the molecules is such that neighbours make a number of close contacts as shown in Fig. 2. The closest approaches of the copper atom to atoms of the neighbouring molecule are 3·59 and 3·51 Å between the copper atom at (0,0,0) and two benzene carbon atoms of the adjacent molecule, situated at (0,0,1). As a consequence, the two molecules involved have the same orientation. This situation is intermediate between the edge-to-edge contacts present in bis-salicylaldiminatocopper(II) (Baker, Hall & Waters, 1966) and the axial separation from the copper atom to the aromatic ring of the next molecule of 3·21 Å found in bis-salicylaldehydatocopper(II) (McKinnon, Waters & Hall, 1964), which was interpreted in terms of polarization bonds, the copper atom acting as acceptor and the π-bond system as donor.

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Establishment of the stable geometric isomer of an α-arylidenelactone: α-(2-hydroxy-3,5-dibromobenzylidene)-γ-butyrolactone*.

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Crystals of α-(2-hydroxy-3,5-dibromobenzylidene)-γ-butyrolactone were found to be orthorhombic, with unit-cell dimensions $a=16{\cdot}32$, $b=10{\cdot}46$, $c=6{\cdot}81$ Å, probable space group $Pca2_1$, $Z=4$. The structure was determined from diffractometer data by non-centric symbolic phase addition. The tangent-refined phases differ by 11° (average) from the final phases despite strong violation of the statistical assumptions underlying the symbolic addition procedure. Full-matrix least-squares refinement yielded an agreement index $R=0{\cdot}059$. The largely planar molecule is in the *trans* configuration, *i.e.* the substituted phenyl moiety is *trans* to the carbonyl group of the lactone.

Introduction

Several indirect lines of evidence have suggested that α-2-hydroxy- and α-2-aminoarylidene-substituted five-membered lactones and lactams are *trans* isomers, *i.e.* the substituted phenyl moiety on carbon 7 of Fig. 1 is *trans* to the carbonyl group on carbon 8, and, once *trans-cis* isomerization has taken place, the *cis* isomers undergo cyclization reactions immediately. To establish the geometry of the stable isomer, we have determined the crystal structure of a representative compound, α-(2-hydroxy-3,5-dibromobenzylidene)-γ-butyrolactone (Fig. 1).

Experimental

The compound, prepared by the procedure of Zimmer & Rothe (1959) was recovered in 86% yield after recrystallization from ethanol.

Analyses: Calculated, for $C_{11}H_8Br_2O_3$: C, 37·9; H, 2·32; Br, 45·9. Found: C, 38·1; H, 2·44; Br, 46·2.

Single crystals (m.p. 210–211 °C) elongated along **c** and bounded by {210} faces were obtained from benzene solution by evaporation for 10 days in darkness at 25 °C. All data were collected from a crystal 0·06 × 0·07 × 0·81 mm. Dimensions of the orthorhombic cell are: $a=16{\cdot}32$, $b=10{\cdot}46$ and $c=6{\cdot}81$ Å. Reflections with indices $0kl$ for odd l, and $h0l$ for odd h are systematically absent, compatible with space groups $Pca2_1$ and $Pcam$. $D_m=1{\cdot}99$ g.cm^{-3} (flotation in a chloroform–bromoform mixture); $D_c=2{\cdot}00$ g.cm^{-3} for $Z=4$. There are then four molecules in general positions in $Pca2_1$ or four on mirror planes in $Pcam$. Since five-membered lactone rings are non-planar (Fridrichsons & Mathieson, 1962; Jeffrey & Kim, 1966), $Pca2_1$ was chosen as the probable space group (see *Discussion*).

Integrated intensities of 473 reflections with $d_{\min}=1{\cdot}1$ Å were collected by ω scan by means of a counter diffractometer with Cu $K\alpha$ radiation. Since the extreme variation in absorption correction of intensities is 9% for the data collected (although $\mu \simeq 98$ cm^{-1} for the crystal) no correction was applied. The absolute scale and overall B(2·10 Å^2) were estimated from a Wilson plot.

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Structure determination

Attempts to interpret the Patterson function were unsuccessful. The roughly planar molecules lie normal to **c** (see *Discussion*) so that all peaks fall at $w=0$ or $\frac{1}{2}$ and the two bromine atoms in each molecule are about $\frac{1}{4}$ apart in both their x and y coordinates. The two bromine atoms, which do 80% of the scattering, could not be located.

The structure was then solved by the symbolic addition method (Karle & Karle, 1964, 1966). Four starting symbols, for 10 3 1, 9 2 0, 1 2 1 and 4 3 1, generated 32 symbolic phases to $E=2{\cdot}0$. Starting phase assignments of 45, 0, 135 and −90 degrees, respectively, fixed the origin and hand. Ten cycles of simultaneous phase extension and tangent refinement led to stable phases for all the 269 independent reflections of $E>0{\cdot}60$. The assigned phases refined to values of 87·0, 0·1, 87·1, and −92·4 degrees respectively. Although the distribution of E values differs strikingly from that expected for a random (centrosymmetric or noncentrosymmetric) electron density distribution, the refined phases differ from those of the final least-squares cycle by only 10·30° (average) or 32·0° (root mean square). If the 11 reflections ($E<1{\cdot}2$) with discrepancies greater than 45° are excluded, the values fall to 4·5° and 7·2°.

The E map displayed a plausible structure, but the two bromine atoms alone (moved to give one a fixed z coordinate of zero) were used to begin a series of three F_o–F_c syntheses which yielded all 16 non-hydrogen atoms. Two

Table 1. *Structure amplitudes*

h	|F$_o$|	|F$_c$|
	H,0,0	
2	427	380
4	1066	1021
6	246	230
8	638	548
10	651	630
12	276	271
14	882	897
	H,1,0	
0	701	765
1	430	436
2	791	775
3	37	39
4	764	714
5	1152	1102
6	47	47
7	128	126
8	100	89
9	1189	1149
11	230	214
12	311	316
13	100	113
14	460	460
	H,2,0	
0	630	666
1	131	122
2	159	148
3	886	902
4	549	544
5	1345	1422
6	215	183
7	161	145
8	254	234
9	1205	1200
10	299	294
11	384	390
12	125	123
13	276	297
14	147	177
	H,3,0	
0	1299	1461
1	154	178
2	624	601
3	312	330
4	1021	1004
5	75	45
6	78	84
7	123	109
8	202	179
9	118	116
10	659	624
11	49	47
12	556	549
13	96	93
14	734	796
	H,4,0	
0	1143	1153
1	547	541
2	313	296
3	94	47
4	1035	981
5	846	843
6	341	351
7	131	125
8	280	262
9	767	779
10	228	228
11	39	30
12	68	80
13	337	373
	H,5,0	
0	423	382
1	101	96
2	452	415
3	517	470
4	178	193
5	1089	1066
6	191	216
7	121	113
8	88	76
9	868	855
10	191	186
11	66	66
12	69	49
	H,6,0	
0	1266	1259
1	93	90
2	33	26
3	439	434
4	690	670
5	110	130
6	64	16
7	89	81
8	51	37
9	281	292
10	207	223
11	250	265
	H,7,0	
0	451	453
1	443	458
2	118	107
3	59	17
4	278	258
5	584	564
6	142	144
7	46	54
8	146	162
9	310	341
10	152	142
	H,8,0	
0	354	396
1	341	355
2	117	100
3	56	61
4	255	242
5	520	533
6	301	288
7	177	177
8	248	291
	H,9,0	
0	430	394
1	229	238
2	205	206
3	142	118
4	285	286
5	235	227
	H,0,1	
4	1488	1340
6	1384	1271
8	1765	1676
10	847	825
12	141	147
14	239	214
	H,1,1	
1	846	840
2	194	233
3	838	772
4	1013	941
5	398	393
6	697	673
7	402	360
8	379	420
9	354	345
10	293	299
11	180	192
12	47	31
13	705	726
14	91	70
	H,2,1	
1	1406	1594
2	296	296
3	557	548
4	441	452
5	959	937
6	482	494
7	27	48
8	277	278
9	384	385
10	98	70
11	53	52
12	315	321
13	613	666
14	66	56
	H,3,1	
1	437	443
2	109	109
3	157	165
4	1366	1370
5	131	113
6	823	791
7	389	397
8	807	789
9	213	226
10	931	916
11	139	138
12	111	120
13	48	28
14	122	113
	H,4,1	
1	1016	1030
2	64	60
3	491	520
4	152	194
5	523	507
6	446	425
7	301	302
8	713	676
9	305	305
10	739	727
11	317	316
12	304	299
13	395	419
	H,5,1	
1	979	949
2	575	549
3	571	533
4	57	59
5	182	175
6	108	87
7	80	70
8	327	319
9	388	375
10	244	215
11	16	21
12	239	176
	H,6,1	
1	316	319
2	136	126
3	31	33
4	718	639
5	349	332
6	621	552
7	293	298
8	687	661
9	197	170
10	560	521
11	196	185
	H,7,1	
1	301	310
2	39	54
3	500	470
4	461	429
5	101	116
6	269	262
7	422	413
8	196	182
9	136	132
	H,8,1	
1	731	676
2	405	404
3	356	354
4	86	50
5	359	342
6	14	9
7	150	117
	H,9,1	
1	79	76
2	171	147
3	97	100
4	282	252
	H,0,2	
2	220	265
4	839	835
6	193	224
8	469	474
10	490	524
12	244	250
	H,1,2	
0	672	667
1	296	332
2	491	513
3	87	95
4	579	592
5	946	922
6	67	56
7	88	113
8	105	93
9	945	957
10	145	162
11	192	190
12	223	273
13	154	97
	H,2,2	
0	457	494
1	98	109
2	119	137
3	643	693
4	414	436
5	1119	1143
6	130	138
7	120	114
8	167	182
9	976	1013
10	237	248
11	316	345
12	109	112
13	246	244
	H,3,2	
0	1195	1233
1	117	154
2	410	479
3	243	278
4	796	848
5	50	62
6	89	104
7	83	83
8	154	174
9	105	108
10	482	515
11	76	52
12	424	477
13	98	89
	H,4,2	
0	884	931
1	372	433
2	248	262
3	38	36
4	742	770
5	660	712
6	270	292
7	104	95
8	233	248
9	599	659
10	181	197
11	81	27
12	62	74
	H,5,2	
0	272	298
1	73	91
2	329	346
3	417	415
4	136	159
5	824	883
6	144	183
7	83	76
8	60	73
9	673	734
10	140	161
11	62	67
	H,6,2	
0	1007	1061
1	89	77
2	41	64
3	344	359
4	509	549
5	93	121
6	29	36
7	66	68
8	44	53
9	238	260
10	.177	192
	H,7,2	
0	393	402
1	359	389
2	102	111
3	27	20
4	225	222
5	430	473
6	135	147
7	55	59
8	141	143
	H,8,2	
0	299	342
1	288	301
2	91	79
3	60	57
4	196	215
5	444	467
6	246	244
	H,0,3	
2	166	155
4	1001	944
6	986	859
8	1190	1143
10	657	622
12	67	73
	H,1,3	
1	643	646
2	58	139
3	484	473
4	633	625
5	303	304
6	414	421
7	247	263
8	315	332
9	239	236
10	237	223
11	118	110
12	24	18
	H,2,3	
1	995	1034
2	189	209
3	298	326
4	272	283
5	604	605
6	299	311
7	106	112
8	225	213
9	307	301
10	75	77
11	63	51
12	234	224
	H,3,3	
1	251	281
2	32	49
3	57	80
4	955	937
5	29	43
6	540	546
7	287	288
8	614	577
9	160	150
10	674	671
11	134	130
	H,4,3	
1	681	676
2	63	70
3	312	352
4	196	217
5	329	343
6	340	330
7	187	203
8	473	464
9	198	217
10	581	552
	H,5,3	
1	687	675
2	349	375
3	358	372
4	34	47
5	130	167
6	50	60
7	80	79
8	213	220
9	274	284
	H,6,3	
1	270	252
2	106	93
3	83	50
4	483	455
5	230	229
6	389	386
7	243	238
8	448	474
	H,7,3	
1	245	229
2	178	97
3	346	336
4	367	325
5	88	87
	H,0,4	
2	109	131
4	496	505
6	160	175
8	299	308
10	293	306
	H,1,4	
0	508	470
1	169	196
2	183	208
3	152	152
4	333	341
5	600	560
6	59	58
7	52	64
9	593	581
10	106	98
	H,2,4	
0	294	282
1	43	33
2	62	75
3	376	382
4	248	240
5	668	637
6	56	64
7	79	67
8	88	96
9	679	637
	H,3,4	
0	790	759
1	98	105
2	260	275
3	213	198
4	527	511
5	61	75
6	87	110
7	51	56
8	148	150
9	64	71
	H,4,4	
0	552	528
1	220	230
2	206	179
3	31	28
4	455	442
5	455	445
6	198	187
7	41	48
8	172	183
	H,5,4	
0	150	155
1	46	67
2	235	219
3	316	292
4	97	89
5	531	532
6	110	115
	H,6,4	
0	679	658
1	75	55
2	73	70
3	234	217
4	337	324
	H,0,5	
2	42	47
4	501	545
6	414	451
	H,1,5	
1	311	329
2	17	67
3	199	217
4	298	318
5	184	183
6	214	206
7	165	171
	H,2,5	
1	514	551
2	69	96
3	128	147
4	160	146
5	393	301
6	155	148
	H,3,5	
1	121	138
2	50	68
3	49	35
4	452	484
5	52	22
	H,4,5	
1	346	339
2	76	66
3	167	181

least-squares cycles, with anisotropic bromine temperature factors, lowered the value of R from 0·158 to 0·070. Atomic scattering factors were taken from Cromer & Waber (1964) except those for H (*International Tables for X-ray Crystallography*, 1962). Inclusion of eight hydrogen atoms and full anomalous dispersion corrections for bromine (Cromer, 1965) lowered the value of R to 0·059 (0·064 weighted). The hand was chosen on the basis of smallest r.m.s. structure factor error. Observed and calculated structure factors are given in Table 1.

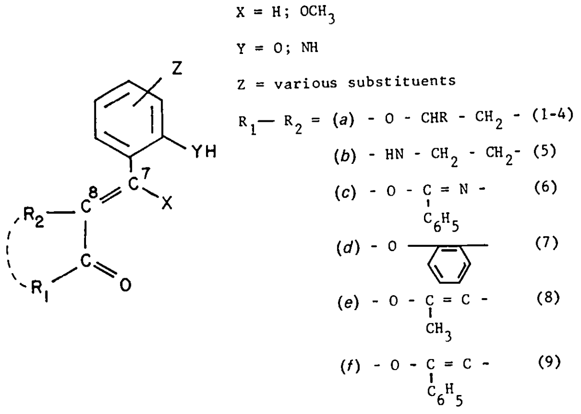

Fig. 1. α-Arylidene-substituted five-membered lactones and lactams: (1–4) α-benzylidene-γ-butyrolactones (Zimmer, Haupter, Rothe, Schrof & Walter, 1963; Zimmer & Walter, 1963*a*,*b*); (5) α-benzylidene-2-pyrrolidinone (Zimmer, Armbruster & Trauth, 1965); (6) α-benzylidene-5-oxazolone (Walter, Purcell & Zimmer, 1966); (7) α-benzylidene-2(3*H*)-coumaranone (Walter, Zimmer & Purcell, 1966); (8) α-benzylidene-Δβ,γ-angelicalactone (Walter & Purcell, 1966); (9) α-benzylidene-Δβ,γ-butenolide (Walter, Theodoropoulos & Purcell, 1967).

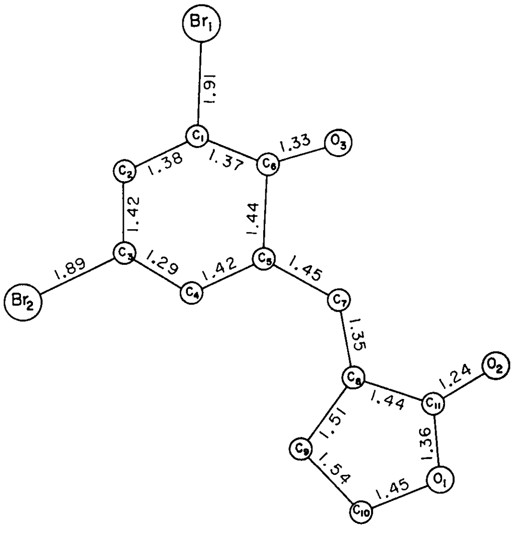

Fig. 2. Structure of α-(2-hydroxy-3,5-dibromobenzylidene)-γ-butyrolactone. Bond distances in Å. Least-squares e.s.d.'s are 0·02 Å for Br–C bonds and 0·03 Å for the others.

Discussion

Final atomic parameters are given in Table 2, bond lengths in Fig. 2, and bond angles in Table 3. Common experience, and inspection of equivalent bond lengths in this structure, indicate that the overall standard deviations are about twice the least-squares estimated standard deviations. Because of the preponderant contribution of the two bromine atoms to the total scattering, highly accurate atomic parameters were neither easily attainable nor sought.

Table 2. *Atomic parameters*

Components of the anisotropic temperature factors for the bromine atoms, defined by

$$\exp\left[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)\right],$$

are listed with least-squares estimated standard deviations in parentheses on the scale of the last digit. $\sigma(x)=0·0001$, $\sigma(y)=0·0002$ and $\sigma(z)=0·0017$ for Br; $\sigma(x)=0·001$, $\sigma(y)=0·002$, and $\sigma(z)=0·010$ for light atoms.

	x	y	z	B
Br(1)	0·0750	0·1464	0·0000	0·0016 (1) 0·0127 (3) 0·0255 (9) 0·0005 (1) 0·0006 (9) −0·0004 (14)
Br(2)	0·3556	−0·1668	−0·0001	0·0027 (1) 0·0074 (3) 0·0352 (10) 0·0007 (1) −0·0004 (10) −0·0037 (13)
C(1)	0·192	0·130	0·007	2·87
C(2)	0·224	0·008	0·009	3·45
C(3)	0·311	0·000	−0·002	2·92
C(4)	0·356	0·101	0·008	2·32
C(5)	0·325	0·228	0·015	2·63
C(6)	0·237	0·240	0·011	3·57
C(7)	0·372	0·344	−0·016	2·97
C(8)	0·453	0·361	0·014	3·05
C(9)	0·526	0·271	0·024	2·91
C(10)	0·596	0·363	−0·030	3·34
C(11)	0·485	0·489	0·027	4·08
O(1)	0·566	0·493	−0·008	3·58
O(2)	0·449	0·593	0·041	4·62
O(3)	0·207	0·358	0·030	3·38

Table 3. *Bond angles*

Least-squares $\sigma \leq 2°$ for all bond angles.

	Angle
C(1)—C(2)—C(3)	116°
C(2)—C(3)—C(4)	121
C(3)—C(4)—C(5)	124
C(4)—C(5)—C(6)	116
C(5)—C(6)—C(1)	118
C(6)—C(1)—C(2)	125
Br(1)-C(1)—C(2)	118
Br(1)-C(1)—C(6)	117
Br(2)-C(3)—C(2)	116
Br(2)-C(3)—C(4)	123
C(4)—C(5)—C(7)	125
C(6)—C(5)—C(7)	117
C(5)—C(6)—O(3)	116
O(3)—C(6)—C(1)	126
C(5)—C(7)—C(8)	128
C(7)—C(8)—C(9)	134

	Angle
C(7)—C(8)—C(11)	119
C(11)-C(8)—C(9)	107
C(8)—C(9)—C(10)	101
C(9)—C(10)-O(1)	108
C(10)-O(1)-C(11)	109
O(1)—C(11)-C(8)	112
O(1)—C(11)-O(2)	117
O(2)—C(11)-C(8)	131

The carbonyl group of the lactone ring is *trans* to the substituted phenyl group on C(7) of the exocyclic double bond (Fig. 2). The phenyl group is planar. In agreement with earlier reports (Mathieson & Taylor, 1961; Fridrichsons & Mathieson, 1962; Jeffrey & Kim, 1966) the $\mathrm{C{-}C{-}O{-}\underset{\underset{O}{\|}}{C}}$ group of the lactone is planar; the carbon atom C(9) of the lactone is 0·3 Å (~6 e.s.d.) above this plane. Least-squares refinement of the structure in space group *Pcam* (the 4 molecules on mirror planes) led to values for *R* of 0·066 (unweighted) and 0·069 (weighted), comparable with those from the $Pca2_1$ refinement. However, temperature factors for atoms C(9), C(10), C(11), O(1), O(2) and O(3) rose by an average of more than 1·0 $Å^2$, so that although a disordered structure containing molecules of each hand cannot be ruled out, the ordered $Pca2_1$ structure seems more probable. In any event, all bond lengths agree within one e.s.d. between the two refined structures, including the unreasonable C(3)–C(4) length of 1·29 Å.

The ester oxygen O(1) of one molecule is hydrogen-bonded to the phenolic oxygen O(3′) of the molecule related to the first one by the *a*-glide plane normal to **b**. The O(1)–O(3′) distance is 2·79 Å (e.s.d. 0·02 Å) and the angle of O(1)–O(3′)–C(6′) is about 144°. The hydrogen-bonded molecules form zigzag chains running along the **a** axis. Perpendicular to **c** and at *c*/2 apart, alternate sheets of parallel chains running in opposite directions are stacked with maximum overlapping of the phenolic rings.

The crystal structure confirms the hypothesis that the initial step in the formation of a coumarin from an α-(2-hydroxybenzylidene)-γ-butyrolactone consists of a *trans,cis* isomerization (Zimmer, Haupter, Rothe, Schrof & Walter, 1963), and lends support to the chemical evidence that all α-arylidene-substituted five-membered lactones and lactams in Fig. 1 are *trans* isomers.

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The absolute structure of $LiIO_3$ crystals.

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Rosenweig & Morosin (*Acta Cryst.* (1966) **20**, 758) concluded that the non-centrosymmetric structure of individual crystals of $LiIO_3$ could not be placed on an absolute basis by use of the anomalous dispersion of the iodine atoms because these particular atoms are related by a point of inversion. This conclusion is erroneous and its implication of such a restriction on the determination of absolute structure is misleading. Numerical evidence that the absolute chirality of individual $LiIO_3$ crystals is capable of experimental confirmation is presented.

Recent re-investigation of the crystal structure of $LiIO_3$ (Rosenweig & Morosin, 1966; Boer, Bolhuis, Olthof-Hazekamp & Vos, 1966), referred to subsequently as RM and BBOV respectively, has unambiguously established its space group as $P6_3$. This space group is non-centrosymmetric, the structure consisting of discrete trigonal iodate groups and Li ions surrounded by six oxygen atoms in a distorted octahedral arrangement. The iodine atoms lie on trigonal