870 (51)	−10790 (35)	4437 (24)	4·12 (65)
H(7)	3425 (52)	−13411 (39)	3137 (25)	4·71 (71)
H(8)	1251 (48)	−11121 (34)	2504 (23)	3·69 (60)

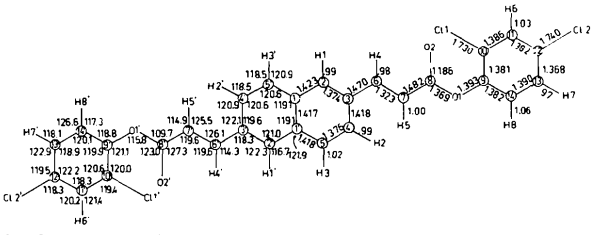

Fig. 2. Observed bond lengths and angles. E.s.d. of bond lengths between non-hydrogen atoms is 0·003 Å, e.s.d. of bond lengths to H atoms is 0·03 Å, e.s.d. of bond angles between non-hydrogen atoms is 0·2°, e.s.d. of bond angles to H atoms is 1·3°.

difference map. All positional parameters were refined with anisotropic thermal motion for the non-hydrogen and isotropic for the H atoms. The final R was 0·048.

No absorption correction was applied. The programs used were those of the XRAY 76 system (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976). Scattering factors for the non-hydrogen atoms were from *International Tables for X-ray Crystallography* (1968) and for H from Stewart, Davidson & Simpson (1965). The final atomic and (for H only) thermal parameters are given in Table 1.*

Discussion. Fig. 1 shows a stereoscopic packing diagram. Polymerization occurs by formation of cyclobutane rings from neighbouring C—C double bonds along *b*. The distance between adjacent double bonds is 3·76 Å, which is consistent with distances observed in highly reactive cinnamic acid derivatives (Schmidt, 1967). Observed bond lengths and angles are shown in Fig. 2. Within experimental error the naphthalene and phenyl rings are planar with an angle of 63·0° between the two ring systems.

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* Lists of structure factors and anisotropic temperature factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33464 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

DECLERCQ, J. P., GERMAIN, G., MAIN, P. & WOOLFSON, M. M. (1973). *Acta Cryst.* A**29**, 231–234.

International Tables for X-ray Crystallography (1968). Vol. III, 2nd ed. Birmingham: Kynoch Press.

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

MEYER, W. & WEGNER, G. (1978). *J. Polym. Sci. Polym. Phys. Ed.* In the press.

SCHMIDT, G. M. J. (1967). *Reactivity of the Photoexcited Molecule*, pp. 227–284. New York: Interscience.

STEWART, J. M., MACHIN, P. A., DICKINSON, C., AMMON, H. L., HECK, H. & FLACK, H. (1976). The XRAY system – version of March 1976. Tech. Rep. TR 446. Computer Science Center, Univ. of Maryland, College Park, Maryland.

STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.