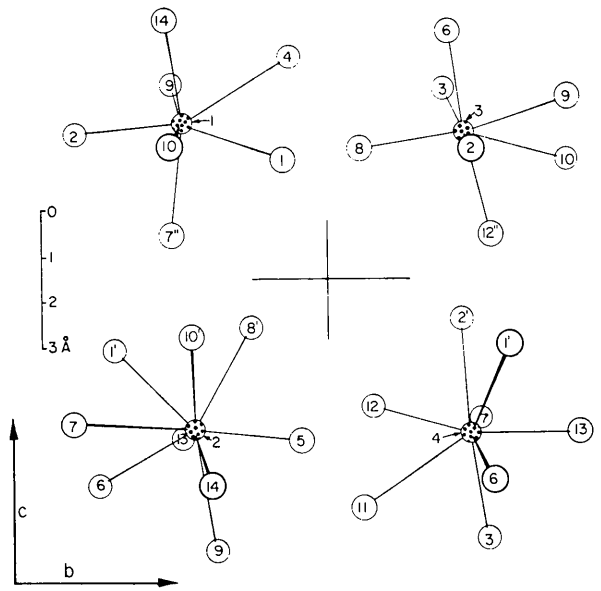

Fig. 7. Calcium–oxygen coordination shells viewed along **a**. Compare with view along **c** in Fig. 1.

can be pictured as a distorted pentagonal bipyramid, as a distorted NbF_7^{2-} configuration (Hoard, 1939) or, perhaps more descriptively, as an octahedron distorted by the approach of O(10) a little farther out than the others. The same description could apply to Ca(1) where O(4) is the distorting atom. Likewise the shell around Ca(4) can be described as an octahedron with two oxygen atoms jammed into edges, O(1′) and O(11). The coordination polyhedron around Ca(2) is a distorted one; it can be pictured as a pentagonal bipyramid with an apical atom replaced by three atoms.

We are indebted to Dr James Stewart for providing us with and instructing us in the use of X-ray 63, the system of crystallographic programs for the IBM 7094 computer developed at the Universities of Washington and Maryland; with the exception of the absorption corrections, this system was used throughout this work. The assistance given by Dr J. S. Cantrell in using X-ray 63 and the many discussions with Dr A. J. Mabis are greatly appreciated. The air-brush art work of Mr H. Thomas Brown is gratefully acknowledged.

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Molecular Structure of Xylerythrin, a Fungus Pigment

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The molecular structure of the red fungus pigment xylerythrin has been determined by X-ray single-crystal analysis of the bisbromoacetate derivative. The *R* value is 10·6% for the 1745 independent observed reflexions.

Introduction

Xylerythrin ($C_{26}H_{15}O_5$) is the main component of the red pigments present in wood infected by the fungus *Peniophora sanguinea* Bres. It has been isolated and studied chemically by Gripenberg (1965). He showed that the compound contained two hydroxyl groups, a lactone group, a conjugated carbonyl group and at least one monosubstituted benzene ring. A single-crystal X-ray analysis was undertaken to provide detailed information about the structure.

Experimental

The bisbromoacetate of xylerythrin ($C_{30}H_{18}O_7Br_2$) was prepared by Prof. Gripenberg who provided us with

excellent single crystals. They are triclinic with the following cell dimensions (precession photographs, Cu $K\alpha$ radiation).

$a = 11{\cdot}16 \pm 0{\cdot}05$ Å	$\alpha = 77{\cdot}86° \pm 0{\cdot}10°$
$b = 9{\cdot}36 \pm 0{\cdot}05$	$\beta = 90{\cdot}00 \pm 0{\cdot}10$
$c = 13{\cdot}29 \pm 0{\cdot}06$	$\gamma = 82{\cdot}65 \pm 0{\cdot}10$

The calculated density is 1·198 g.cm^{-3}, which indicates that there are two molecules per unit cell. The space group was assumed to be $P\bar{1}$. Weissenberg photographs were taken for layers 0–5 about the b axis and for layers 0–2 about the a axis. One crystal (0·27 × 0·36 × 0·09 mm^3) was used to collect all the data. The intensities were estimated visually and corrected for the Lorentz and polarization factors but not for absorption.

Structure determination

The coordinates of the two bromine atoms were derived from a three-dimensional 'point atoms at rest' Patterson synthesis. The light atoms were successively found from three-dimensional electron density series by computer scanning for peaks. All light atoms were at first treated as carbon atoms. When all the atoms of the molecule had been located and included in the structure factor calculation, the oxygen atoms were identified from the peak heights in the electron density series. With the molecular skeleton known, the chemical information also fixes the oxygen atoms to these positions.

The structure was refined by block-diagonal least-squares treatment. The weight assigned to each observation was

$$w = \left(1/1 + \left\{\frac{|F_o| - a}{b}\right\}^2\right), \quad \text{(Mills \& Rollett, 1960)}$$

in which the final values of a and b were $10|F_{\min}|$ and $6|F_{\min}|$ respectively.

The hydrogen atoms were included in the structure factor calculations at their expected coordinates and with isotropic temperature factors corresponding to the hydrogen-carrying carbon atoms. The final R value for the 1745 independent observed reflexions was 0·106.

The calculations were performed on a Datasaab D21 computer with the integrated program system developed at this Institute (Abrahamsson, Aleby, Larsson,

Table 1. *Fractional atomic coordinates with standard deviations* × 10^5 *(in brackets) for the heavier atoms of the structure*

	x	$\sigma(x)$	y	$\sigma(y)$	z	$\sigma(z)$
Br(1)	0·19393	(12)	0·25932	(24)	0·35574	(13)
Br(2)	0·14280	(19)	0·88215	(31)	0·63455	(17)
O(1)	0·45487	(58)	0·47003	(100)	0·20518	(65)
O(2)	0·46781	(71)	0·26104	(116)	0·32373	(70)
O(3)	0·49467	(74)	0·27206	(127)	0·08844	(87)
O(4)	0·09229	(58)	0·68013	(104)	0·92866	(54)
O(5)	0·07940	(57)	0·40622	(102)	0·09859	(59)
O(6)	0·10980	(71)	0·83669	(111)	0·40509	(70)
O(7)	0·25491	(86)	0·65108	(137)	0·45368	(95)
C(1)	0·27606	(94)	0·41490	(178)	0·28103	(102)
C(2)	0·41132	(91)	0·36262	(162)	0·27361	(93)
C(3)	0·40734	(116)	0·13669	(190)	0·64159	(125)
C(4)	0·42572	(113)	0·27816	(194)	0·59496	(102)
C(5)	0·40398	(101)	0·39462	(181)	0·64536	(95)
C(6)	0·35927	(83)	0·37109	(137)	0·74758	(88)
C(7)	0·34165	(94)	0·22823	(143)	0·79159	(95)
C(8)	0·35964	(116)	0·10995	(168)	0·74374	(115)
C(9)	0·34015	(92)	0·49418	(144)	0·80465	(86)
C(10)	0·42902	(87)	0·56327	(149)	0·82764	(93)
C(11)	0·41664	(93)	0·67438	(153)	0·89001	(99)
C(12)	0·29920	(86)	0·72405	(158)	0·93033	(87)
C(13)	0·20993	(86)	0·65093	(146)	0·89988	(84)
C(14)	0·21997	(79)	0·53943	(142)	0·84034	(76)
C(15)	0·10914	(83)	0·50232	(133)	0·82890	(75)
C(16)	0·02578	(96)	0·58802	(147)	0·88793	(82)
C(17)	0·27799	(88)	0·83793	(160)	0·98929	(92)
C(18)	0·36315	(99)	0·84624	(165)	0·06535	(100)
C(19)	0·34601	(116)	0·95727	(189)	0·11688	(110)
C(20)	0·24860	(100)	0·06885	(177)	0·09867	(108)
C(21)	0·16472	(101)	0·06496	(157)	0·02081	(105)
C(22)	0·18079	(94)	0·95449	(156)	0·96613	(91)
C(23)	0·05474	(99)	0·74740	(171)	0·34728	(101)
C(24)	0·02977	(100)	0·33456	(167)	0·60575	(87)
C(25)	0·08773	(89)	0·41746	(149)	0·66338	(83)
C(26)	0·05742	(82)	0·40805	(151)	0·76841	(84)
C(27)	0·02444	(92)	0·68056	(152)	0·18594	(85)
C(28)	0·08233	(91)	0·76512	(165)	0·24416	(98)
C(29)	0·21072	(119)	0·77293	(193)	0·46018	(115)
C(30)	0·25137	(121)	0·86193	(201)	0·52843	(123)

Table 2. *Mean-square-amplitude tensors*

Allowance was made for anisotropic vibration with

$$\exp[-2\pi^2(h^2a^{*2}U_{11}+k^2b^{*2}U_{22}+l^2c^{*2}U_{33}+2klb^*c^*U_{23}+2lhc^*a^*U_{31}+2hka^*b^*U_{12})$$

The U_{ij}'s (Å^2) are given together with standard deviations ($\times 10^4$) within brackets.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br(1)	0·0825 (9)	0·1680 (20)	0·0987 (12)	0·0059 (12)	0·0195 (7)	−0·0221 (9)
Br(2)	0·1440 (15)	0·1947 (27)	0·1272 (17)	−0·0611 (18)	−0·0247 (12)	−0·0216 (14)
O(1)	0·0528 (40)	0·0850 (77)	0·0875 (61)	−0·0078 (52)	0·0006 (35)	−0·0050 (38)
O(2)	0·0792 (53)	0·1145 (91)	0·0780 (66)	0·0164 (62)	−0·0035 (43)	0·0071 (49)
O(3)	0·0820 (57)	0·1212 (105)	0·1491 (94)	−0·0757 (83)	0·0106 (55)	−0·0308 (55)
O(4)	0·0621 (42)	0·1117 (83)	0·0521 (48)	−0·0203 (51)	0·0032 (32)	−0·0247 (42)
O(5)	0·0508 (38)	0·1073 (83)	0·0658 (52)	−0·0148 (51)	0·0029 (31)	−0·0183 (39)
O(6)	0·0869 (55)	0·0981 (87)	0·0904 (66)	−0·0177 (59)	−0·0423 (46)	−0·0089 (48)
O(7)	0·0946 (63)	0·1336 (110)	0·1680 (108)	−0·0561 (86)	−0·0556 (65)	−0·0065 (61)
C(1)	0·0534 (61)	0·1194 (139)	0·0866 (94)	−0·0250 (91)	−0·0024 (53)	−0·0143 (65)
C(2)	0·0571 (61)	0·1043 (135)	0·0736 (87)	−0·0073 (84)	−0·0075 (52)	−0·0253 (64)
C(3)	0·0849 (84)	0·0963 (147)	0·1246 (128)	−0·0344 (107)	−0·0070 (75)	−0·0301 (78)
C(4)	0·0942 (89)	0·1322 (165)	0·0780 (95)	−0·0555 (104)	−0·0049 (66)	−0·0232 (83)
C(5)	0·0716 (72)	0·1313 (148)	0·0582 (84)	0·0112 (88)	0·0024 (55)	−0·0255 (73)
C(6)	0·0520 (56)	0·0627 (104)	0·0758 (82)	−0·0116 (70)	−0·0163 (48)	−0·0126 (51)
C(7)	0·0733 (67)	0·0434 (108)	0·0832 (88)	−0·0055 (73)	−0·0137 (55)	−0·0272 (57)
C(8)	0·0972 (87)	0·0615 (125)	0·1094 (112)	−0·0311 (92)	−0·0153 (72)	−0·0080 (70)
C(9)	0·0743 (67)	0·0532 (112)	0·0617 (77)	−0·0110 (72)	0·0023 (50)	−0·0100 (58)
C(10)	0·0571 (60)	0·0739 (117)	0·0799 (84)	−0·0223 (77)	−0·0125 (51)	−0·0061 (57)
C(11)	0·0647 (65)	0·0737 (118)	0·0791 (89)	0·0099 (76)	−0·0067 (54)	−0·0279 (60)
C(12)	0·0530 (58)	0·1075 (130)	0·0629 (78)	−0·0097 (80)	−0·0143 (49)	−0·0100 (61)
C(13)	0·0589 (59)	0·0736 (114)	0·0586 (76)	−0·0076 (72)	−0·0006 (47)	0·0018 (55)
C(14)	0·0519 (54)	0·0806 (109)	0·0435 (64)	−0·0061 (65)	−0·0090 (41)	−0·0112 (52)
C(15)	0·0647 (59)	0·0519 (101)	0·0424 (64)	−0·0063 (62)	−0·0030 (42)	−0·0155 (51)
C(16)	0·0855 (74)	0·0648 (116)	0·0392 (68)	0·0126 (67)	−0·0069 (49)	−0·0128 (61)
C(17)	0·0536 (59)	0·1033 (128)	0·0739 (84)	−0·0198 (81)	−0·0097 (50)	−0·0148 (60)
C(18)	0·0736 (73)	0·0953 (131)	0·0891 (97)	−0·0358 (91)	−0·0243 (62)	−0·0117 (68)
C(19)	0·0894 (87)	0·1191 (156)	0·0800 (98)	−0·0041 (98)	−0·0133 (67)	−0·0167 (82)
C(20)	0·0655 (69)	0·1159 (149)	0·0938 (101)	−0·0258 (97)	−0·0005 (60)	−0·0287 (72)
C(21)	0·0802 (76)	0·0708 (122)	0·0865 (97)	−0·0073 (84)	0·0058 (62)	−0·0129 (66)
C(22)	0·0686 (67)	0·0780 (120)	0·0648 (83)	−0·0017 (76)	−0·0102 (52)	−0·0018 (61)
C(23)	0·0693 (69)	0·0900 (126)	0·0869 (93)	−0·0245 (85)	−0·0198 (59)	−0·0063 (66)
C(24)	0·0793 (74)	0·1032 (132)	0·0478 (73)	−0·0115 (78)	−0·0136 (52)	−0·0116 (67)
C(25)	0·0654 (63)	0·0820 (118)	0·0505 (72)	−0·0033 (71)	0·0016 (47)	−0·0115 (58)
C(26)	0·0496 (55)	0·0910 (120)	0·0560 (72)	−0·0016 (73)	−0·0047 (44)	−0·0074 (56)
C(27)	0·0663 (64)	0·0861 (122)	0·0539 (72)	−0·0053 (72)	−0·0115 (48)	−0·0209 (59)
C(28)	0·0543 (61)	0·1036 (131)	0·0798 (89)	−0·0092 (83)	−0·0075 (52)	−0·0181 (63)
C(29)	0·0941 (90)	0·1135 (154)	0·0927 (105)	−0·0263 (100)	−0·0183 (71)	−0·0241 (82)
C(30)	0·0857 (86)	0·1320 (168)	0·1159 (126)	−0·0278 (115)	−0·0356 (77)	−0·0314 (86)

Table 3. *Fractional coordinates and isotropic temperature factors for the hydrogen atoms*

The first appended number refers to the parent atom

	x	y	z	B
H(11)	0·7384	0·4943	0·6790	4·26 Å^2
H(12)	0·7617	0·5507	0·7955	4·26
H(31)	0·4310	0·0481	0·6027	5·80
H(41)	0·4545	0·3072	0·5131	5·57
H(51)	0·4204	0·5100	0·6086	4·80
H(71)	0·3098	0·2052	0·8741	4·46
H(81)	0·3444	0·0036	0·7800	5·90
H(181)	0·4433	0·7676	1·0787	4·64
H(191)	0·4078	0·9543	1·1806	6·05
H(201)	0·2384	1·1654	1·1369	4·90
H(211)	0·0814	1·1450	1·0054	5·06
H(221)	0·1190	0·9506	0·9056	4·34
H(241)	0·0535	0·3311	0·5244	4·33
H(251)	0·1499	0·4918	0·6291	3·54
H(271)	−0·0507	0·3213	0·8921	3·52
H(281)	−0·1411	0·1543	0·7919	4·64
H(301)	−0·3424	0·1795	0·4437	6·32
H(302)	−0·2545	0·0257	0·5233	6·32

Nilsson, Selin & Westerdahl, 1965). The form factors used are those given in *International Tables for X-ray Crystallography* (1962).

Results and discussion

The final parameters are given in Tables 1–3. Observed and calculated structure factors are listed in Table 4.

A spatial drawing of xylerythrin bisbromoacetate is shown in Fig. 1. Distances and angles are given in Fig. 2 and in Tables 5 and 6 with standard deviations calculated according to Ahmed & Cruickshank (1953) and Darlow (1960). The structure analysis determines the molecular formula of the bromo derivative as (I) and hence of the pigment itself as (II) (see page 953).

The pigment is thus a quinone methide, as has earlier been found in fungi, *e.g.* citrinin (Brown, Robertson, Whalley & Cartwright, 1949) and purpurogenone (Robert & Warren, 1955).

Table 4. *Observed and calculated structure factors* (× 100)

h	k	l	Fobs	Fcalc
0	0	2	3732	-3177
0	0	3	6912	7922
0	0	4	10052	-12147
0	0	5	1809	1317
0	0	6	1037	1151
0	0	7	6431	-7539
0	0	8	2425	2647
0	0	9	971	968
0	0	10	1209	-1041
0	0	11	2212	2514
0	0	13	676	-648
1	0	1	1352	-1267
1	0	2	5319	6204
1	0	3	3925	4043
1	0	4	5332	-5948
1	0	5	1681	1856
1	0	6	3152	3520
1	0	7	2228	-2457
1	0	8	2650	2941
1	0	10	1355	-1305
1	0	11	681	598
1	0	-1	5030	-5453
1	0	-2	1648	-1430
1	0	-3	4373	4593
1	0	-4	3151	-3442
1	0	-5	2053	1835
1	0	-6	1596	-1403
1	0	-7	2169	-2126
1	0	-8	795	639
1	0	-9	504	506
2	0	0	3821	-3904
2	0	1	1327	169
2	0	2	3732	-3169
2	0	3	920	-1078
2	0	4	2252	2306
2	0	5	1421	-1045
2	0	6	2206	-2250
2	0	7	1203	1053
2	0	8	808	-811
2	0	10	558	810
2	0	11	969	-1053
2	0	-1	4668	4974
2	0	-2	6292	-6167
2	0	-3	4417	-4300
2	0	-4	2731	-2664
2	0	-6	2075	-2180
2	0	-8	2151	-2260
2	0	-9	614	515
2	0	-10	1915	2120
2	0	-11	1113	-1218
2	0	-12	978	1159
2	0	-14	757	-798
3	0	0	6357	-7388
3	0	1	8815	11401
3	0	2	8196	-8412
3	0	3	4563	-4668
3	0	4	6935	7308
3	0	5	4759	-5007
3	0	6	1835	-2070
3	0	7	2639	2773
3	0	8	2858	-2862
3	0	9	1285	1520
3	0	10	669	653
3	0	11	1397	-1324
3	0	-1	669	256
3	0	-2	4518	4861
3	0	-3	8784	-11057
3	0	-4	5651	6290
3	0	-5	1927	2031
3	0	-6	5902	-5946
3	0	-7	3523	3513
3	0	-9	1768	-1737
3	0	-10	2238	2416
4	0	0	3379	-3330
4	0	1	4048	3728
4	0	2	956	695
4	0	3	6372	-6265
4	0	4	3146	3564
4	0	5	2024	-2056
4	0	6	2654	2550
4	0	7	3313	3412
4	0	8	2833	-3042
4	0	9	1075	1196
4	0	10	1078	937
4	0	11	692	-599
4	0	-1	2492	-1546
4	0	-2	4761	5260
4	0	-3	1286	-1386
4	0	-5	2270	-1774
4	0	-6	2004	-1926
4	0	-8	1405	1243
4	0	-10	1072	812
5	0	0	2592	2143
5	0	1	8509	-7607
5	0	2	1499	1422
5	0	3	3915	3154
5	0	4	2210	-2254
5	0	5	1452	1415
5	0	6	703	629
5	0	7	748	-638
5	0	8	2150	2658
5	0	11	687	634
5	0	12	1142	-1325
5	0	-1	1496	1103
5	0	-2	3586	-2904
5	0	-3	476	300
5	0	-4	3390	-2910
5	0	-5	1225	1069
5	0	-6	3368	3283
5	0	-7	1206	-928
5	0	-8	1105	962
5	0	-10	1789	-1592
5	0	-11	1091	1006
5	0	-13	874	-843
6	0	0	792	-670
6	0	1	1312	-1327
6	0	2	2479	2266
6	0	3	1000	-761
6	0	4	2900	-2905
6	0	5	4768	4437
6	0	6	1066	-853
6	0	7	2450	-2353
6	0	8	1912	1825
6	0	9	1089	-1127
6	0	10	1092	1108
6	0	11	671	575
6	0	12	1174	-1290
6	0	-1	736	833
6	0	-2	4052	-3728
6	0	-3	5497	5319
6	0	-4	898	716
6	0	-5	1645	-1477
6	0	-6	3422	3405
6	0	-8	815	-667
6	0	-9	1578	1398
6	0	-10	1593	-1328
6	0	-13	819	-706
7	0	0	1882	-1511
7	0	1	3581	-2913
7	0	2	2548	2425
7	0	3	722	851
7	0	4	1639	-1493
7	0	5	4536	4306
7	0	7	675	-724
7	0	8	1395	1367
7	0	9	1553	-1539
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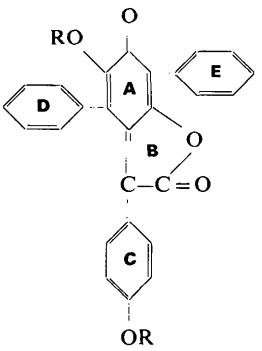
9	-3	-5	636	611
10	-3	-5	1147	-1305
10	-3	-6	937	-870
10	-3	-7	628	546
10	-3	-8	609	-654
1	-3	0	1357	1413
1	-3	1	1513	1360
1	-3	2	1832	-1981
1	-3	3	1321	1457
1	-3	4	644	544
1	-3	5	1356	-1334
1	-3	7	1076	-1044
1	-3	8	933	-806
1	-3	9	1014	1122
1	-3	10	1692	-1715
1	-3	14	908	-909

The distances in Fig. 2 indicate clearly the quinoid character of ring *A*. The values for the bonds O(3)–C(11), C(9)–C(10), C(10)–C(11), C(11)–C(12) and C(9)–C(14) compare well with the corresponding bonds in tetrahydroxy-*p*-benzoquinone (Klug, 1965). The differences in the remaining ring bonds are probably significant: C(12)–C(13) is 0·06 Å longer than the C(9)–C(10) double bond and C(13)–C(14) is 0·05 Å shorter than the corresponding bond in the quinone. Such deviations are expected as the attached lactone ring *B* is coplanar with ring *A* and an extended π-electron system is formed. The bond O(4)–C(13) is also about 0·1 Å shorter than usual for lactones (*e.g.* Mathieson & Taylor, 1963) whereas the other lactone distances are normal. The ring system *A*–*B* is planar within 0·025 Å. The distances to the best least-squares plane are given



(I) R = $COCH_2Br$
(II) R = H

in Table 7. The attached oxygen atoms O(1), O(3) and O(5) and the bond to the benzene ring *E* are also in this plane. However the bonds to the other rings (*C* and *D*) are directed considerably out of the plane. C(6) is 0·127 Å above and C(26) 0·169 Å below the *A–B* ring plane as given in Fig. 2. Table 7 also contains information for the other planar groups of the structure.

The three benzene rings and the carboxyl group cannot be coplanar with the *A–B* ring system to which they are attached, because of steric hindrance. Ring *E* forms an angle of 43° with the *A–B* ring plane. The distances C(18)–O(3) and C(22)–O(4) are then 2·90 and 3·00 Å respectively. Similar intramolecular contact distances to oxygen atoms also result for the other benzene rings (Fig. 3) with a twist of 47° for ring *C* and 63°

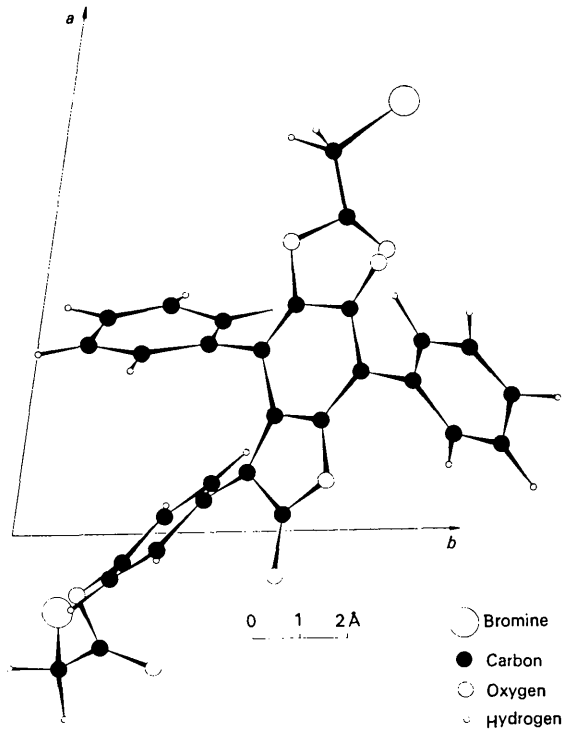


Fig. 1. Stereochemistry of xylerythrin bisbromoacetate.

Table 5. *Bond distances with standard deviations*

	Length	σ
Br(1)–C(1)	1·918 Å	0·014 Å
Br(2)–C(30)	1·883	0·016
O(1)—C(2)	1·347	0·015
–C(10)	1·386	0·012
O(2)—C(2)	1·151	0·015
O(3)—C(11)	1·225	0·016
O(4)—C(13)	1·377	0·012
–C(16)	1·395	0·017
O(5)—C(16)	1·184	0·013
O(6)—C(23)	1·438	0·019
–C(29)	1·344	0·015
O(7)—C(29)	1·204	0·021
C(1)—C(2)	1·536	0·015
C(3)—C(4)	1·380	0·024
–C(8)	1·442	0·022
C(4)—C(5)	1·391	0·025
C(5)—C(6)	1·430	0·017
C(6)—C(7)	1·381	0·018
–C(9)	1·501	0·019
C(7)—C(8)	1·382	0·022
C(9)—C(10)	1·320	0·018
–C(14)	1·464	0·014
C(10)–C(11)	1·454	0·021
C(11)–C(12)	1·473	0·015
C(12)–C(13)	1·384	0·018
–C(17)	1·447	0·021
C(13)–C(14)	1·430	0·019
C(14)–C(15)	1·344	0·014
C(15)–C(16)	1·483	0·016
–C(26)	1·479	0·019
C(17)–C(18)	1·408	0·018
–C(22)	1·420	0·016
C(18)–C(19)	1·354	0·024
C(19)–C(20)	1·391	0·019
C(20)–C(21)	1·405	0·019
C(21)–C(22)	1·378	0·022
C(23)–C(24)	1·361	0·018
–C(28)	1·385	0·018
C(24)–C(25)	1·409	0·020
C(25)–C(26)	1·424	0·016
C(26)–C(27)	1·369	0·017
C(27)–C(28)	1·425	0·021
C(29)–C(30)	1·462	0·026

Table 6. *Bond angles with standard deviations*

Angle		σ
C(2)—O(1)—C(10)	116·3°	0·9°
C(13)–O(4)—C(16)	106·6	0·9
C(23)–O(6)—C(29)	116·5	1·2
Br(1)–C(1)—C(2)	111·2	0·9
O(1)—C(2)—O(2)	126·0	1·0
–C(1)	105·9	1·0
O(2)—C(2)—C(1)	127·6	1·1
C(4)—C(3)—C(8)	119·1	1·6
C(3)—C(4)—C(5)	121·8	1·3
C(4)—C(5)—C(6)	120·5	1·3
C(5)—C(6)—C(7)	116·1	1·3
–C(9)	121·1	1·2
C(7)—C(6)—C(9)	122·7	1·1
C(6)—C(7)—C(8)	125·4	1·2
C(3)—C(8)—C(7)	117·1	1·4
C(6)—C(9)—C(10)	122·7	1·0
–C(14)	120·3	1·1
C(10)–C(9)—C(14)	117·0	1·2
O(1)—C(10)–C(9)	120·9	1·3
–C(11)	114·5	1·0

Table 5 (*cont.*)

Angle		σ
C(9)—C(10)–C(11)	124·6	1·0
O(3)—C(11)–C(10)	120·2	1·1
–C(12)	118·2	1·4
C(10)–C(11)–C(12)	121·7	1·1
C(11)–C(12)–C(13)	110·4	1·2
–C(17)	125·2	1·1
C(13)–C(12)–C(17)	124·3	0·9
O(4)—C(13)–C(12)	120·5	1·2
–C(14)	110·4	1·0
C(12)–C(13)–C(14)	129·1	1·0
C(9)—C(14)–C(13)	117·2	1·0
–C(15)	134·7	1·2
C(13)–C(14)–C(15)	108·1	0·9
C(14)–C(15)–C(16)	107·1	1·1
–C(26)	134·6	1·0
C(16)–C(15)–C(26)	118·2	0·9
O(4)—C(16)–O(5)	119·5	1·2
–C(15)	107·8	0·9
O(5)—C(16)–C(15)	132·6	1·3
C(12)–C(17)–C(18)	120·0	1·0
–C(22)	122·6	1·1
C(18)–C(17)–C(22)	117·0	1·3
C(17)–C(18)–C(19)	119·8	1·2
C(18)–C(19)–C(20)	124·1	1·4
C(19)–C(20)–C(21)	116·9	1·5
C(20)–C(21)–C(22)	120·3	1·1
C(17)–C(22)–C(21)	121·8	1·1
O(6)—C(23)–C(24)	118·0	1·2
–C(28)	116·7	1·2
C(24)–C(23)–C(28)	125·0	1·4
C(23)–C(24)–C(25)	118·2	1·1
C(24)–C(25)–C(26)	118·4	1·1
C(15)–C(26)–C(25)	120·0	1·0
–C(27)	118·4	1·0
C(25)–C(26)–C(27)	121·6	1·2
C(26)–C(27)–C(28)	119·9	1·1
C(23)–C(28)–C(27)	116·7	1·2
O(6)—C(29)–O(7)	119·9	1·6
–C(30)	113·3	1·4
O(7)—C(29)–C(30)	126·7	1·3
Br(2)–C(30)–C(29)	112·5	1·0

for ring *D* to the central ring system. Rings *C* and *D* come very close together, introducing considerable strain in the molecule. The C(7)–C(25) distance is only 3·39 Å and it is clear from the large angles at C(14), C(15) and C(16) (Fig. 2) that ring *C* has been forced away from ring *D*, thereby also requiring O(5) to move. A corresponding displacement of ring *D* in the opposite direction would be more difficult as it would affect not

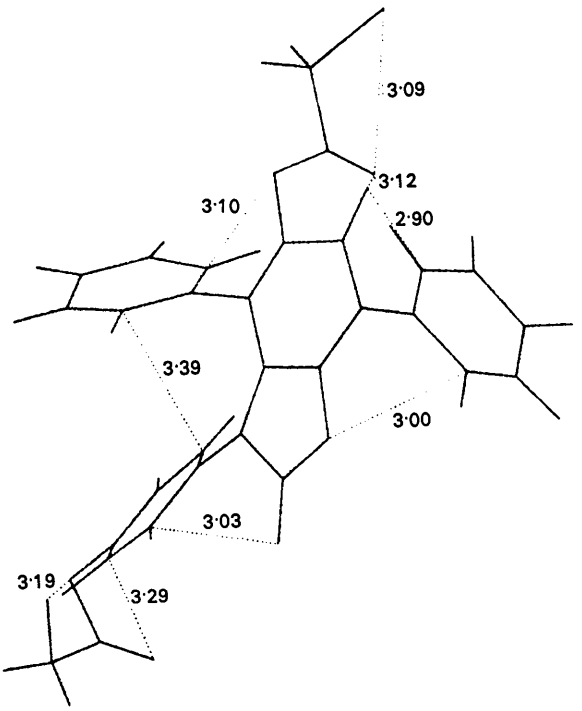


Fig. 3. Some short intramolecular contacts.

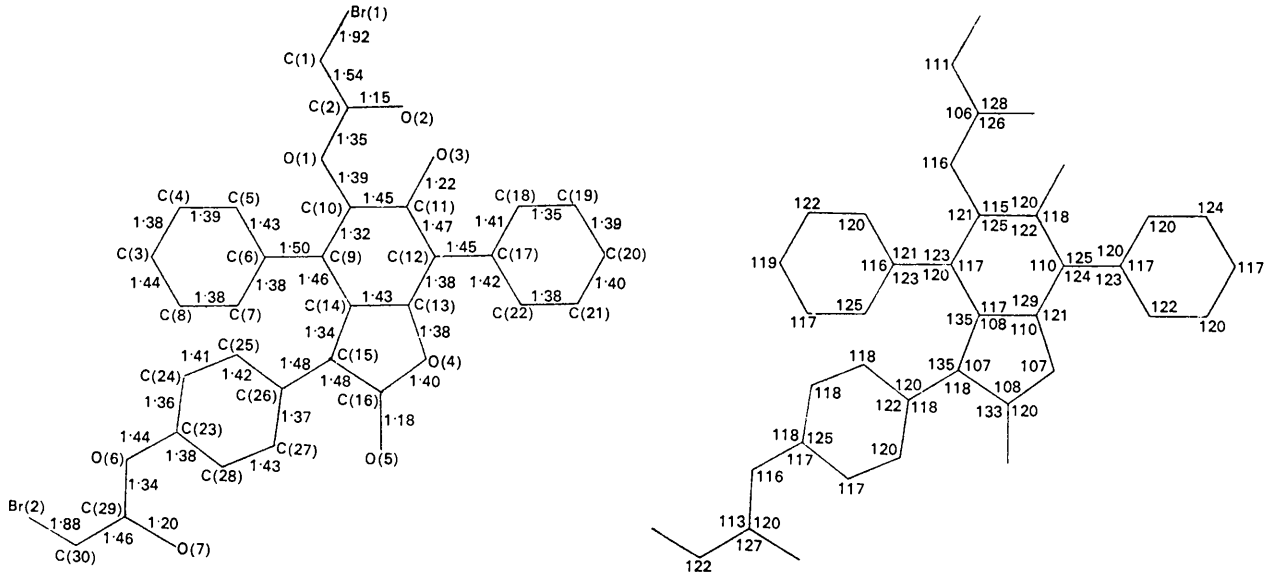


Fig. 2. Bond distances and angles of xylerythrin bisbromoacetate. The atomic numbering used is indicated.

Table 7. *Least-squares planes*

Plane	Atoms involved	Equation of plane (referred to crystal axes)	Out-of-plane deviations (Å) for atoms defining plane	Out-of-plane deviations (Å) for other atoms
A, *B*	C(9)–C(16), O(4)	$0{\cdot}09570X-0{\cdot}47053Y+0{\cdot}87718Z-0{\cdot}50355=0$	C(9) 0·024, C(10) −0·016, C(11) −0·003 C(12) 0·005, C(13) −0·004, C(14) 0·009 C(15) −0·025, C(16) 0·012, O(4) −0·001	C(6) 0·127, C(17) −0·036 C(26) −0·169, O(1) −0·037 O(3) 0·020, O(5) 0·002
C	C(15), C(23)–C(28), O(6)	$0{\cdot}76618X-0{\cdot}62153Y+0{\cdot}16330Z+0{\cdot}08729=0$	C(15) −0·056, C(23) −0·047 C(24) 0·010, C(25) 0·032, C(26) 0·030 C(27) 0·028, C(28) 0·016, O(6) −0·011	C(14) 0·543, C(16) −1·067 C(29) −1·196
D	C(3)–C(9)	$0{\cdot}91973X-0{\cdot}00709Y+0{\cdot}39249Z-0{\cdot}62317=0$	C(3) 0·026, C(4) −0·001, C(5) −0·013 C(6) −0·022, C(7) 0·001, C(8) −0·014 C(9) 0·022	C(10) 1·032, C(14) −1·061
E	C(12), C(17)–C(22)	$-0{\cdot}60914X-0{\cdot}41436Y+0{\cdot}67620Z-0{\cdot}14864=0$	C(12) −0·020, C(17) 0·042, C(18) −0·001 C(19) −0·009, C(20) 0·000, C(21) 0·000, C(22) −0·010	C(11) −0·894, C(13) 0·695
Carboxyl group 1	C(1), C(2), O(1), O(2)	$0{\cdot}20803X+0{\cdot}49094Y+0{\cdot}84599Z-1{\cdot}04690=0$	C(1) −0·011, C(2) 0·039, O(1) −0·012 O(2) −0·017	Br(1) 0·386, C(10) 0·250
Carboxyl group 2	C(29), C(30), O(6), O(7)	$-0{\cdot}60291X-0{\cdot}27611Y+0{\cdot}74850Z-0{\cdot}46687=0$	C(29) 0·018, C(30) −0·005 O(6) −0·005, O(7) −0·007	Br(2) −1·630, C(23) −0·176

only O(1) but also O(3) and ring *E* (Fig. 3). The only indication of distortion at ring *D* is, as discussed earlier, the direction of the bond C(6)–C(9).

Except for the large angles mentioned above, the remaining bond distances and angles in the structure are normal. The average benzene bond distance is 1·397 Å and the average angle 119·9°.

The planes of the two carboxyl groups are roughly at right angles to the planar groups to which they are attached. The conformations of the two bromoacetate residues are different as indicated in Fig. 4. The bromine atom and the carbonyl oxygen are in a *trans* conformation about the C(29)–C(30) bond whereas the more usual *gauche* arrangement is valid in the other acetate group.

The molecular packing is illustrated in Fig. 5 with some of the shorter intermolecular H–H distances indicated. Ring *E* lies roughly at right angles to, and is in packing contact with, rings *C* and *D*. Close packing with parallel ring planes also exists around centres of symmetry. All benzene rings are in contact with the bromoacetate hydrogen atoms.

The strong colour of certain quinone compounds, *e.g.* choranil (Chu, Jeffrey & Sakurai, 1962) and tetrahydroxy-*p*-benzoquinone (Klug, 1965), has been attributed to charge transfer self-complexing, made possible by short intermolecular carbon–oxygen distances (< 3·0 Å). Such a short distance (2·97 Å) also exists in xylerythrin bisbromoacetate between O(5) and C(16) over a centre of symmetry. The conditions are favourable for strong charge transfer interaction as – in the two parallel *A*–*B* ring planes – each carbonyl oxygen atom approaches an sp^2-hybridized carbon atom almost exactly along the axis of the π-orbital. No other short intermolecular C–O distances are found.

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Fig. 4. Conformation of the two bromoacetate groups as seen along the C(1)–C(2) and C(30)–C(29) bonds.

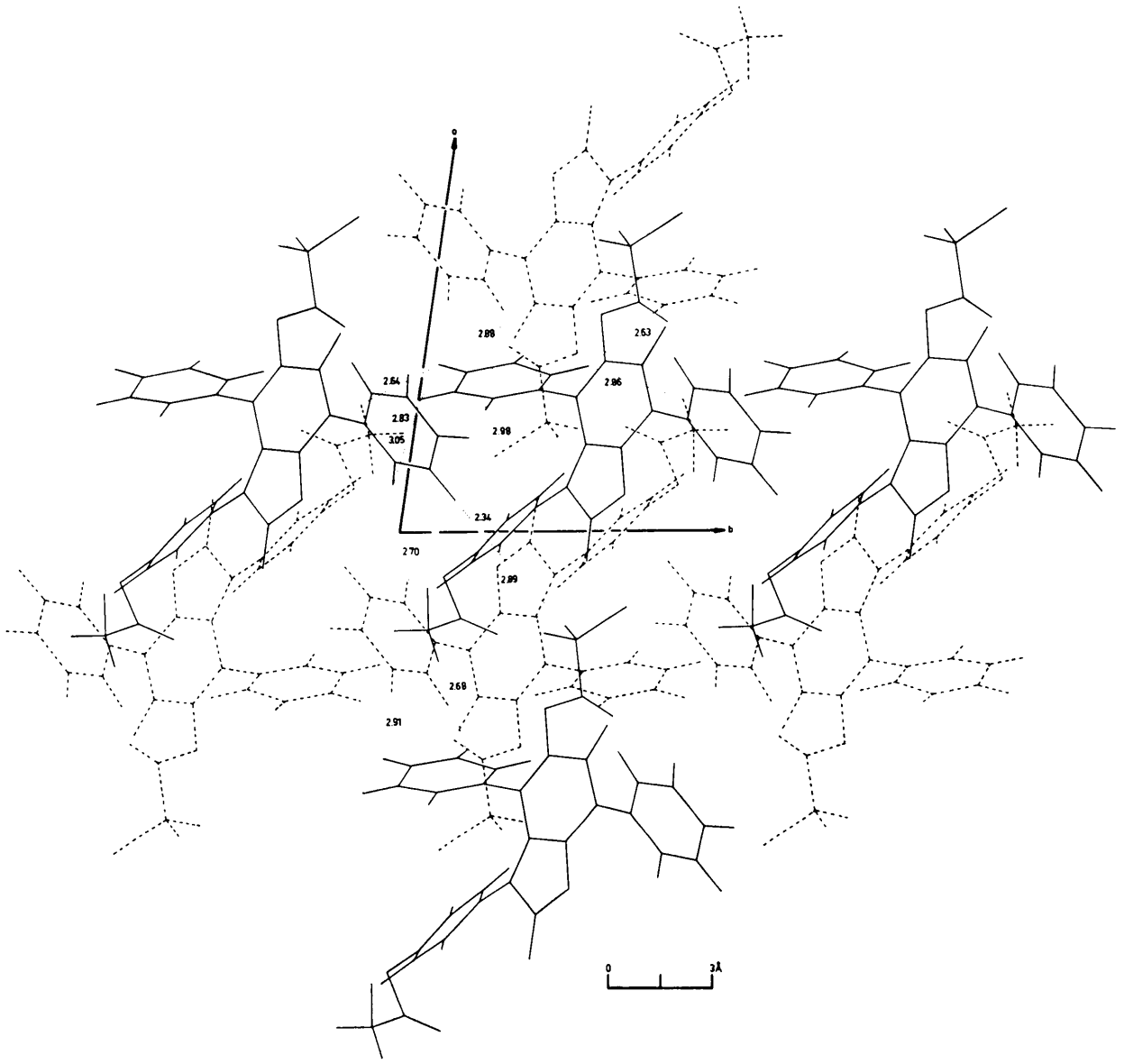

Fig. 5. Molecular packing of xylerythrin bisbromoacetate as seen along the *c* axis. Dashed lines belong to symmetry-related molecules. Some short intermolecular H–H distances are indicated by dotted lines.

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