[O(2)—C(3)—O(4)], together with the atomic numbering scheme. The bond distances and angles are listed in Table 2.

The configuration of the C=N bond was proved to be Z and the geometry of the nitrone chromophore [R—CH=N(O)R'] was found to be essentially the same as those of other aldonitrones (see Inouye, 1983).

The dihedral angle between the ester plane [O(2)—C(3)—O(4)] and the nitrone plane [C(5)—N(6)—O(7)] is $31.0 (3)°$, which is larger than that $(8.4°)$ of the N-benzyl derivative (Inouye, 1983).

The dihedral angle between the two phenyl rings is $109.2 (3)°$ and the conformation of the diphenylmethyl group is such that C(5) is eclipsed with H(4) and that C(9) and C(15) atoms are *gauche* to O(7). A similar orientation of phenyl rings was recently reported in phenyl α-[(α-phenylbenzyl)imino]benzyl ketone (Fonseca, Martínez-Carrera & García-Blanco, 1982).

All the intermolecular atomic contacts are slightly larger than usual van der Waals distances; the shortest are O(2) (x, y, z)—C(18) $(1—x, 1—y, 1—z)$ [$3.463 (4)$ Å] between non-hydrogen atoms, O(2) (x, y, z)—H(13)

$(1—x, 1—y, 1—z)$ [$2.86 (3)$ Å] involving hydrogen atoms, and H(6) (x, y, z)—H(2) $(x, y, z + 1)$ [$2.39 (5)$ Å] between hydrogen atoms.

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Acetyltriphenylmethane,* $C_{21}H_{18}O$

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Abstract. $M_r = 286.37$, monoclinic, $C2/c$, $a = 16.276 (4)$, $b = 7.067 (1)$, $c = 27.389 (7)$ Å, $\beta = 99.78 (1)°$, $V = 3104.6 (12)$ Å³, $Z = 8$, D_m(flotation) $= 1.209$, $D_x = 1.225$ g cm⁻³, Mo $K\alpha$, $\lambda = 0.71073$ Å, $\mu = 0.39$ cm⁻¹, $F(000) = 1216$, room temperature, final $R = 0.033$ for 1086 significant reflections. The acetyl and three phenyl groups are arranged tetrahedrally around the central carbon atom. Two distinct C(central)—C bond lengths are found, C—C(Ph) = $1.538 (2)$ Å and C—C(Ac) = $1.555 (3)$ Å, the lengthening of the latter bond being explicable in terms of the electronic structure of the molecule.

Introduction. Crystal structure studies of acetyltriphenylgermane (Harrison & Trotter, 1968) and -silane (Chieh & Trotter, 1969) (Ia) (X = Ge, Si) have revealed lengthenings of the X—C(Ac) bonds, which are explicable in terms of canonical resonance forms, (Ic), and which are in accord with the spectral and basicity studies (Brook, 1957; Brook, Quigley, Peddle, Schwartz & Warner, 1960). The present study shows a
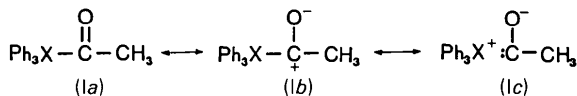
similar but less extreme lengthening in the carbon analogue, (Ia) (X = C).

Experimental. Colorless crystals, $0.2 \times 0.4 \times 0.2$ mm, CAD-4 diffractometer; graphite-monochromatized Mo $K\alpha$ radiation, $\theta \le 25°$, ω–2θ scan, ω-scan width $(0.70 + 0.35 \tan\theta)°$ extended 25% on each side for background measurement, horizontal aperture $(2.00 + \tan\theta)$ mm, vertical aperture 4 mm; intensity and orientation controls regularly, $< \pm 0.5\%$ deviation for three reference reflections throughout data collection; cell parameters from least-squares fit on $\sin^2\theta$ values for 20 centered reflections with $10 < \theta < 18°$; Lp corrections (no absorption); 2741 independent reflections, 1086 with $I \ge 3\sigma(I)$ where $\sigma^2(I) = S + 2B + [0.04(S - B)]^2$, S = the scan count and B = the time-averaged background [$\theta \le 20°$, 871 of 1457 (59.8%), $20 < \theta \le 25°$, 215 of 1284 (16.7%) observed reflections, $\theta \le 25°$, 39.6%]. *MULTAN*80 (Main, Fiske, Hull, Lessinger,

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* 1,1,1-Triphenylacetone, 1,1,1-triphenyl-2-propanone.

Germain, Declercq & Woolfson, 1980); full-matrix least-squares refinement, anisotropic, H atoms from a difference synthesis, isotropic; $\sum w(|F_o| - |F_c|)^2$ minimized; final $R = 0.033$, $R_w = 0.033$ for 1086 reflections, 271 variables, $w = 1/\sigma^2(F)$, $R = 0.145$, $R_w = 0.033$ for all data; reflections to variables ratio ~4; $(\Delta/\sigma)_{mean} = 0.01$, $(\Delta/\sigma)_{max} = 0.04$; $S = 1.44$; random fluctuations of $\pm 0.10\,\mathrm{e\,\AA^{-3}}$ on final difference map; scattering factors from Cromer & Mann (1968) and Stewart, Davidson & Simpson (1965); local adaptations of standard computer programs, ORFLS (Busing, Martin & Levy, 1962), ORFFE (Busing, Martin & Levy, 1964), and ORTEPII (Johnson, 1976).

Discussion. Final atomic parameters are in Table 1.*

The molecular structure (Fig. 1) is quite similar to that of the Ge and Si analogues (Harrison & Trotter, 1968; Chieh & Trotter, 1969), with a central carbon atom, C(1), bonded tetrahedrally to the acetyl and three phenyl groups. There are small deviations from exact tetrahedral geometry, with angles at C(1) ranging from 103·1 (2) to 113·7 (2)° (Table 2), and angles between C(Ac)—C—C(Ph) planes of 121·8 (2), 120·4 (2), and 117·7 (3)°. The phenyl rings are approximately planar – maximum deviation from mean planes 0·025 (2) Å – and are oriented in a propeller fashion. The angles between the ring planes and the C(Ac)—C—C(Ph) planes are 56, 3, and 61° ($\sigma = 0.2°$) for the C(4), C(10), and C(16) rings, respectively; this arrangement is less symmetrical than those in the Ge and Si compounds (angles 62, 41, 58 and 58, 55, 55°, respectively). The acetyl group is approximately planar [maximum deviation 0·026 (3) Å], with its plane almost parallel to the C(2)—C(1)—C(16) plane [angle 3·1 (2)°, see Fig. 1].

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* Lists of structure factors, anisotropic thermal parameters, bond distances and angles involving hydrogen atoms, torsion angles, least-squares planes and the packing diagram have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38851 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
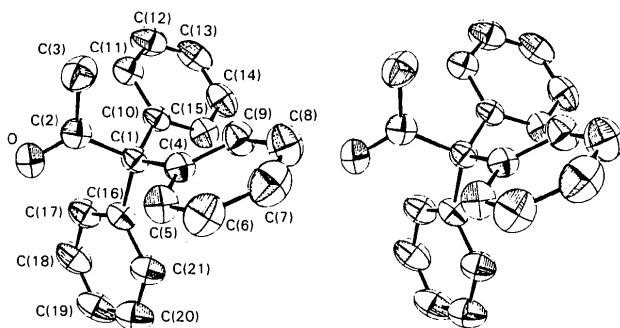

Fig. 1. Stereodiagram of acetyltriphenylmethane (thermal ellipsoids are 50% probability).

Table 1. *Final positional (fractional* $\times 10^5$, H $\times 10^4$) *and isotropic thermal* ($\mathrm{\AA}^2 \times 10^3$) *parameters with estimated standard deviations in parentheses*

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

	x	y	z	U_{eq}/U_{iso}
O	3702 (12)	37129 (29)	69967 (7)	63
C(1)	−6517 (15)	22931 (34)	63573 (8)	38
C(2)	−3388 (18)	37472 (38)	67737 (9)	46
C(3)	−9194 (25)	53030 (49)	68662 (15)	60
C(4)	−9246 (15)	35496 (35)	59020 (9)	41
C(5)	−3580 (20)	48502 (42)	57709 (11)	53
C(6)	−5710 (22)	60701 (44)	53779 (11)	61
C(7)	−13562 (23)	60331 (48)	51060 (12)	67
C(8)	−19278 (23)	47905 (49)	52296 (12)	64
C(9)	−17177 (17)	35615 (41)	56248 (10)	51
C(10)	−13607 (14)	10762 (36)	64984 (10)	40
C(11)	−16217 (17)	11655 (44)	69525 (11)	50
C(12)	−22552 (20)	194 (52)	70613 (15)	67
C(13)	−26326 (20)	−12639 (51)	67216 (15)	66
C(14)	−23645 (18)	−14287 (42)	62746 (14)	60
C(15)	−17271 (17)	−2953 (39)	61676 (11)	48
C(16)	643 (14)	9375 (33)	62947 (10)	42
C(17)	4007 (18)	−1959 (42)	66926 (13)	55
C(18)	10297 (19)	−14765 (47)	66564 (15)	68
C(19)	13338 (20)	−16357 (49)	62231 (16)	74
C(20)	10071 (21)	−5495 (48)	58245 (16)	67
C(21)	3736 (19)	7386 (41)	58587 (13)	54
H1(C3)	−743 (21)	6448 (54)	6719 (12)	118 (14)
H2(C3)	−1509 (19)	5115 (42)	6715 (11)	85 (11)
H3(C3)	−879 (18)	5552 (42)	7239 (13)	92 (10)
H(C5)	194 (17)	4852 (38)	5948 (9)	61 (9)
H(C6)	−131 (18)	6943 (43)	5300 (10)	86 (10)
H(C7)	−1497 (15)	6921 (39)	4821 (10)	70 (9)
H(C8)	−2486 (18)	4755 (39)	5071 (11)	75 (10)
H(C9)	−2144 (17)	2722 (39)	5716 (9)	67 (9)
H(C11)	−1336 (15)	2019 (35)	7203 (9)	55 (8)
H(C12)	−2402 (18)	110 (45)	7389 (12)	83 (11)
H(C13)	−3109 (20)	−1988 (42)	6794 (10)	84 (10)
H(C14)	−2617 (14)	−2386 (36)	6021 (8)	49 (8)
H(C15)	−1546 (13)	−438 (31)	5851 (9)	38 (7)
H(C17)	179 (15)	−61 (39)	7005 (10)	64 (9)
H(C18)	1248 (17)	−2244 (44)	6940 (10)	81 (11)
H(C19)	1774 (18)	−2526 (45)	6188 (10)	83 (10)
H(C20)	1132 (17)	−673 (43)	5493 (12)	82 (11)
H(C21)	106 (17)	1406 (38)	5576 (10)	66 (10)

Table 2. *Bond lengths* (Å) *and angles* (°) *with estimated standard deviations in parentheses*

O—C(2)	1·211 (3)	C(10)—C(11)	1·382 (4)
C(1)—C(2)	1·555 (3)	C(10)—C(15)	1·390 (4)
C(1)—C(4)	1·534 (3)	C(11)—C(12)	1·383 (4)
C(1)—C(10)	1·540 (3)	C(12)—C(13)	1·368 (5)
C(1)—C(16)	1·541 (3)	C(13)—C(14)	1·373 (4)
C(2)—C(3)	1·499 (4)	C(14)—C(15)	1·381 (4)
C(4)—C(5)	1·392 (4)	C(16)—C(17)	1·388 (4)
C(4)—C(9)	1·382 (3)	C(16)—C(21)	1·380 (4)
C(5)—C(6)	1·377 (4)	C(17)—C(18)	1·383 (4)
C(6)—C(7)	1·366 (4)	C(18)—C(19)	1·366 (5)
C(7)—C(8)	1·363 (4)	C(19)—C(20)	1·366 (5)
C(8)—C(9)	1·385 (4)	C(20)—C(21)	1·391 (4)
C(2)—C(1)—C(4)	103·1 (2)	C(1)—C(10)—C(11)	123·9 (3)
C(2)—C(1)—C(10)	110·5 (2)	C(1)—C(10)—C(15)	118·9 (2)
C(2)—C(1)—C(16)	109·4 (2)	C(11)—C(10)—C(15)	117·1 (3)
C(4)—C(1)—C(10)	113·7 (2)	C(10)—C(11)—C(12)	121·4 (3)
C(4)—C(1)—C(16)	112·9 (2)	C(11)—C(12)—C(13)	120·5 (4)
C(10)—C(1)—C(16)	107·1 (2)	C(12)—C(13)—C(14)	119·3 (3)
O—C(2)—C(1)	121·5 (2)	C(13)—C(14)—C(15)	120·3 (3)
O—C(2)·C(3)	120·2 (3)	C(10)·C(15)—C(14)	121·4 (3)
C(1)—C(2)—C(3)	118·1 (2)	C(1)—C(16)—C(17)	118·5 (2)
C(1)—C(4)—C(5)	118·6 (2)	C(1)—C(16)—C(21)	123·6 (2)
C(1)·C(4)—C(9)	124·4 (2)	C(17)—C(16)—C(21)	117·9 (3)
C(5)—C(4)·C(9)	116·9 (3)	C(16)·C(17)—C(18)	121·3 (3)
C(4)—C(5)—C(6)	121·7 (3)	C(17)—C(18)—C(19)	119·9 (4)
C(5)—C(6)—C(7)	120·2 (3)	C(18)—C(19)—C(20)	119·9 (3)
C(6)·C(7)—C(8)	119·5 (3)	C(19)—C(20)—C(21)	120·4 (4)
C(7)—C(8)·C(9)	120·7 (3)	C(16)—C(21)—C(20)	120·6 (3)
C(4)—C(9)—C(8)	121·1 (3)		

Table 3. *Comparison of the bond lengthenings for C, Si and Ge analogues*

Bond	Length (Å)	X–C(Ph$_{ave}$) Å	Difference	Reference
C—C(Ac)	1·555 (3)			
C—C(Ph₁)	1·534 (3)			
C—C(Ph₂)	1·540 (3)	X = C, 1·538 (2)	0·017 Å	(1)
C—C(Ph₃)	1·541 (3)			
Si—C(Ac)	1·926 (14)			
Si—C(Ph₁)	1·860 (14)			
Si—C(Ph₂)	1·864 (14)	X = Si, 1·864 (8)	0·062 Å	(2)
Si—C(Ph₃)	1·867 (14)			
Ge—C(Ac)	2·011 (15)			
Ge—C(Ph₁)	1·940 (14)			
Ge—C(Ph₂)	1·945 (14)	X = Ge, 1·945 (8)	0·066 Å	(3)
Ge—C(Ph₃)	1·950 (14)			

References: (1) Present work; (2) Chieh & Trotter (1969); (3) Harrison & Trotter (1968).

The C(1)—C(Ph) bond distances are 1·534 (3), 1·540 (3), 1·541 (3) Å (Table 2); the mean length of 1·538 (2) Å is somewhat longer than the value of 1·51 Å which might be expected for a C(sp^3)—C(sp^2) single bond, but is quite close to the 1·53 (1) Å quoted as a mean for C—C₆H₅ bonds (*Molecular Structures and Dimensions*, 1972). The · C(1)—C(Ac) bond, 1·555 (3) Å, is 0·017 Å (5σ) longer than the mean C(1)—C(Ph) distance; this lengthening is similar to, but much less prominent, than the lengthenings of about 0·06 Å in the Ge and Si compounds (Table 3). The canonical form (Ic) therefore makes a smaller contribution to the resonance hybrid of the carbon compound, relative to the Ge and Si analogues. This conclusion is in accord with spectroscopic and basicity data (Brook, 1957; Allred & Rochow, 1958; Brook, Quigley, Peddle, Schwartz & Warner, 1960; Yates & Agolini, 1966).

Other molecular dimensions are normal. In the acetyl group C=O is 1·211 (3) and C—CH₃, 1·499 (4) Å; the

C—C distances in the phenyl rings are in the range 1·363–1·392 (4) Å, the shorter distances probably being subject to thermal-libration errors.

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Structure of 5-Benzoyl-4-(p-chlorophenyl)-2,2,5-triphenyl-Δ³-1,3-oxazoline,C₃₄H₂₄ClNO₂

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Abstract. $M_r = 514·02$, orthorhombic, *Pbca*, $a = 16·354$ (7), $b = 17·464$ (9), $c = 18·599$ (9) Å, $V = 5312$ (4) Å³, $Z = 8$, $D_x = 1·286$ Mg m⁻³, μ(Mo $K\alpha$) = 1·721 mm⁻¹, $\lambda = 0·71069$ Å, $F(000) = 2144$, $T = 292$ K, $R = 0·054$ for 1171 observed reflexions. Bond lengths and angles are normal. The structure analysis confirms that the reaction mechanism leading to the title photoproduct involves a 1,2-acyl migration.

Introduction. The photochemical reactions of enol esters are dominated by 1,3-acyl migration (Bellus, 1971; Muzart & Pete, 1978). Up to the recent work of Armesto, Ortiz, Perez-Ossorio & Horspool (1983) no example of a 1,2-acyl migration has been reported for such systems although 1,2-acyl migrations do occur in the related oxa-di-π-methane systems (Hixson, Mariano & Zimmerman, 1973). The irradiation of 4-benzoyloxy-