

The two independent molecules are related by a pseudo inversion centre which exactly relates the Br and Si atoms and nearly relates the remainder of the molecules. The main exception is the orientations of the phenyl rings C(15) → (20) and C(47) → (52) which differ by 37°. This is obvious from the torsion angles C(1)–Si(1)–C(15)–C(16) and C(27)–Si(2)–C(47)–C(48) which are –104 and 141° respectively. The equivalent bond lengths and angles in the two molecules are equal within experimental error. Br(2)–C(1) and Br(4)–C(27), average 1.93 (1) Å, are systematically shorter than Br(1)–C(2) and Br(3)–C(28), average 1.99 (1) Å. For comparison, the C–Br lengths in hexabromoethane average 1.944 (5) Å (Mandel & Donohue, 1972), but quite a wide variation in C–Br lengths is found in other structures. A value of 1.909 (12) Å occurs in (4-bromo-1,2,3,4-tetraphenyl-*cis*-1,3-butadienyl)dimethylphenyltin (Boer, van Remoortere, North & Reeke, 1971), and 2.00 (3) Å in (+)-1,2-dibromo-2-phenethyl *p*-tolyl sulphoxide (Iwasaki, Mitamura & Tsuchihashi, 1975). In 3-bromo-2,2-diphenyl-2-sila- $\Delta$ 3-1-tetralone (Vidal, Galigné & Falgueirettes, 1972) where a C atom is bonded to both Br

and Si, the C–Br length is 1.911 (5) Å, although in this case the C atom is trigonally hybridized.

### References

- BOER, F. P., VAN REMOORTERE, F. P., NORTH, P. P. & REEKE, G. N. (1971). *Inorg. Chem.* **10**, 529–537.  
 BROOK, A. G., DUFF, J. M., HITCHCOCK, P. B. & MASON, R. (1976). *J. Organomet. Chem.* **113**, C11–C12.  
 BROOK, A. G., DUFF, J. M. & REYNOLDS, W. F. (1976). *J. Organomet. Chem.* **121**, 293–306.  
 CROMER, D. T. (1965). *Acta Cryst.* **18**, 17–23.  
 CROMER, D. T. & WABER, J. T. (1965). *Acta Cryst.* **18**, 104–109.  
 IWASAKI, F., MITAMURA, S. & TSUCHIHASHI, G. I. (1975). *Bull. Chem. Soc. Jpn*, **48**, 944–948.  
 MANDEL, G. & DONOHUE, J. (1972). *Acta Cryst.* **B28**, 1313–1316.  
 STEWART, J. M. (1972). The XRAY system – version of June 1972. Tech. Rep. TR 72-192. 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.  
 VIDAL, J. P., GALIGNÉ, J. L. & FALGUEIRETTES, J. (1972). *Acta Cryst.* **B28**, 3130–3137.

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## Bis(triphenylmethyl) Ether

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**Abstract.** C<sub>38</sub>H<sub>30</sub>O, monoclinic, *P*2<sub>1</sub>/*c*, *a* = 14.791 (2), *b* = 10.598 (2), *c* = 17.521 (3) Å,  $\beta$  = 96.528 (12)°; *M<sub>r</sub>* = 502.62; *D<sub>c</sub>* = 1.223, *D<sub>m</sub>* = 1.220 g cm<sup>-3</sup>; *Z* = 4;  $\mu$ (Mo *K* $\alpha$ ) = 0.37 cm<sup>-1</sup>. The final residual from 3020 observed reflections was 0.041. The COC angle is 127.9 (1)°, and the C–O bond distances are 1.454 (2) and 1.465 (2) Å.

**Introduction.** The compound was prepared by reaction of chlorotriphenylmethane with mercury(II) oxide (Gomberg, 1913) and crystals were grown from toluene solution. The space group was assigned uniquely from the systematic absences: *h*0*l*, *l* = 2*n* + 1; 0*k*0, *k* = 2*n* + 1. A crystal in the shape of a thick plate of approximate dimensions 0.5 × 0.32 × 0.13 mm was used for data collection. Data were collected on a Philips PW 1100 four-circle diffractometer with graphite-monochromated Mo *K* $\alpha$  radiation. Unit-cell dimensions were

derived from least-squares fits to the reflecting positions of 25 reflections each measured 15 times during data collection. The intensities of 5279 reflections within the quadrant  $\pm h$ ,  $+k$ ,  $+l$ , with  $3 \leq \theta \leq 25^\circ$  were measured using the  $\omega$ – $2\theta$  scan technique with a scan speed of 0.05° s<sup>-1</sup> in  $\omega$  and a scan width of (0.9 + 0.1 tan  $\theta$ )° in  $\omega$ . Backgrounds were measured at both ends of each scan. Three reference reflections were measured every 6 h during data collection and showed only small random deviations about their mean intensities. Lorentz and polarization corrections were applied to the data, but no corrections for absorption were made.

The structure was solved with the fast, centrosymmetric direct-methods program in the *SHELX* system (Sheldrick, 1976) and refined by blocked-full-matrix least squares with complex neutral-atom scattering factors (Cromer & Mann, 1968) and a weighting scheme  $w = 1/\sigma^2(F)$ , with 3020 unique reflections

Table 1. Atom coordinates ( $\times 10^4$ ; for H  $\times 10^3$ )

	x	y	z		x	y	z
O	1898 (1)	3743 (1)	3942 (1)	C(233)	1639 (2)	7224 (2)	4892 (2)
C(1)	1565 (1)	2462 (2)	4011 (1)	C(234)	2214 (2)	7603 (2)	5515 (2)
C(2)	2794 (1)	4248 (2)	4233 (1)	C(235)	2995 (2)	6925 (2)	5728 (2)
C(111)	1281 (1)	2206 (2)	4818 (1)	C(236)	3195 (2)	5848 (2)	5330 (1)
C(112)	1132 (1)	3193 (2)	5311 (1)	H(112)	125 (2)	407 (2)	517 (1)
C(113)	837 (2)	2968 (2)	6021 (1)	H(113)	76 (2)	377 (2)	635 (2)
C(114)	675 (2)	1758 (2)	6254 (1)	H(114)	49 (2)	162 (2)	674 (2)
C(115)	776 (1)	770 (2)	5758 (1)	H(115)	64 (2)	-9 (2)	590 (1)
C(116)	1060 (1)	994 (2)	5043 (1)	H(116)	110 (2)	26 (2)	470 (1)
C(121)	2208 (1)	1482 (2)	3711 (1)	H(122)	206 (1)	219 (2)	262 (1)
C(122)	2360 (1)	1550 (2)	2939 (1)	H(123)	299 (1)	77 (2)	208 (1)
C(123)	2893 (2)	663 (2)	2618 (2)	H(124)	362 (1)	-99 (2)	286 (1)
C(124)	3276 (2)	-322 (3)	3055 (2)	H(125)	339 (1)	-110 (2)	414 (1)
C(125)	3139 (2)	-396 (2)	3819 (2)	H(126)	258 (1)	47 (2)	468 (1)
C(126)	2627 (1)	506 (2)	4146 (1)	H(132)	68 (1)	63 (2)	308 (1)
C(131)	644 (1)	2483 (2)	3488 (1)	H(133)	-74 (1)	67 (2)	238 (1)
C(132)	316 (1)	1423 (2)	3080 (1)	H(134)	-170 (2)	252 (2)	235 (1)
C(133)	-540 (1)	1434 (2)	2659 (1)	H(135)	-117 (2)	432 (2)	308 (1)
C(134)	-1083 (1)	2480 (2)	2642 (1)	H(136)	29 (1)	427 (2)	378 (1)
C(135)	-771 (1)	3539 (2)	3061 (1)	H(212)	282 (1)	340 (2)	570 (1)
C(136)	80 (1)	3536 (2)	3482 (1)	H(213)	374 (1)	196 (2)	640 (1)
C(211)	3425 (1)	3302 (2)	4691 (1)	H(214)	494 (1)	98 (2)	583 (1)
C(212)	3298 (1)	3001 (2)	5446 (1)	H(215)	518 (1)	146 (2)	457 (1)
C(213)	3845 (2)	2131 (2)	5865 (2)	H(216)	424 (1)	288 (2)	385 (1)
C(214)	4541 (2)	1549 (3)	5543 (2)	H(222)	216 (2)	437 (2)	272 (1)
C(215)	4691 (2)	1847 (2)	4803 (2)	H(223)	282 (2)	512 (2)	165 (1)
C(216)	4134 (1)	2698 (2)	4374 (1)	H(224)	430 (1)	610 (2)	186 (1)
C(221)	3219 (1)	4765 (2)	3533 (1)	H(225)	508 (2)	620 (2)	314 (1)
C(222)	2767 (2)	4731 (2)	2797 (1)	H(226)	438 (2)	540 (2)	417 (1)
C(223)	3174 (2)	5210 (2)	2181 (1)	H(232)	140 (2)	586 (2)	404 (1)
C(224)	4022 (2)	5738 (3)	2294 (2)	H(233)	108 (2)	768 (2)	474 (1)
C(225)	4466 (2)	5817 (3)	3023 (2)	H(234)	206 (2)	837 (2)	580 (1)
C(226)	4068 (2)	5354 (2)	3639 (2)	H(235)	343 (2)	719 (2)	614 (2)
C(231)	2600 (1)	5425 (2)	4712 (1)	H(236)	373 (2)	536 (2)	550 (1)
C(232)	1831 (1)	6150 (2)	4490 (1)				

having  $F_o \geq 6\sigma(F_o)$ . Anisotropic temperature factors were used for the O and C atoms. H atom positions were obtained from a difference synthesis and were refined with a common isotropic temperature factor. The refinement converged to  $R_G [= (\sum w\Delta^2/\sum wF_o^2)^{1/2}]$  of 0.046 and  $R [= \sum \Delta/\sum F_o]$  of 0.041 for 443 refined parameters. The final atom coordinates are listed in Table 1, and the geometry of the central  $C_3COCC_3$  fragment is listed in Table 2.\*

**Discussion.** The two independent C—O distances, 1.454 (2) and 1.465 (2) Å, and the COC angle, 127.9 (1)°, are all significantly greater than those in  $(CH_3)_2O$  [ $r(C—O)$  1.416 (3) Å;  $\angle(COC)$  111.5 (15)°] (Kimura & Kubo, 1959). The C(aryl)—C(quaternary) distances, mean 1.543 (6) Å, are comparable with those

\* Lists of structure factors, anisotropic thermal parameters and the geometrical parameters for the phenyl rings have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33142 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 2. Geometry of the COC bridge

(a) Bond distances (Å)			
C(1)—O	1.454 (2)	C(2)—O	1.465 (2)
C(1)—C(111)	1.544 (3)	C(2)—C(211)	1.533 (3)
C(1)—C(121)	1.540 (3)	C(2)—C(221)	1.541 (3)
C(1)—C(131)	1.552 (2)	C(2)—C(231)	1.548 (3)
(b) Bond angles (°)			
O—C(1)—C(111)	111.7 (1)	O—C(2)—C(211)	114.6 (1)
O—C(1)—C(121)	111.9 (1)	O—C(2)—C(221)	106.8 (1)
O—C(1)—C(131)	102.7 (1)	O—C(2)—C(231)	105.5 (1)
C(111)—C(1)—C(121)	115.9 (1)	C(211)—C(2)—C(221)	111.6 (2)
C(121)—C(1)—C(131)	110.0 (1)	C(221)—C(2)—C(231)	105.2 (1)
C(131)—C(1)—C(111)	103.4 (1)	C(231)—C(2)—C(211)	112.5 (1)

in  $CPh_4$ , 1.550 (3) Å (Robbins, Jeffrey, Chesick, Donohue, Cotton, Frenz & Murillo, 1975), and in  $HCPH_3$ , mean 1.524 (23) Å (Riche & Pascard-Billy, 1974).

There are no fewer than 15 non-bonded C...C distances between the two  $CPh_3$  groups, which are less

Table 3. *Intramolecular non-bonded distances between the two CPh<sub>3</sub> groups, which are less than the sum of the van der Waals radii (Å)*

C(1)···C(211)	3.006	C(121)···C(216)	3.221
C(1)···C(212)	3.428	C(122)···C(222)	3.438
C(2)···C(111)	3.356	C(126)···C(211)	3.291
C(2)···C(112)	3.451	C(126)···C(215)	3.445
C(2)···C(121)	3.162	C(126)···C(216)	3.213
C(111)···C(211)	3.408	C(111)···H(216)	2.894
C(111)···C(212)	3.174	C(112)···H(216)	2.519
C(112)···C(212)	3.191	C(222)···H(122)	2.891
C(112)···C(231)	3.454	H(122)···H(222)	2.320
C(121)···C(211)	3.034	H(136)···H(232)	2.370

than twice the van der Waals radius of aromatic C (Bondi, 1964) (Table 3). C(1) and C(2) participate in two and three, respectively, while the C atoms of rings *A*, *B* and *D* (Fig. 1) participate in six, seven and ten, respectively, of these presumably repulsive interactions; however, rings *E* and *F* are involved in only one short C···C distance each, and ring *C* in none at all. By contrast with the C···C distances, there are only one C···H and two H···H distances between CPh<sub>3</sub> groups shorter than the van der Waals sum (Bondi, 1964). The steric stress is thus distributed between interactions involving, in all, 13 C atoms, although the occurrence of so many short C···C distances involving atoms of rings *A*, *B* and *D* does not cause the C(aryl)–C(quaternary) distances or the C(aryl)–C(quaternary)–O angles associated with these rings to be any greater than those associated with rings *C*, *E* and *F* (Table 2).

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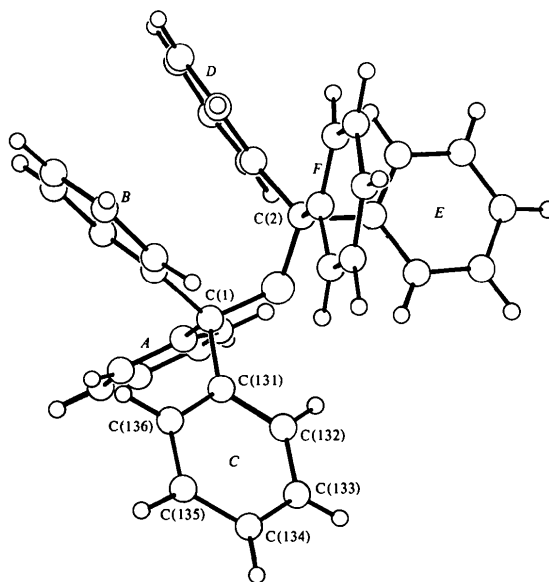


Fig. 1. Molecular structure with numbering scheme.

### References

- BONDI, A. (1964). *J. Phys. Chem.* **68**, 441–451.  
 CROMER, D. T. & MANN, J. B. (1968). *Acta Cryst.* **A24**, 321–324.  
 GOMBERG, M. (1913). *J. Am. Chem. Soc.* **35**, 200–210.  
 KIMURA, K. & KUBO, M. (1959). *J. Chem. Phys.* **30**, 151–158.  
 RICHE, C. & PASCARD-BILLY, C. (1974). *Acta Cryst.* **B30**, 1874–1876.  
 ROBBINS, A., JEFFREY, G. A., CHESICK, J. P., DONOHUE, J., COTTON, F. A., FRENZ, B. A. & MURILLO, C. A. (1975). *Acta Cryst.* **B31**, 2395–2399.  
 SHELDRIK, G. M. (1976). Personal communication.