Structures of Vicinal Polyketones

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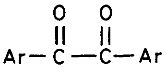
The crystal structures of mesitil, dimesityl triketone, and dimesityl tetraketone have been determined by X-ray diffraction methods and refined by least squares techniques to residuals of 0.087, 0.070, 0.053, respectively. Crystals of mesitil are monoclinic, $P2_1/n$, a = 17.666(8), b = 6.232(3), c = 17.514(8) Å, β = 117.58(2)°, Z = 4. Crystals of dimesityl triketone are monoclinic, $C2/c$, a = 29.625(15), b = 9.329(5), c = 15.182(8) Å, β = 121.07(2)°, Z = 8. Crystals of dimesityl tetraketone are monoclinic, $C2/c$, a = 14.295(7), b = 8.411(4), c = 16.190(8) Å, β = 105.20(2)°, Z = 4. The two carbonyl groups of mesitil assume an *s-trans* conformation with the aromatic rings approximately perpendicular to the plane defined by the carbonyl groups. In contrast, the tri- and tetra-ketone had torsion angles >100° and of identical sign along the chain of carbonyl groups and torsion angles of 25—40° between aromatic rings and adjacent groups. The geometrical parameters of a series of open-chain di-, tri-, and tetra-ketones are compared.

The structures of vicinal polycarbonyl compounds have been of interest for many years.[1] Bond lengths, bond angles, and torsion angles in such molecules can deviate from ' normal ' values in order to minimize (a) the repulsive interactions resulting from juxtaposition of dipolar carbonyl groups and (b) the steric interactions of the chain of carbonyl groups with the end groups present.

Crystallographic investigations of benzil [2a] (1) and recently [2b] of 1,3-diphenylpropane-1,2,3-trione (diphenyl triketone) (2) and 1,4-diphenylbutane-1,2,3,4-tetrone (diphenyl tetraketone) (3) provided an interesting comparison in a series of polyketones; the unexpected observation of a nearly eclipsed relationship between the central carbonyl groups (torsion angle 24.2°) of (3) is particularly noteworthy. We now report crystal structures of mesitil (4), dimesityl triketone (5), and dimesityl tetraketone (6). In contrast to the diphenyl series (1)—(3) where benzene rings are approximately coplanar with adjacent carbonyl groups, the *ortho*-methyl groups in the mesityl series prevent such coplanarity. It appeared of interest to determine the effect of this change on the structures of the polyketones. Certain generalizations on structures of vicinal polyketones emerge from these new results taken with results of earlier investigations.

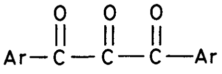
Preparation of Compounds.—Compounds (4)—(6) were prepared by literature procedures.[1] Good crystals of (4) were obtained by crystallization from anhydrous ethanol and of (5) and (6) by crystallization from ligroin (b.p. 100—120 °C).

Crystal Structure Analysis.—Crystallographic data and details of intensity measurement and structure refinement are given in Table 1. The intensities were collected on a Philips PW 1100 four-circle computer-controlled diffractometer with graphite-monochromated Mo-K_α radiation (λ 0.71069 Å) or Cu-K_α radiation (λ 1.5418 Å). The crystal structures were solved by MULTAN 77 [3] and refined by full-matrix least squares [4] with anisotropic thermal parameters for C and O atoms, isotropic for H. Scattering factors for C and O were taken from Cromer and Mann [5] and for H from Stewart *et al.*[6] Final positional parameters for (4)—(6) are given in Tables 2—4, respectively. In the stereoviews (Figures 1, 3, and 5), vibration ellipsoids are drawn at the 50% probability level.[7] The list of observed and calculated structure factors is contained in Supplementary Publication No. SUP 23449 (30 pp.).†



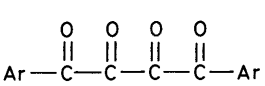
$$\mathrm{Ar{-}\overset{\displaystyle O}{\overset{\|}{C}}{-}\overset{\displaystyle O}{\overset{\|}{C}}{-}Ar}$$

(1) Ar = C_6H_5
(4) Ar = 2,4,6-$(CH_3)_3C_6H_2$



$$\mathrm{Ar{-}\overset{\displaystyle O}{\overset{\|}{C}}{-}\overset{\displaystyle O}{\overset{\|}{C}}{-}\overset{\displaystyle O}{\overset{\|}{C}}{-}Ar}$$

(2) Ar = C_6H_5
(5) Ar = 2,4,6-$(CH_3)_3C_6H_2$
(7) Ar = 4-BrC_6H_4



$$\mathrm{Ar{-}\overset{\displaystyle O}{\overset{\|}{C}}{-}\overset{\displaystyle O}{\overset{\|}{C}}{-}\overset{\displaystyle O}{\overset{\|}{C}}{-}\overset{\displaystyle O}{\overset{\|}{C}}{-}Ar}$$

(3) Ar = C_6H_5
(6) Ar = 2,4,6-$(CH_3)_3C_6H_2$

Structural Commentary.—*Mesitil* (4). The unit cell contains two crystallographically independent molecules which occupy the space group special positions (centre of inversion) at (000) and $(\frac{1}{2}00)$. Bond lengths and angles involving C and O atoms are given in Figures 2a and b; the C–H distances (not shown) lie in the range 0.76—1.07 Å. The e.s.d.s of bond distances are typically 0.007—0.01 Å, of bond angles 0.4—0.6°.

Dimesityl triketone (5). A stereoview of the molecule is shown in Figure 3. Bond lengths and angles involving C and O atoms are given in Figure 4; the C–H bond distances (not shown) lie in the range 0.88—1.06 Å. The e.s.d.s of bond distances are typically 0.005—0.009 Å, of bond angles 0.4—0.6°.

Dimesityl tetraketone (6). The molecule has crystallographic two-fold symmetry. A stereoview is shown in Figure 5, bond lengths and angles involving C and O atoms in Figure 6; the C–H bond distances (not shown) lie in the range 0.85—1.11 Å. The e.s.d.s of bond distances are typically 0.002—0.003 Å, of bond angles 0.1—0.2°.

Discussion

Conformations.—The contrast between absorption spectra (in solution) of benzil (1) (broad maximum at 370 nm) and of mesitil (4) (maximum at 493 nm with fine structure at shorter wavelengths) has been attributed [8] to differences in the ground-state conformations of these two diketones. Benzil, both in the crystal [2a] and in solution, can be regarded as composed of two approximately planar benzoyl groups joined together with a torsion angle of 108°. Mesitil, on the other hand, has been assumed to possess an *s-trans*-dicarbonyl conformation. The results obtained with the crystal (Figure 1) indeed show tor-

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† For details of Supplementary Publication, see Notice to Authors No. 7 in *J. Chem. Soc., Perkin Trans. 2*, 1981, Index Issue.

Table 1. Crystallographic and experimental details of (4)—(6)

	(4)	(5)	(6)
Formula	$C_{20}H_{22}O_2$	$C_{21}H_{22}O_3$	$C_{22}H_{22}O_4$
Mol. wt.	294.38	322.39	350.40
a (Å)	17.666(8)	29.625(15)	14.295(7)
b (Å)	6.232(3)	9.329(5)	8.411(4)
c (Å)	17.514(8)	15.182(8)	16.190(8)
β (°)	117.58(2)	121.07(2)	105.20(2)
U (Å^3)	1 709.08	3 593.92	1 878.51
Z	4	8	4
Space group	$P2_1/n$	$C2/c$	$C2/c$
D_x (g cm^{-3})	1.145	1.192	1.239
λ (Å)	0.710 69	0.710 69	1.5418
Scan mode	ω/θ	ω/θ	ω/θ
Δω (°)	1.2	1.4	1.2
Scan time (s)	30.0	28.0	24.0
Background time (s) [a]	20.0	28.0	20.0
$\theta_{max.}$ (°)	24.0	23.0	62.0
Reflections measured	2 547	1 969	1 503
Significant [$F_o > 1.5\sigma(F_o)$]	1 478	1 465 [b]	1 379 [c]
Weighting coefficients (k;g) [d]	1.829; 0.001	1.457; 0.001	2.236; 0.002
R_w	0.085	0.064	0.065
R	0.087	0.070	0.053

[a] Total background counting time. [b] $F_o > 2.0\,\sigma$. [c] Four reflections were omitted due to extinction errors. [d] $w = k/[\sigma^2(F_o) + g^*F_o^2]$.

Table 2. Positional parameters of (4), for non-hydrogen atoms (× 10^4) and for hydrogen atoms (× 10^3) with estimated standard deviations in parentheses

(A)

	x	*y*	*z*		*x*	*y*	*z*
O(1)	59(3)	1 645(9)	784(3)	H(4)	304(3)	51(8)	83(3)
C(1)	318(3)	417(9)	441(3)	H(6)	247(3)	−420(8)	209(3)
C(2)	1 220(3)	−387(9)	836(3)	H(81)	122(4)	350(11)	21(4)
C(3)	1 813(3)	632(9)	642(3)	H(82)	127(4)	221(9)	−43(4)
C(4)	2 621(3)	−239(11)	965(3)	H(83)	206(5)	338(12)	18(5)
C(5)	2 861(3)	−2 051(11)	1 481(3)	H(91)	401(4)	−268(13)	141(5)
C(6)	2 270(4)	−2 968(10)	1 689(4)	H(92)	365(4)	−456(11)	172(4)
C(7)	1 446(4)	−2 186(10)	1 371(3)	H(93)	406(6)	−258(15)	234(6)
C(8)	1 595(4)	2 631(10)	95(4)	H(101)	103(5)	−468(14)	186(5)
C(9)	3 747(4)	−3 027(12)	1 805(4)	H(102)	39(9)	−212(24)	170(9)
C(10)	819(4)	−3 208(12)	1 625(4)	H(103)	49(4)	−378(12)	120(5)

(B)

	x	*y*	*z*		*x*	*y*	*z*
O(1)	4 168(3)	−1 421(9)	9 961(3)	H(4)	420(3)	−54(8)	696(3)
C(1)	4 544(3)	−338(9)	9 681(3)	H(6)	291(3)	433(8)	752(3)
C(2)	4 168(3)	446(9)	8 777(3)	H(81)	478(4)	−345(11)	793(4)
C(3)	4 349(3)	−568(10)	8 181(3)	H(82)	494(5)	−308(13)	888(5)
C(4)	4 020(3)	250(11)	7 356(3)	H(83)	50(5)	−267(11)	368(5)
C(5)	3 511(4)	2 035(11)	7 109(4)	H(91)	319(5)	438(13)	629(5)
C(6)	3 306(4)	3 013(10)	7 699(4)	H(92)	257(6)	284(14)	588(5)
C(7)	3 623(3)	2 244(10)	8 538(4)	H(93)	352(6)	270(14)	596(5)
C(8)	4 901(4)	−2 548(11)	8 411(4)	H(101)	392(3)	387(9)	961(3)
C(9)	3 171(4)	2 955(13)	6 205(4)	H(102)	303(9)	279(25)	924(9)
C(10)	3 383(5)	3 290(13)	9 161(5)	H(103)	315(6)	460(19)	901(6)

sion angles * of 180° between the carbonyls as well as torsion angles * of 86.9 and 79.3° between each carbonyl group and the plane defined by the adjacent aromatic ring. Thus, in the absence of a stabilizing interaction between carbonyl and adjacent aromatic ring, mesitil assumes the *s-trans*-conformation characteristic of simple 1,2-diketones such as biacetyl. The overall effect is to maximize the distances (3.35, 3.38 Å) between the two electronegative oxygen atoms and to allow orbital overlap of the dione π system. Further, the planes of the two mesityl groups are separated by *ca.* 1.6 Å and displaced between C(2) and C(2)* (see Figure 2) by *ca.* 3.9 Å so that all potential steric interactions are minimized.

An analogous planar, all-*trans* geometry in vicinal triketones would result in a very short distance (*ca.* 2.5 Å) between the first (O_2) and third (O_2') oxygen atoms of the trione chain [conformations (A)] while other planar conformations (B) and (C) would lead to severe interactions involving end group(s). Thus the conformation of dimesityl triketone (5) is of necessity very different from that of (4). The torsion angles pro-

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* These angles obtained for the two independent molecules of the asymmetric unit.

Table 3. Positional parameters of (5), for non-hydrogen atoms (× 10^4) and for hydrogen atoms (× 10^3), with estimated standard deviations in parentheses

	x	*y*	*z*
O(1)	3 508(1)	502(4)	1 825(3)
O(2)	4 230(1)	3 422(4)	2 057(2)
O(3)	3 519(1)	2 965(5)	3 107(3)
C(1)	3 561(2)	1 598(6)	1 458(4)
C(2)	3 956(2)	2 674(6)	2 242(3)
C(3)	3 959(2)	2 806(5)	3 248(4)
C(4)	4 448(2)	2 876(5)	4 259(3)
C(5)	4 893(2)	2 077(6)	4 463(4)
C(6)	5 338(2)	2 156(6)	5 432(4)
C(7)	5 365(2)	2 980(6)	6 197(4)
C(8)	4 929(2)	3 784(6)	5 986(4)
C(9)	4 465(2)	3 747(5)	5 039(4)
C(10)	4 910(2)	1 079(6)	3 686(4)
C(11)	5 866(2)	3 037(7)	7 252(4)
C(12)	4 007(2)	4 653(6)	4 873(4)
C(13)	3 330(2)	1 857(6)	343(3)
C(14)	3 064(2)	3 134(6)	−101(4)
C(15)	2 848(2)	3 330(6)	−1 149(4)
C(16)	2 911(2)	2 329(6)	−1 750(4)
C(17)	3 178(2)	1 088(6)	−1 286(4)
C(18)	3 381(2)	798(5)	−252(4)
C(19)	2 979(2)	4 294(6)	500(4)
C(20)	2 685(2)	2 587(7)	−2 885(4)
C(21)	3 654(2)	−610(6)	187(4)
H(6)	564(2)	155(4)	552(3)
H(8)	495(1)	444(4)	656(3)
H(101)	455(1)	62(4)	320(3)
H(102)	517(2)	33(5)	402(3)
H(103)	502(2)	167(4)	329(3)
H(111)	604(2)	226(6)	729(4)
H(112)	573(2)	300(6)	777(4)
H(113)	595(2)	393(7)	749(4)
H(121)	386(2)	520(5)	426(4)
H(122)	415(2)	532(5)	543(3)
H(123)	370(2)	400(6)	483(4)
H(15)	268(2)	423(4)	−141(3)
H(17)	322(1)	33(4)	−167(3)
H(191)	296(1)	390(4)	106(2)
H(192)	265(2)	489(5)	2(3)
H(193)	326(1)	489(4)	80(3)
H(201)	286(3)	196(7)	−314(5)
H(202)	276(2)	360(5)	−297(3)
H(203)	232(2)	230(5)	−324(3)
H(211)	401(1)	−47(4)	90(3)
H(212)	373(2)	−105(5)	−34(4)
H(213)	340(2)	−126(6)	19(4)

Table 4. Positional parameters of (6), for non-hydrogen atoms (× 10^4) and for hydrogen atoms (× 10^3), with estimated standard deviations in parentheses

	x	*y*	*z*
O(1)	−715(1)	2 569(2)	3 157(1)
O(2)	1 192(1)	163(2)	3 318(1)
C(1)	−25(1)	2 039(2)	2 964(1)
C(2)	846(1)	1 283(2)	3 613(1)
C(3)	1 105(1)	1 789(2)	4 508(1)
C(4)	1 149(1)	3 422(2)	4 708(1)
C(5)	1 347(1)	3 855(2)	5 567(1)
C(6)	1 487(1)	2 753(2)	6 215(1)
C(7)	1 470(1)	1 147(3)	6 008(1)
C(8)	1 298(1)	636(2)	5 163(1)
C(9)	1 049(2)	4 701(2)	4 041(1)
C(10)	1 668(2)	3 258(4)	7 137(1)
C(11)	1 296(2)	−1 121(2)	4 987(2)
H(5)	140(2)	488(3)	573(2)
H(7)	157(2)	35(3)	641(2)
H(91)	40(2)	512(3)	382(2)
H(92)	125(2)	436(3)	355(2)
H(93)	152(2)	558(5)	431(2)
H(101)	202(3)	422(6)	723(3)
H(102)	229(4)	286(8)	753(3)
H(103)	116(2)	326(4)	732(2)
H(111)	181(2)	−142(3)	473(2)
H(112)	63(2)	−157(3)	453(2)
H(113)	132(2)	−170(4)	548(2)

ceeding along the carbonyl chain are 145.4 and 127.1° (see Figure 3), values close to those observed for (2) (107.4 and 123.2°) and for bis-*p*-bromophenyl triketone (7), (130.9, 130.9°) despite the difference in end groups. The mesityl groups in (5) adopt torsion angles of 27 and 40° with the adjacent carbonyl groups in contrast to the much larger values observed with (4). This appears to be due to relief of interactions between the *ortho*-methyl groups and the more remote oxygen atoms.

The conformation of dimesityl tetraketone (6) is a direct extension of that of (5) without the unexpected features observed in the structure of (3). Torsion angles along the carbonyl chain were 144.1, 128.5, and 144.1° (see Figure 5) and torsion angles between mesityl groups and neighbouring carbonyl groups were 38.5°. From examination of space-filling molecular models, the conformation observed for (6) appears to minimize repulsive interactions of oxygen atoms with one another and with the end groups. A small torsion angle between the central carbonyl groups would lead to severe interactions of oxygen atoms with *ortho*-methyl groups. Examination of models does not provide a rationalization for the fact that (3) assumes a conformation in the crystal in which the torsion angle between the central carbonyl groups is small (27.2°) and the distance between oxygen atoms is 2.77 Å (the van der Waals radius of oxygen is 1.4 Å) instead of a conformation similar to that of (6). It seems likely that the rotational barrier in polycarbonyl chains is small * so that packing forces in the crystal may become dominant. This question might be resolved by crystallographic studies of additional tetraketones provided that such compounds assumed different crystal packings.

Structural Parameters.—The geometry of a polyketone skeleton is described by the bond lengths between adjacent carbonyl carbon atoms (d_1, d_1', d_2'), CO bond lengths (l_1, l_1', l_2, l_2'), bond lengths (s_1, s_1') between terminal CO groups and the end groups, by bond angles (α,β) and oxygen–oxygen

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* An attempt [9] to detect helical conformations in 4,4-dimethyl-1,4-diphenylbutane-1,2,3-trione using low temperature ^{1}H n.m.r. spectroscopy (down to −140 °C) was unsuccessful. It was concluded that the rotational barrier between the dimethylbenzyl group and the adjacent carbonyl group was larger than the rotational barrier between vicinal carbonyl groups.

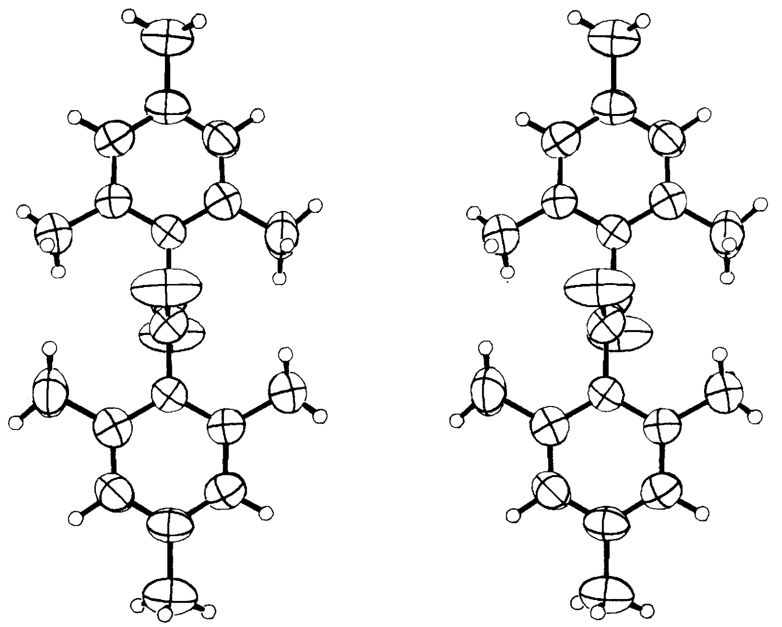


Figure 1. Stereoscopic view of (4) [7]

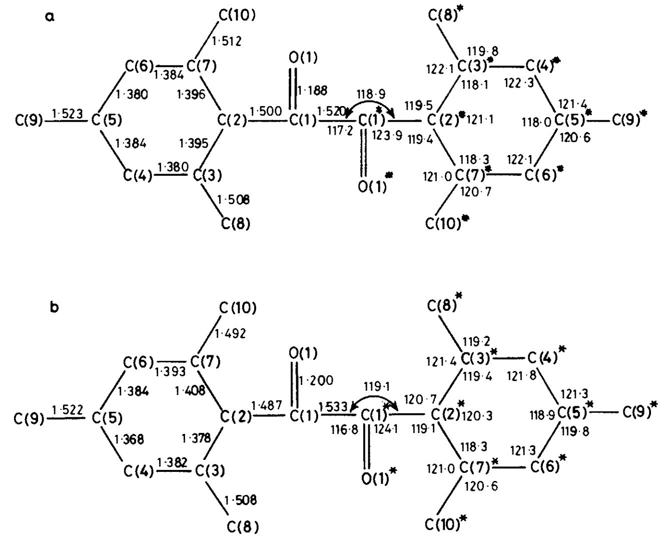


Figure 2. Bond lengths and angles in (4): 2a, in molecule (A); 2b, in molecule (B)

non-bonded distances. Table 4 summarizes these values for the compounds reported in this study together with results obtained in investigations of other vicinal polyketones.

A *Bond distances between carbonyl carbon atoms* ($d^1{}_1,d^2{}_2$) These bond distances lie in the range 1.520—1.565 Å for the eight diketones, three triketones, and two tetraketones in Table 5. The values are slightly larger than those in formally sp^2–sp^2 single bonds, such as in butadiene, possibly as a means of decreasing the unfavourable interaction between the positive ends of vicinal CO dipoles. Similar values have been observed with cyclic polyketones. The observation that the central CO–CO bond in (3) is longer (1.552 Å) than the outer ones (1.512, 1.522 Å) may reflect the nearly eclipsed conformation of (3). The opposite situation obtained in (6) (central CO–CO 1.523 Å, outer CO–CO 1.541 Å).

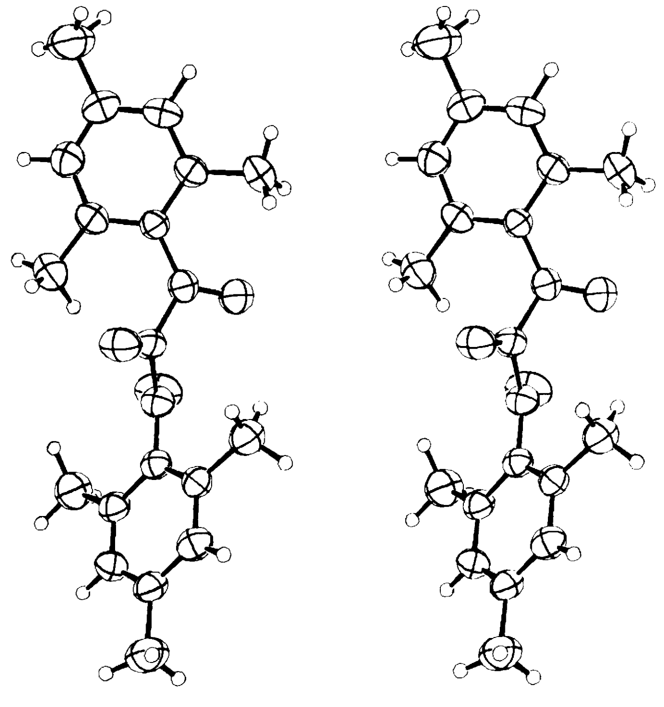


Figure 3. Stereoscopic view of (5) [7]

B *Distances between end and carbonyl groups* ($s_1,s_{1'}$). With the exception of (8a), where the end group is diazomethyl, the values of s_1 and $s_{1'}$ lie in the range 1.463—1.500 Å, independent of the length of the polycarbonyl chain. This is true even with mesityl compounds where conjugation of the aromatic ring with the adjacent carbonyl group is inhibited by steric hindrance.

C *Carbonyl–oxygen bond lengths* ($l_1,l_{1'},l_2,l_{2'}$). Values for C–O bond lengths were 1.188—1.225 Å; the slight shorten-

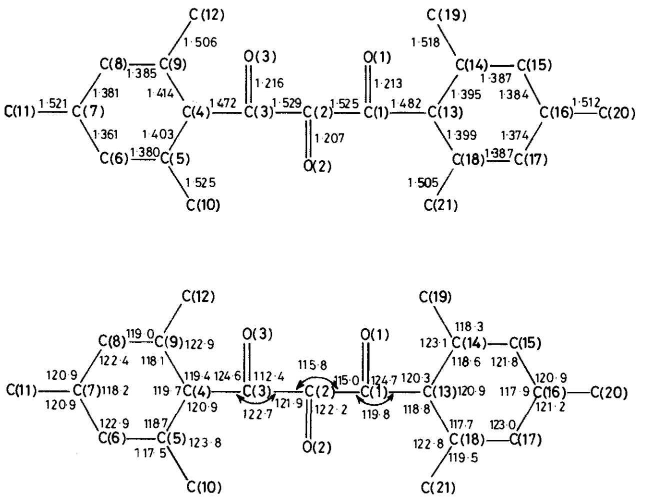


Figure 4. Bond lengths and angles in (5)

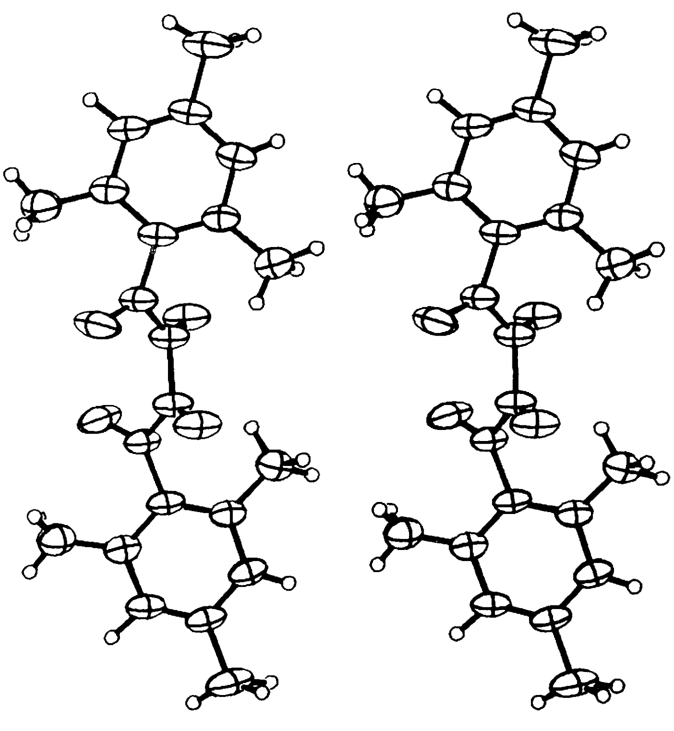


Figure 5. Stereoscopic view of (6) [7]

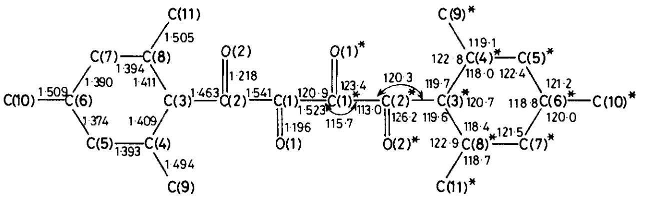
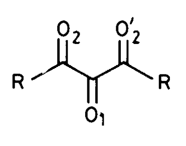
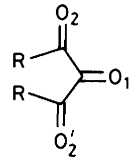


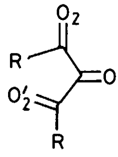
Figure 6. Bond lengths and angles in (6)



(A)



(B)



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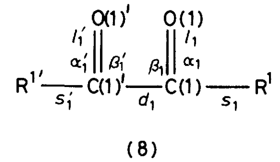
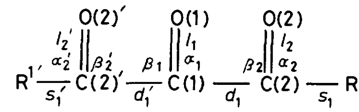


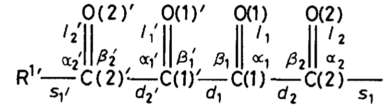
(8)

a; $R^1 = R^{1'} = CHN_2$
b; $R^1 = C_6H_5$, R^1 =2-(3-cyano-*N*-methoxyaziridinyl)
c; $R^1 = R^{1'}$= cyclopropyl
d; $R^1 = C_6H_5$, $R^{1'}$= 2-pyridyl
e; $R^1 = R^{1'}$ = 2-pyridyl
f; $R^1 = R^{1'}$ = 4-$NO_2C_6H_4$
g; = (1)
h; = (4)



(9)

a = (7) b = (2) c = (5)



(10)

a = (3) b = (6)

ing of values for inner carbonyl groups (1.194—1.200 Å) compared to terminal ones (1.218—1.220 Å) in tetraketones could be interpreted as a reduction in the polar character of the CO group. However, no such differences were observed with triketones where inner CO values (1.207—1.221 Å) were identical with those for outer groups (1.209—1.220 Å).

D ***Bond angles of carbonyl groups*** ($\alpha_1,\alpha_2,\beta_1,\beta_2$). The sum of the bond angles for each CO group was 360° in all compounds, indicating that these groups are invariably planar. Bond angles (α_1,β_1) about the central CO group of triketones and the two central CO groups of tetraketones were close to the ideal value of 120°. However, the outer angles (α) of terminal CO groups were invariably appreciably larger than the inner angles (β). This results in a decreased interaction with the end group and appears to reflect the size of the end group.

E *Oxygen–oxygen distances.* The non-bonded O–O contacts were 3.00—3.55 Å for oxygen atoms on adjacent CO groups and 3.00—3.80 Å for other oxygen atoms. These values are greater than twice the van der Waals radius of oxygen (1.4 Å). The exceptional case of compound (3) was discussed earlier.

Table 5. Comparison of geometrical parameters in various polyketones (8)—(10)

(A) Diketones

Ketone	α_1, α_1' (°)	β_1, β_1' (°)	d_1 (Å)	l_1, l_1' (Å)	s_1, s_1' (Å)	Molecular symmetry	Ref.
(8a)	125.2	120.8	1.531	1.221	1.418	$\bar{1}$	10
	125.2	120.8		1.221	1.418		
(8b)	124.2	114.7	1.565	1.225	1.487	1	11
	123.1	121.4		1.208	1.489		
(8c)	123.7	118.7	1.536	1.213	1.455	$\bar{1}$	12
	123.7	118.7		1.213	1.455		
(8d)	124.5	117.9	1.549	1.199	1.477	1	13
	124.6	116.9		1.205	1.479		
(8e)	124.0	118.7	1.522	1.219	1.478	1	14
	123.6	118.8		1.216	1.494		
(8f)	123.1	117.0	1.532	1.212	1.490	1	15
	123.0	117.2		1.212	1.490		
(8g)	122.4	118.2	1.522	1.211	1.482	2	2*a*
	122.4	118.2		1.211	1.482		
(8h) (A)	123.9	117.2	1.520	1.188	1.500	$\bar{1}$	Present work
	123.9	117.2		1.188	1.500		
(8h) (B)	124.1	116.8	1.533	1.200	1.487	$\bar{1}$	Present work
	124.1	116.8		1.200	1.487		

(B) Triketones

Ketone	α_2, α_2' (°)	β_2, β_2' (°)	α_1 (°)	β_1 (°)	d_1, d_1' (Å)	l_2, l_2' (Å)	l_1' (Å)	s_1, s_1' (Å)	Molecular symmetry	Ref.
(9a)	125.8	114.8	120.3	120.3	1.540	1.220	1.221	1.464	$\bar{1}$	16
	125.8	114.8			1.540	1.220		1.464		
(9b)	124.0	114.1	120.5	122.2	1.522	1.209	1.213	1.450	1	2*b*
	124.7	114.8			1.523	1.216		1.469		
(9c)	124.7	115.0	122.2	121.9	1.525	1.213	1.207	1.482	1	Present work
	124.6	112.4			1.529	1.216		1.472		

(C) Tetraketones

Ketone	α_1, α_1' (°)	β_1, β_1' (°)	α_2, α_2' (°)	β_2, β_2' (°)	d_1 (Å)	d_2, d_2' (Å)	l_1, l_1' (Å)	l_2, l_2' (Å)	s_1, s_1'	Molecular symmetry	Ref.
(10a)	123.9	119.7	125.1	113.4	1.552	1.512	1.200	1.220	1.465	1	2*b*
	125.2	119.8	124.4	112.7		1.522	1.194	1.221	1.465		
(10b)	123.4	120.9	126.2	113.0	1.523	1.541	1.196	1.218	1.463	2	Present work
	123.4	120.9	126.2	113.0		1.541	1.196	1.218	1.463		

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Received 21*st June* 1982; *Paper* 2/1033