Table 2. *Selected geometric parameters* (Å, °)

O—C5	1.364 (4)	C9—C10	1.412 (4)
O—C1	1.458 (4)	C10—C11	1.353 (5)
N—C12	1.307 (4)	C11—C12	1.404 (5)
N—C8	1.364 (5)	C13—C18	1.377 (4)
C1—C19	1.504 (4)	C13—C14	1.379 (5)
C1—C2	1.515 (4)	C14—C15	1.388 (5)
C1—C13	1.528 (4)	C15—C16	1.353 (6)
C2—C3	1.312 (5)	C16—C17	1.370 (6)
C3—C4	1.457 (4)	C17—C18	1.386 (5)
C4—C5	1.374 (4)	C19—C20	1.386 (4)
C4—C9	1.422 (5)	C19—C24	1.393 (5)
C5—C6	1.399 (4)	C20—C21	1.363 (5)
C6—C7	1.352 (5)	C21—C22	1.374 (5)
C7—C8	1.413 (4)	C22—C23	1.354 (5)
C8—C9	1.418 (4)	C23—C24	1.370 (5)
C5—O—C1	118.5 (2)	C10—C9—C4	123.8 (3)
C12—N—C8	117.5 (3)	C8—C9—C4	120.0 (3)
O—C1—C19	108.6 (2)	C11—C10—C9	120.2 (3)
O—C1—C2	109.7 (2)	C10—C11—C12	118.9 (3)
C19—C1—C2	111.1 (3)	N—C12—C11	124.0 (3)
O—C1—C13	104.2 (2)	C18—C13—C14	118.6 (3)
C19—C1—C13	112.5 (2)	C18—C13—C1	120.2 (2)
C2—C1—C13	110.5 (2)	C14—C13—C1	121.2 (3)
C3—C2—C1	120.6 (2)	C13—C14—C15	120.6 (4)
C2—C3—C4	121.5 (3)	C16—C15—C14	120.4 (4)
C5—C4—C9	118.3 (2)	C15—C16—C17	119.8 (3)
C5—C4—C3	116.6 (3)	C16—C17—C18	120.4 (4)
C9—C4—C3	125.0 (3)	C13—C18—C17	120.2 (3)
O—C5—C4	121.8 (2)	C20—C19—C24	117.7 (3)
O—C5—C6	116.0 (2)	C20—C19—C1	120.0 (3)
C4—C5—C6	122.1 (3)	C24—C19—C1	122.4 (2)
C7—C6—C5	119.8 (3)	C21—C20—C19	120.2 (3)
C6—C7—C8	121.3 (3)	C20—C21—C22	121.2 (3)
N—C8—C7	118.4 (3)	C23—C22—C21	119.4 (3)
N—C8—C9	123.1 (3)	C22—C23—C24	120.3 (3)
C7—C8—C9	118.4 (3)	C23—C24—C19	121.1 (3)
C10—C9—C8	116.2 (3)		

Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1994). Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *Word* 5.0 on a Macintosh LCII.

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Diethyl Methano-C60-fullerene-61,61-dicarboxylate Chloroform Solvate at 193 K, C60C(CO2C2H5)2.CHCl3

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Abstract

The structure of fullerene can be interpreted as a condensation of 20 cyclohexatriene rings [with single- and double-bond lengths of 1.450 (4) Å and 1.390 (4) Å, respectively] to form a highly symmetrical sphere. The addition of the bis(ethoxycarbonyl)methano group to a double bond prevents the known disorder of the unsubstituted fullerene molecule in the solid phase.

Comment

The title compound (I) crystallizes with two molecules in the asymmetric unit together with two chloroform solvent molecules. The fullerene molecule can be interpreted as an arrangement of 12 five-membered rings on the surface of a sphere connected by double bonds. In this way, 20 six-membered rings are generated, all of which are formal cyclohexatriene rings.

(I)
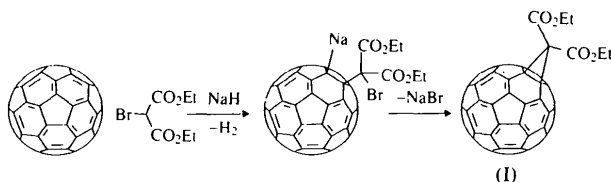
Even at low temperature (249 K), the crystal structure of unsubstituted C60-fullerene is disordered (Bürgi *et al.*, 1992). Because in this case the malonic acid diethyl ester group is added to a double bond of the fullerene molecule, the orientation of the fullerene molecule is fixed in the cell. It is therefore possible to determine the dimensions of the fullerene molecule quite accurately because the coordinates of C atoms having the same local symmetry are determined many times. This situation is further enhanced by the fact that there are two molecules in the asymmetric unit.

The addition of the malonic acid diethyl ester group increases the C—C bond distance involved in the cyclopropane ring fusion from 1.393 (5) Å to an average of 1.606 (4) Å. This is contrary to the theory that the fullerene ring system is opened by the addition

of a substituent (Wudl, 1992) and is similar to the results obtained for a Diels–Alder adduct where a C—C distance of 1.62 (4) Å was found (Rubin, Khan, Freedberg & Yeretzian, 1993). In the Pt–C_{60} complex, where the Pt atom is bridging, a distance of 1.4979 (7) Å was found (Fagan, Calabrese & Malone, 1991a,b).

The C—C bond lengths in the immediate environment of the generated cyclopropane ring (two five-membered and two six-membered rings) are influenced strongly. The single-bond lengths (excluding those within the cyclopropane ring) vary from 1.435 (4) to 1.503 (4) Å, and the double-bond lengths vary from 1.373 (4) to 1.384 (4) Å, the average values being 1.47 (2) and 1.378 (3), respectively. On the other side of the sphere (around the C51=C34 double bond), the single bonds vary in length between 1.442 (4) and 1.461 (4) Å, with an average of 1.453 (4) Å, and the double bonds vary between 1.384 (5) and 1.401 (4) Å, with an average of 1.393 (5) Å. These latter values are almost congruent with the bond lengths (1.401 and 1.458 Å) found by electron diffraction in a gas-phase study (Hedberg *et al.*, 1991).

This comparison shows that the addition of malonic acid diethyl ester affects the single bonds of the fullerene molecule much more than it does the double bonds.

The average distance of an atom from the best plane through its associated five- or six-membered ring becomes smaller as the distance from the cyclopropane ring increases, and varies between 0.0001 and 0.044 Å. It is concluded that the five- and six-membered rings in unsubstituted and undistorted fullerene are fully planar but not aromatic, the location of the double bonds being fixed. Fig. 1 shows the antiprismatic arrangement of two five-membered rings with practically no distortion and Fig. 2 shows an antiprismatic arrangement with maximum distortion. In the first case, the angle between the two five-membered rings is 0.3 (1)°; in the second this angle is 5.1 (2)°.
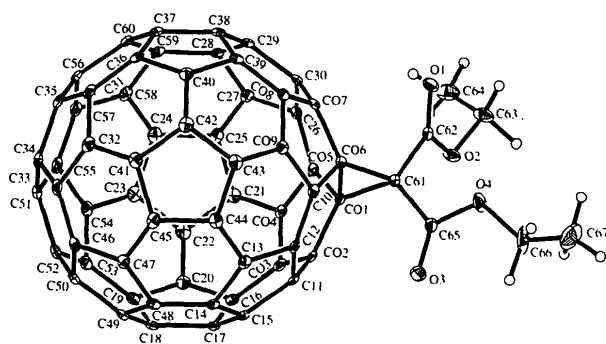

Fig. 1. Projection of the title compound showing the most ideal antiprismatic arrangement of two five-membered rings. Displacement ellipsoids are at the 20% probability level. Atom numbers correspond to those of Table 1 without the prefixes 1 or 2, which indicate different molecules in the asymmetric unit.

Fig. 3 is a projection of the crystal structure along the c axis, perpendicular to (1$\bar{1}$0), showing alternate polar and non-polar regions. One carbonyl group of the malonic ester is involved in a very weak hydrogen bond to the chloroform solvent molecule with distances of 3.351 (7) and 3.395 (7) Å.
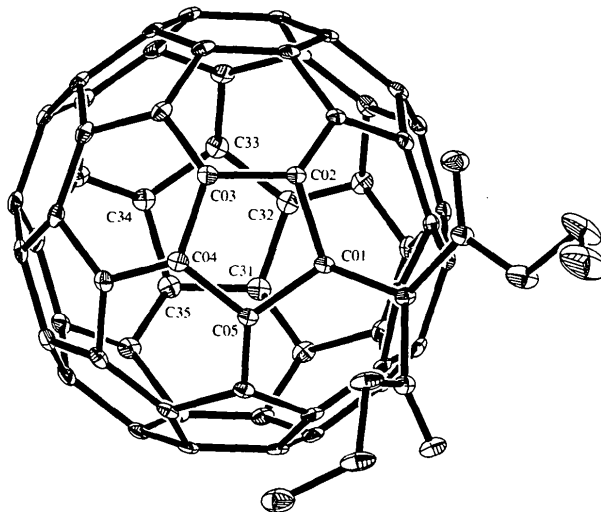
Fig. 2. Projection of the title compound showing the most non-ideal antiprismatic arrangement of two five-membered rings. Displacement ellipsoids are at the 20% probability level.
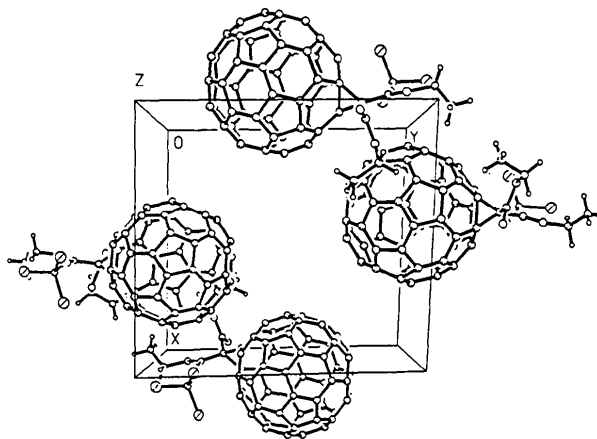
Fig. 3. Projection of the structure along the c axis.

Experimental

The compound was synthesized according to the procedure of Bingel (1993) (see scheme above). The crystals were obtained by evaporation from chloroform solution. The density was measured by flotation in aqueous K_2HgI_4.

Crystal data

$C_{67}H_{10}O_4.CHCl_3$	Mo $K\alpha$ radiation
$M_r = 998.12$	$\lambda = 0.71073$ Å

Triclinic
$P\bar{1}$
$a = 13.665 (1)$ Å
$b = 14.680 (2)$ Å
$c = 19.539 (2)$ Å
$\alpha = 94.965 (6)°$
$\beta = 104.131 (7)°$
$\gamma = 90.482 (8)°$
$V = 3784.9 (7)$ Å^3
$Z = 4$
$D_x = 1.752$ Mg m^{-3}
$D_m = 1.72$ Mg m^{-3}

Cell parameters from 25
reflections
$\theta = 5.5–18.2°$
$\mu = 0.312$ mm^{-1}
$T = 193 (2)$ K
Rectangular columns
$0.75 \times 0.21 \times 0.14$ mm
Black

Data collection

Siemens $R3m/V$ four-circle
  diffractometer
$2\theta/\theta$ scans
Absorption correction:
  none
15 687 measured reflections
13 408 independent
  reflections
8198 observed reflections
  $[I > 2\sigma(I)]$

$R_{int} = 0.0229$
$\theta_{max} = 25.06°$
$h = -16 \rightarrow 2$
$k = -17 \rightarrow 17$
$l = -22 \rightarrow 23$
1 standard reflection
  monitored every 65
  reflections
  intensity variation: 2.3%

Refinement

Refinement on F^2
$R(F) = 0.045$
$wR(F^2) = 0.125$
$S = 0.931$
13 401 reflections
1401 parameters
H atoms refined as riding
  model
$w = 1/[\sigma^2(F_o^2) + (0.0733P)^2]$
  where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.072$
$\Delta\rho_{max} = 0.901$ e Å^{-3}
$\Delta\rho_{min} = -0.620$ e Å^{-3}
Atomic scattering factors
  from *International Tables*
  for Crystallography (1992,
  Vol. C, Tables 4.2.6.8 and
  6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent*
isotropic displacement parameters (Å^2)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
C101	-0.0209 (2)	0.3218 (2)	0.18903 (15)	0.0195 (6)
C102	-0.0047 (2)	0.3238 (2)	0.26777 (15)	0.0186 (6)
C103	-0.0797 (2)	0.3810 (2)	0.2878 (2)	0.0217 (6)
C104	-0.1356 (2)	0.4242 (2)	0.2263 (2)	0.0212 (6)
C105	-0.0953 (2)	0.3943 (2)	0.16672 (14)	0.0194 (6)
C106	0.0795 (2)	0.3260 (2)	0.16027 (14)	0.0202 (6)
C107	0.0865 (2)	0.4026 (2)	0.11580 (14)	0.0213 (6)
C108	0.1888 (2)	0.4388 (2)	0.13535 (15)	0.0212 (6)
C109	0.2438 (2)	0.3956 (2)	0.1967 (2)	0.0211 (6)
C110	0.1763 (2)	0.3311 (2)	0.21567 (15)	0.0208 (6)
C111	0.0897 (2)	0.3205 (2)	0.31275 (15)	0.0198 (6)
C112	0.1817 (2)	0.3241 (2)	0.28647 (15)	0.0197 (6)
C113	0.2577 (2)	0.3770 (2)	0.3403 (2)	0.0231 (7)
C114	0.2143 (2)	0.4052 (2)	0.39957 (15)	0.0220 (6)
C115	0.1103 (2)	0.3707 (2)	0.38215 (14)	0.0219 (7)
C116	-0.0608 (2)	0.4282 (2)	0.3552 (2)	0.0232 (6)
C117	0.0365 (2)	0.4222 (2)	0.40353 (15)	0.0234 (7)
C118	0.0627 (2)	0.5117 (2)	0.44209 (14)	0.0239 (7)
C119	-0.0188 (2)	0.5719 (2)	0.4177 (2)	0.0265 (7)
C120	-0.0960 (2)	0.5206 (2)	0.3632 (2)	0.0254 (7)
C121	-0.1687 (2)	0.5128 (2)	0.2347 (2)	0.0237 (7)
C122	-0.1486 (2)	0.5623 (2)	0.3049 (2)	0.0266 (7)
C123	-0.1267 (2)	0.6570 (2)	0.2974 (2)	0.0257 (7)
C124	-0.1341 (2)	0.6664 (2)	0.2227 (2)	0.0252 (7)
C125	-0.1602 (2)	0.5765 (2)	0.1841 (2)	0.0242 (7)
C126	-0.0847 (2)	0.4554 (2)	0.11914 (14)	0.0209 (6)
C127	-0.1179 (2)	0.5488 (2)	0.12805 (15)	0.0223 (7)
C128	-0.0475 (2)	0.6098 (2)	0.10815 (14)	0.0228 (7)
C129	0.0302 (2)	0.5560 (2)	0.08721 (14)	0.0228 (7)
C130	0.0077 (2)	0.4602 (2)	0.09346 (14)	0.0222 (7)
C131	0.2722 (2)	0.7214 (2)	0.2575 (2)	0.0256 (7)
C132	0.3277 (2)	0.6784 (2)	0.3193 (2)	0.0256 (7)
C133	0.2841 (2)	0.7065 (2)	0.3781 (2)	0.0250 (7)
C134	0.2022 (2)	0.7669 (2)	0.3531 (2)	0.0253 (7)
C135	0.1945 (2)	0.7762 (2)	0.2788 (2)	0.0254 (7)
C136	0.2527 (2)	0.6742 (2)	0.1907 (2)	0.0252 (7)
C137	0.1546 (2)	0.6791 (2)	0.14201 (15)	0.0237 (7)
C138	0.1287 (2)	0.5899 (2)	0.10315 (14)	0.0236 (7)
C139	0.2105 (2)	0.5305 (2)	0.12827 (15)	0.0232 (7)
C140	0.2883 (2)	0.5818 (2)	0.1823 (2)	0.0236 (7)
C141	0.3611 (2)	0.5895 (2)	0.3106 (2)	0.0260 (7)
C142	0.3403 (2)	0.5401 (2)	0.2409 (2)	0.0243 (7)
C143	0.3179 (2)	0.4449 (2)	0.2481 (2)	0.0239 (7)
C144	0.3256 (2)	0.4355 (2)	0.3219 (2)	0.0240 (7)
C145	0.3515 (2)	0.5246 (2)	0.3612 (2)	0.0246 (7)
C146	0.2754 (2)	0.6441 (2)	0.4263 (2)	0.0256 (7)
C147	0.3094 (2)	0.5516 (2)	0.4173 (2)	0.0240 (7)
C148	0.2393 (2)	0.4907 (2)	0.43706 (14)	0.0244 (7)
C149	0.1620 (2)	0.5449 (2)	0.45899 (14)	0.0246 (7)
C150	0.1844 (2)	0.6402 (2)	0.45216 (15)	0.0268 (7)
C151	0.1151 (2)	0.7631 (2)	0.3777 (2)	0.0259 (7)
C152	0.1056 (2)	0.6985 (2)	0.4283 (2)	0.0263 (7)
C153	0.0019 (2)	0.6636 (2)	0.4111 (2)	0.0254 (7)
C154	-0.0530 (2)	0.7068 (2)	0.3495 (2)	0.0260 (7)
C155	0.0167 (2)	0.7684 (2)	0.3291 (2)	0.0254 (7)
C156	0.1005 (2)	0.7813 (2)	0.2321 (2)	0.0251 (7)
C157	0.0095 (2)	0.7772 (2)	0.2578 (2)	0.0253 (7)
C158	-0.0675 (2)	0.7251 (2)	0.2036 (2)	0.0254 (7)
C159	-0.0236 (2)	0.6962 (2)	0.1446 (2)	0.0242 (7)
C160	0.0808 (2)	0.7311 (2)	0.1625 (2)	0.0256 (7)
C161	0.0048 (2)	0.2461 (2)	0.13905 (15)	0.0217 (6)
C162	-0.0609 (2)	0.2374 (2)	0.0633 (2)	0.0246 (7)
C163	-0.2250 (3)	0.1926 (3)	-0.0061 (2)	0.0449 (10)
C164	-0.2879 (3)	0.2739 (4)	-0.0148 (2)	0.0524 (11)
C165	0.0366 (2)	0.1550 (2)	0.1667 (2)	0.0270 (7)
C166	0.0631 (4)	0.0001 (2)	0.1292 (2)	0.085 (2)
C167	-0.0137 (5)	-0.0572 (3)	0.0887 (3)	0.106 (2)
O11	-0.0343 (2)	0.2601 (2)	0.01307 (11)	0.0345 (5)
O12	-0.1513 (2)	0.2022 (2)	0.06239 (11)	0.0388 (6)
O13	0.0572 (2)	0.13985 (15)	0.22694 (12)	0.0475 (7)
O14	0.0397 (3)	0.0948 (2)	0.11355 (13)	0.0674 (10)
C201	-0.4660 (2)	-0.1738 (2)	0.15826 (14)	0.0208 (6)
C202	-0.5295 (2)	-0.1686 (2)	0.21018 (15)	0.0201 (6)
C203	-0.6081 (2)	-0.1040 (2)	0.1878 (2)	0.0224 (7)
C204	-0.5887 (2)	-0.0605 (2)	0.12837 (15)	0.0229 (7)
C205	-0.4984 (2)	-0.0970 (2)	0.11285 (14)	0.0222 (6)
C206	-0.3467 (2)	-0.1785 (2)	0.19128 (15)	0.0208 (6)
C207	-0.2828 (2)	-0.1062 (2)	0.1724 (2)	0.0219 (6)
C208	-0.2046 (2)	-0.0764 (2)	0.2348 (2)	0.0227 (6)
C209	-0.2245 (2)	-0.1200 (2)	0.2942 (2)	0.0236 (7)
C210	-0.3149 (2)	-0.1770 (2)	0.27067 (15)	0.0201 (6)
C211	-0.4920 (2)	-0.1750 (2)	0.28176 (15)	0.0214 (6)
C212	-0.3828 (2)	-0.1796 (2)	0.31194 (14)	0.0215 (7)
C213	-0.3604 (2)	-0.1294 (2)	0.38156 (14)	0.0248 (7)
C214	-0.4531 (2)	-0.0950 (2)	0.39504 (15)	0.0255 (7)
C215	-0.5346 (2)	-0.1227 (2)	0.3331 (2)	0.0249 (7)
C216	-0.6500 (2)	-0.0543 (2)	0.2368 (2)	0.0254 (7)
C217	-0.6121 (2)	-0.0638 (2)	0.3114 (2)	0.0276 (7)
C218	-0.6123 (2)	0.0251 (2)	0.3500 (2)	0.0270 (7)
C219	-0.6506 (2)	0.0902 (2)	0.2988 (2)	0.0287 (7)
C220	-0.6749 (2)	0.0409 (2)	0.2286 (2)	0.0273 (7)
C221	-0.6127 (2)	0.0310 (2)	0.1203 (2)	0.0256 (7)
C222	-0.6568 (2)	0.0824 (2)	0.1715 (2)	0.0261 (7)
C223	-0.6137 (2)	0.1751 (2)	0.1814 (2)	0.0286 (7)
C224	-0.5432 (2)	0.1798 (2)	0.1367 (2)	0.0267 (7)
C225	-0.5435 (2)	0.0905 (2)	0.09844 (15)	0.0243 (7)
C226	-0.4309 (2)	-0.0398 (2)	0.09399 (14)	0.0230 (7)
C227	-0.4545 (2)	0.0558 (2)	0.08640 (14)	0.0237 (7)

C228	−0.3608 (2)	0.1093 (2)	0.11122 (15)	0.0241 (7)
C229	−0.2798 (2)	0.0480 (2)	0.1344 (2)	0.0252 (7)
C230	−0.3211 (2)	−0.0447 (2)	0.12429 (14)	0.0206 (6)
C231	−0.2046 (2)	0.2062 (2)	0.3563 (2)	0.0279 (7)
C232	−0.2237 (2)	0.1630 (2)	0.4159 (2)	0.0280 (7)
C233	−0.3172 (3)	0.1977 (2)	0.4291 (2)	0.0285 (7)
C234	−0.3562 (3)	0.2629 (2)	0.3774 (2)	0.0278 (7)
C235	−0.2862 (2)	0.2679 (2)	0.3325 (2)	0.0286 (7)
C236	−0.1629 (2)	0.1562 (2)	0.3070 (2)	0.0289 (7)
C237	−0.2014 (2)	0.1656 (2)	0.2315 (2)	0.0283 (7)
C238	−0.2014 (2)	0.0757 (2)	0.1933 (2)	0.0260 (7)
C239	−0.1633 (2)	0.0122 (2)	0.2449 (2)	0.0268 (7)
C240	−0.1393 (2)	0.0614 (2)	0.3148 (2)	0.0277 (7)
C241	−0.2013 (2)	0.0710 (2)	0.4235 (2)	0.0274 (7)
C242	−0.1578 (2)	0.0199 (2)	0.3720 (2)	0.0274 (7)
C243	−0.2009 (2)	−0.0723 (2)	0.3617 (2)	0.0261 (7)
C244	−0.2708 (2)	−0.0782 (2)	0.40618 (15)	0.0250 (7)
C245	−0.2710 (2)	0.0111 (2)	0.44458 (15)	0.0278 (7)
C246	−0.3839 (3)	0.1400 (2)	0.44958 (15)	0.0301 (8)
C247	−0.3595 (3)	0.0447 (2)	0.45778 (15)	0.0282 (7)
C248	−0.4528 (2)	−0.0098 (2)	0.43225 (15)	0.0267 (7)
C249	−0.5346 (2)	0.0521 (2)	0.4086 (2)	0.0277 (7)
C250	−0.4922 (2)	0.1444 (2)	0.4196 (2)	0.0277 (7)
C251	−0.4590 (3)	0.2672 (2)	0.3489 (2)	0.0287 (7)
C252	−0.5293 (2)	0.2070 (2)	0.3700 (2)	0.0290 (7)
C253	−0.6097 (2)	0.1791 (2)	0.3085 (2)	0.0283 (7)
C254	−0.5905 (2)	0.2218 (2)	0.2488 (2)	0.0289 (7)
C255	−0.4974 (2)	0.2767 (2)	0.2737 (2)	0.0279 (7)
C256	−0.3224 (2)	0.2768 (2)	0.2603 (2)	0.0270 (7)
C257	−0.4298 (3)	0.2812 (2)	0.2307 (2)	0.0277 (7)
C258	−0.4532 (3)	0.2310 (2)	0.1608 (2)	0.0275 (7)
C259	−0.3609 (2)	0.1958 (2)	0.1471 (2)	0.0257 (7)
C260	−0.2794 (2)	0.2243 (2)	0.2090 (2)	0.0275 (7)
C261	−0.4063 (2)	−0.2541 (2)	0.13936 (15)	0.0241 (7)
C262	−0.3903 (2)	−0.2627 (2)	0.0649 (2)	0.0260 (7)
C263	−0.2738 (3)	−0.3046 (3)	−0.0035 (2)	0.0476 (11)
C264	−0.2198 (4)	−0.2203 (4)	−0.0145 (2)	0.0569 (12)
C265	−0.4236 (3)	−0.3452 (2)	0.1664 (2)	0.0282 (7)
C266	−0.4639 (5)	−0.5029 (2)	0.1290 (3)	0.098 (2)
C267	−0.4191 (5)	−0.5601 (3)	0.0855 (3)	0.093 (2)
O21	−0.4530 (2)	−0.2442 (2)	0.01329 (11)	0.0371 (6)
O22	−0.2993 (2)	−0.2931 (2)	0.06487 (11)	0.0414 (6)
O23	−0.4161 (2)	−0.3586 (2)	0.22603 (13)	0.0583 (8)
O24	−0.4477 (3)	−0.4081 (2)	0.11365 (13)	0.0778 (11)
C111	0.23956 (7)	0.16721 (5)	0.42762 (4)	0.0351 (2)
C112	0.05230 (7)	0.14908 (8)	0.46774 (5)	0.0526 (3)
C113	0.11899 (8)	−0.00036 (6)	0.38398 (6)	0.0578 (3)
C1	0.1168 (3)	0.1190 (2)	0.4016 (2)	0.0324 (8)
C121	−0.25251 (6)	−0.33583 (5)	0.42978 (4)	0.0329 (2)
C122	−0.38478 (8)	−0.49729 (6)	0.38741 (5)	0.0478 (2)
C123	−0.44317 (7)	−0.33913 (7)	0.46707 (5)	0.0475 (2)
C2	−0.3783 (3)	−0.3767 (2)	0.4026 (2)	0.0298 (7)

Although $\langle |E^2-1| \rangle$ was 1.04, the phase problem could be solved only in the non-centrosymmetric space group $P1$ with four molecules of fullerene per unit cell. In the course of the investigation it was found that one molecule of chloroform crystallizes with one molecule of fullerene and that the structure has, in reality, the centrosymmetric space group $P\bar{1}$. During parameter refinement in the non-centrosymmetric space group it was not possible to distinguish between single and double bonds in the fullerene molecule without extensive use of restraints. Refinement in the correct space group, however, produced average bond lengths with relatively low e.s.d.'s for the single and double bonds at a 'respectful' distance from the cyclopropane ring [1.453 (4) and 1.393 (5) Å].

Siemens $P3$ diffractometer software was used for data collection, data reduction and cell refinement. SHELXS86 (Sheldrick, 1990) was used for the solution of the phase problem and SHELXL93 (Sheldrick, 1993) was used for the refinement of parameters. SHELXTL-Plus (Sheldrick, 1991) was used for molecular graphics and SHELXL93 for the preparation of the published material.

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(–)-(S,S)-α-Phenyl-2-(p-tolylsulfinyl)-3-furanmethanol

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Abstract

The structure determination of the title compound, $C_{18}H_{16}O_3S$, based on X-ray single crystal diffraction data, confirms that the absolute configuration is S at the two asymmetric centres; it facilitated the establishment of the absolute configuration of the chiral C centre of the parent molecule, after cleaveage of the sulfoxide group, which had been postulated but not confirmed in the literature until now.