Table 3. *Dihedral angles* (°) *between planes* I *and* II
and the carboxylate group, plane —COO—

	I, II	I, —COO—	II, —COO—
Pannarin	123.6	39.2	41.9
Eriodermin	115.0	44.7	45.5
Variolaric acid	120.5	49.8	41.3
2-Chlorounguinol	117.5	42.7	45.5

There is a relatively strong intramolecular hydrogen bond involving the formyl substituent at C(3) and the hydroxyl substituent at C(4); see Table 2 and Fig. 1.

The Cambridge Structural Database (1991, Version 4.20) contains information on five depsidones only; namely, the iodoacetate derivative of vicanicin, nidulin (McMillan, 1964), eriodermin (Connolly, Freer, Kalb & Huneck, 1984), the diacetate derivative of variolaric acid (Brassy, Bodo & Molho, 1977), and 2-chlorounguinol monohydrate (Kawahara, Nakajima, Satoh, Yamazaki & Kawai, 1988). Atomic coordinates were available for the last three only and showed the bond lengths and angles in rings I and II and the heterocycle to be very similar to those in pannarin. The overall conformations of eriodermin and 2-chlorounguinol are very similar, but different to those in variolaric acid and pannarin as shown in Table 3.

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Structure and Coloration of 1,1'-Spirobiindan-4,4',7,7'-tetrol

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Abstract. Mo $K\alpha$, $\lambda = 0.71073$ Å. Dihydrate, (I), $C_{17}H_{16}O_4.2H_2O$, $M_r = 320.33$, monoclinic, $I2/a$, $a = 14.371$ (2), $b = 10.229$ (2), $c = 10.469$ (1) Å, $\beta = 99.44$ (1)°, $V = 1518.1$ (4) Å^3, $Z = 4$, D_m (CH_2Cl_2/ CCl_4) = 1.40 (2), $D_x = 1.40$ Mg m^{-3}, $\mu = 0.099$ mm^{-1}, $F(000) = 680$, $T = 297$ (2) K, $R = 0.044$ for 926 unique reflections. Monohydrate, (II), $C_{17}H_{16}O_4.H_2O$, $M_r = 302.31$, monoclinic, $P2_1/c$, $a = 10.562$ (2), $b = 13.131$ (2), $c = 9.921$ (2) Å, $\beta = 91.13$ (1)°, $V = 1375.7$ (4) Å^3, $Z = 4$, $D_x = 1.46$ Mg m^{-3}, $\mu = 0.100$ mm^{-1}, $F(000) = 640$, $T = 120$ (2) K, $R = 0.049$ for 2268 unique reflections. Sesquidioxane solvate, (III), $C_{17}H_{16}O_4.1.5C_4H_8O_2$, $M_r = 416.45$, triclinic, $P\bar{1}$, $a = 9.351$ (1), $b = 12.394$ (1), $c =$

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9·338 (1) Å, $\alpha = 108·79$ (1), $\beta = 93·80$ (1), $\gamma = 85·08$ (1)°, $V = 1019·9$ (2) Å^3, $Z = 2$, $D_x = 1·36$ Mg m^{-3}, $\mu = 0·093$ mm^{-1}, $F(000) = 444$, $T = 120$ (2) K, $R = 0·053$ for 2197 unique reflections. Crystals of (I) are deep blue and have stacking of the hydroquinone moieties with an interplanar distance of 3·25 Å. Such a π–π close contact does not exist in the pale-yellow crystals of (II) and (III). The coloration of (I) seems to be due to an excimer fluorescence.

Introduction. The title compound was synthesized by the rearrangement of 2,2'-spirobichroman derivatives. Unexpectedly, deep-blue crystals, (I), were grown from ether–benzene (1:5) in the ambient atmosphere. Formation of radicals or of a quinoid structure were not detected by the ESR and ^{1}H NMR spectra (Tanaka, 1980; Tanaka, Miyaguchi, Mochisuki, Tanaka, Okamoto, Kitajima & Miyazaki, 1987). On the other hand, pale-yellow crystals, (II) and (III), were grown from anhydrous ether–benzene or ether–dioxane solution. Crystal structure analyses have been performed to investigate the mechanism of the coloration.

Experimental. Crystals of (II) are slightly hygroscopic and gradually change from pale yellow to deep blue in the air. Specimens of (II) and (III) were maintained at 120 K with a stream of cold nitrogen gas in order to keep them dry. X-ray intensity data were collected on a Rigaku AFC-5 four-circle diffractometer with Mo $K\alpha$ radiation monochromatized by a graphite plate. ω–2θ scan. Cell parameters were refined by least squares for 26–46 2θ values ($20 < 2\theta < 30°$). No absorption correction. Structures were solved using MULTAN78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). All H atoms were found from difference syntheses. Positional parameters of all atoms, anisotropic thermal parameters of non-H atoms and isotropic thermal parameters of H atoms were refined by block-diagonal least squares, $\Sigma w||F_o| - |F_c||^2$ minimized, $w^{-1} = \sigma^2(|F_o|) + (0·015|F_o|)^2$. Complex neutral-atom scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). Calculations were carried out on a FACOM M-380R computer at Keio University using UNICSIII computation program system (Sakurai & Kobayashi, 1979). Atomic coordinates are listed in Table 1,* bond lengths and bond angles

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* Lists of structure factors, anisotropic thermal parameters, atomic parameters for H atoms, bond lengths and bond angles, and projections of the crystal structures of (II) and (III) have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54326 (62 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

of (I) in Table 2. Experimental details are given below.

(I): Deep-blue prismatic crystal, $0·30 \times 0·20 \times 0·20$ mm. Intensity measurement performed up to $2\theta = 50°$ ($h - 15 \rightarrow 15$, $k - 11 \rightarrow 11$, $l\ 0 \rightarrow 11$ for $4 < 2\theta \leq 45°$; $h - 17 \rightarrow 17$, $k\ 0 \rightarrow 13$, $l\ 0 \rightarrow 13$ for $45 < 2\theta \leq 50°$). Variation of $|F_o|$ of five standard reflections, $0·990 < \Sigma(|F_o|/|F_o|_{initial})/5 < 1·002$. 2759 reflections measured, 2026 observed with $|F_o| > 3\sigma(|F_o|)$, 926 unique ($R_{int} = 0·013$). Systematic absences ($h + k + l = 2n + 1$ for hkl and $h, l = 2n + 1$ for $h0l$) indicated either space groups Ia (noncentrosymmetric) or $I2/a$ (centrosymmetric). In this case, the I-centered unit cell is preferred to the standard C-centered one to make β close to 90°. Assuming a twofold symmetry of the molecule, a successful refinement confirmed $I2/a$ [$(c, b, -a - c)$ setting of $C2/c$] as the correct space group. The water molecule lies near the twofold axis and forms a hydrogen bond with its symmetry-related molecule:
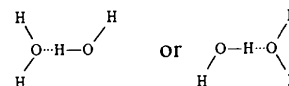
Therefore, one of the H atoms of the water molecule takes two possible positions with an occupancy factor of 0·5. The disordered H atoms were located from the difference Fourier map. $R = 0·044$, $wR = 0·052$, $S = 2·4$ for 926 unique reflections. Reflection/ parameter ratio 6·2, $\Delta/\sigma = 0·38$, $-0·33 < \Delta\rho < 0·18$ e Å^{-3}. (II): A pale-yellow prismatic crystal, $0·40 \times 0·30 \times 0·30$ mm. $2\theta_{max} = 55°$ ($h\ 0 \rightarrow 13$, $k - 17 \rightarrow 17$, $l - 12 \rightarrow 12$). $0·993 < \Sigma(|F_o|/|F_o|_{initial})/5 < 1·009$. 6506 reflections measured, 4496 observed, [$|F_o| > 3\sigma(|F_o|)$], 2268 unique ($R_{int} = 0·019$). Space group, $P2_1/c$, was unambiguously determined from the systematic absences, $h0l$, l odd; $0k0$, k odd. $R = 0·049$, $wR = 0·054$, $S = 2·2$ for 2268 unique reflections. Reflection/parameter ratio 8·3, $\Delta/\sigma = 0·27$, $-0·40 < \Delta\rho < 0·59$ e Å^{-3}. (III): A pale-yellow prismatic crystal, $0·30 \times 0·20 \times 0·15$ mm. $2\theta_{max} = 55°$ ($h - 12 \rightarrow 12$, $k - 16 \rightarrow 16$, $l\ 0 \rightarrow 12$). $0·997 < \Sigma(|F_o|/ |F_o|_{initial})/5 < 1·006$. No absorption correction. 4964 reflections measured, 2341 observed, [$|F_o| > 3\sigma(|F_o|)$], 2197 unique ($R_{int} = 0·022$). The normalized structure-factor statistics favored the centrosymmetric space group, $P\bar{1}$, which was confirmed by the subsequent refinement. $R = 0·053$, $wR = 0·045$, $S = 1·3$ for 2197 unique reflections. Reflection/parameter ratio 5·7, $\Delta/\sigma = 0·27$, $-0·27 < \Delta\rho < 0·29$ e Å^{-3}. One of the dioxane molecules lies on a general position and the other at the center of symmetry.

Discussion. Molecular structures are shown in Fig. 1. There is no evidence for the quinoid structure of the

Table 1. *Atomic positional and equivalent isotropic displacement parameters*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{eq}(\text{Å}^2)$
(I)				
O(1)	−0·06235 (8)	−0·1758 (1)	0·0927 (1)	0·0305
O(2)	0·28817 (9)	0·0628 (1)	0·1809 (1)	0·0427
C(1)	¼	−0·1720 (3)	0	0·0359
C(2)	0·1813 (1)	−0·2565 (2)	−0·0968 (2)	0·0315
C(3)	0·0921 (1)	−0·2746 (2)	−0·0355 (2)	0·0294
C(4)	0·0225 (1)	−0·1120 (2)	0·1144 (2)	0·0356
C(5)	0·0391 (1)	−0·0048 (2)	0·1958 (2)	0·0384
C(6)	0·1269 (1)	−0·0545 (2)	0·2153 (2)	0·0423
C(7)	0·1995 (1)	0·0075 (2)	0·1553 (2)	0·0275
C(8)	0·1825 (1)	−0·0980 (2)	0·0708 (2)	0·0328
C(9)	0·0944 (1)	−0·1578 (2)	0·0520 (2)	0·0342
O(W)	−0·1701 (1)	−0·3645 (2)	−0·0685 (2)	0·0803
H(O1)	−0·113 (1)	−0·124 (2)	0·128 (2)	0·095
H(O2)	0·304 (1)	0·093 (2)	0·276 (3)	0·122
O(OW)1	−0·117 (2)	−0·306 (2)	−0·021 (2)	0·122
H(OW)2a*	−0·216 (3)	−0·367 (5)	−0·009 (7)	0·143
H(OW)2b*	−0·206 (3)	−0·289 (4)	−0·097 (5)	0·089
(II)				
O(1)	0·8563 (2)	0·1802 (1)	0·3378 (2)	0·0224
O(2)	0·9093 (2)	0·5875 (1)	0·1928 (2)	0·0266
O(3)	0·7330 (2)	0·8924 (1)	0·4857 (2)	0·0308
O(4)	0·5490 (2)	0·5512 (1)	0·2126 (2)	0·0252
C(1)	0·7505 (2)	0·5296 (2)	0·4321 (2)	0·0216
C(2)	0·6583 (2)	0·4553 (2)	0·5004 (2)	0·0278
C(3)	0·7212 (2)	0·3498 (2)	0·4942 (2)	0·0222
C(4)	0·8638 (2)	0·2818 (2)	0·3012 (2)	0·0166
C(5)	0·9423 (2)	0·3078 (2)	0·1956 (2)	0·0212
C(6)	0·9571 (2)	0·4092 (2)	0·1591 (2)	0·0220
C(7)	0·8935 (2)	0·4855 (2)	0·2271 (2)	0·0191
C(8)	0·8135 (2)	0·4598 (2)	0·3314 (2)	0·0169
C(9)	0·7995 (2)	0·3578 (2)	0·3693 (2)	0·0165
C(10)	0·8563 (3)	0·5738 (2)	0·5300 (3)	0·0381
C(11)	0·8253 (2)	0·6839 (2)	0·5582 (2)	0·0215
C(12)	0·6831 (2)	0·8073 (2)	0·4198 (2)	0·0204
C(13)	0·5902 (2)	0·8186 (2)	0·3205 (2)	0·0223
C(14)	0·5442 (2)	0·7332 (2)	0·2515 (2)	0·0227
C(15)	0·5918 (2)	0·6367 (2)	0·2804 (2)	0·0201
C(16)	0·6858 (2)	0·6260 (2)	0·3803 (2)	0·0192
C(17)	0·7289 (2)	0·7114 (2)	0·4511 (2)	0·0188
O(W)	0·3474 (2)	0·9109 (1)	0·5276 (2)	0·0285
H(O1)	0·796 (3)	0·164 (2)	0·389 (3)	0·065
H(O2)	0·920 (4)	0·623 (3)	0·240 (4)	0·114
H(O3)	0·684 (5)	0·964 (4)	0·482 (5)	0·168
H(O4)	0·490 (3)	0·566 (2)	0·142 (3)	0·052
H(OW)1	0·360 (3)	0·887 (2)	0·439 (3)	0·061
H(OW)2	0·305 (3)	0·957 (2)	0·508 (3)	0·066
(III)				
O(1)	0·4906 (2)	0·9045 (2)	0·7800 (3)	0·0286
O(2)	−0·0353 (2)	0·7950 (2)	1·0648 (3)	0·0258
O(3)	−0·2636 (2)	0·3630 (2)	0·7540 (3)	0·0253
O(4)	−0·1765 (2)	0·7889 (2)	0·7095 (3)	0·0260
C(1)	0·0752 (3)	0·6335 (3)	0·7725 (4)	0·0180
C(2)	0·1362 (3)	0·6156 (3)	0·6141 (4)	0·0175
C(3)	0·2671 (3)	0·6873 (3)	0·6443 (4)	0·0217
C(4)	0·2971 (3)	0·8839 (3)	0·8550 (4)	0·0205
C(5)	0·2489 (4)	0·9579 (3)	0·9917 (4)	0·0230
C(6)	0·1386 (3)	0·9298 (3)	1·0629 (4)	0·0213
C(7)	0·0743 (3)	0·8264 (3)	0·9991 (4)	0·0201
C(8)	0·1216 (3)	0·7526 (3)	0·8611 (4)	0·0175
C(9)	0·2319 (3)	0·7814 (3)	0·7894 (4)	0·0184
C(10)	0·1396 (3)	0·5420 (3)	0·8437 (4)	0·0202
C(11)	0·0346 (3)	0·4457 (3)	0·7947 (4)	0·0212
C(12)	−0·2447 (3)	0·4698 (3)	0·7437 (4)	0·0195
C(13)	−0·3573 (3)	0·5380 (3)	0·7081 (4)	0·0210
C(14)	−0·3334 (3)	0·6449 (3)	0·6976 (4)	0·0213
C(15)	−0·1965 (3)	0·6832 (3)	0·7224 (4)	0·0188
C(16)	−0·0835 (3)	0·6142 (3)	0·7573 (3)	0·0148
C(17)	−0·1061 (3)	0·5081 (3)	0·7681 (4)	0·0182
O(71)	0·5540 (3)	0·8743 (2)	0·1769 (3)	0·0374
C(72)	0·5298 (5)	0·7684 (3)	0·0618 (4)	0·0407
C(73)	0·6047 (5)	0·6710 (3)	0·1054 (5)	0·0473
O(74)	0·5554 (3)	0·6699 (2)	0·2469 (3)	0·0351
C(75)	0·5809 (6)	0·7753 (4)	0·3606 (5)	0·0642
C(76)	0·5031 (6)	0·8721 (3)	0·3149 (5)	0·0603
O(81)	0·0632 (3)	0·0736 (2)	0·6334 (3)	0·0306
C(82)	−0·0507 (4)	0·1147 (3)	0·5490 (4)	0·0337
C(83)	−0·1452 (4)	0·0205 (3)	0·4672 (4)	0·0305
H(O1)	0·438 (4)	0·979 (3)	0·837 (5)	0·084

Table 1 (*cont.*)

	x	y	z	$U_{eq}(\text{Å}^2)$
H(O2)	−0·055 (4)	0·847 (3)	1·158 (4)	0·054
H(O3)	−0·363 (4)	0·356 (3)	0·736 (4)	0·070
H(O4)	−0·102 (4)	0·826 (3)	0·760 (4)	0·056

* Population parameters of the disordered H atoms = 0·5.

Table 2. *Bond distances (Å) and angles (°) for* (I)

O(1)—C(4)	1·368 (2)	C(4)—C(5)	1·385 (3)
O(2)—C(7)	1·380 (2)	C(4)—C(9)	1·392 (3)
C(1)—C(2)	1·556 (2)	C(5)—C(6)	1·384 (3)
C(1)—C(8)	1·517 (2)	C(6)—C(7)	1·389 (3)
C(2)—C(3)	1·536 (3)	C(7)—C(8)	1·391 (3)
C(3)—C(9)	1·503 (3)	C(8)—C(9)	1·391 (2)

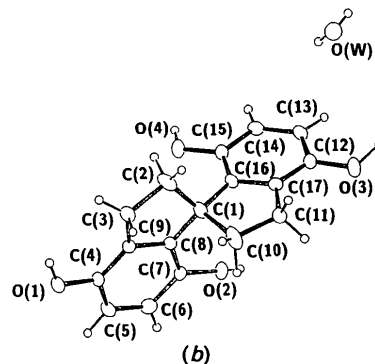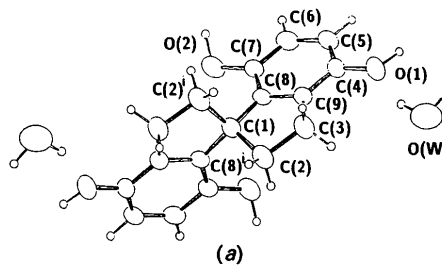|			
C(2)—C(1)—C(8)	102·0 (1)	C(5)—C(6)—C(7)	121·0 (2)
C(2)—C(1)—C(2ⁱ)	112·5 (2)	O(2)—C(7)—C(6)	120·6 (2)
C(8)—C(1)—C(2ⁱ)	110·3 (1)	O(2)—C(7)—C(8)	120·1 (2)
C(8)—C(1)—C(8ⁱ)	120·1 (2)	C(6)—C(7)—C(8)	119·3 (2)
C(1)—C(2)—C(3)	106·2 (1)	C(1)—C(8)—C(7)	129·7 (1)
C(2)—C(3)—C(9)	102·9 (2)	C(1)—C(8)—C(9)	110·6 (1)
O(1)—C(4)—C(5)	122·6 (2)	C(7)—C(8)—C(9)	119·5 (2)
O(1)—C(4)—C(9)	118·1 (2)	C(3)—C(9)—C(4)	127·7 (2)
C(5)—C(4)—C(9)	119·3 (2)	C(3)—C(9)—C(8)	111·4 (2)
C(4)—C(5)—C(6)	119·9 (2)	C(4)—C(9)—C(8)	120·9 (2)

Symmetry code: (i) ½ − x, y, − z.
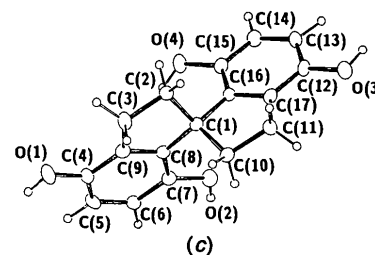
Fig. 1. *ORTEP* (Johnson, 1971) drawing of the molecular structures of (*a*) (I), (*b*) (II) and (*c*) (III) with numbering schemes. Thermal ellipsoids at 50% probability. H atoms not to scale.

phenyl groups in accord with the NMR spectra of the $CDCl_3$ solution (Tanaka, 1980). The C—C bond distances in the phenyl rings range from 1·382 (4) to 1·400 (4) Å. Furthermore, the H atoms of the hydroxy groups were observed by difference synthesis and the C—O bond lengths are 1·367 (2)–1·393 (3) Å. The C—O bond lengths are in good agreement with those reported for the α-modification of hydroquinone, 1·371 (5)–1·384 (4) Å (Wallwork & Powell, 1980). The tendency of phenols to have the C—C—OH bond angle larger on the hydrogen side (Hirshfeld, 1964) is also observed.
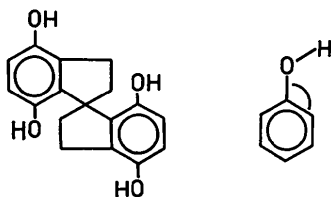
The dihedral angles between the two phenyl groups are (I) 75·92 (7), (II) 83·45 (7) and (III) 73·7 (1)°. The larger dihedral angle of (II) results from a flattened form of one of the five-membered rings. The magnitude of the torsion angle C(1)—C(10)—C(11)—C(17) is − 15·5 (2)°, which is smaller than that of C(1)—C(2)—C(3)—C(9) in (II) [− 28·6 (2)°] and the corresponding angles in (I) [+ 24·9 (2)°] and (III) [−25·6 (3), − 27·4 (3)°]. The

molecular conformation in the colored crystal, (I), is essentially identical with those in the pale-yellow crytals of (II) and (III), despite crystallographic twofold symmetry in (I). Thus the origin of the coloring of (I) cannot be attributed to the molecular structure.

The crystal structure of (I) is illustrated in Fig. 2(a). Stacking of the π-electron systems is observed in (I). As shown in Fig. 2(b), a hydroxy group of one molecule lies above the phenyl ring of the neighboring molecule. The adjacent hydroquinone groups are related by a center of symmetry and are parallel to each other. The interplanar distance is 3·25 Å and the closest C···C distance is 3·301 (4) Å, which is significantly shorter than the van der Waals contact of 3·54 Å for the aromatic rings (Bondi, 1964). A similar stacking mode with ring-over-bond overlap is also observed in charge-transfer complexes, α-quinhydrone and phenoquinone (Sakurai, 1968), which have the interplanar distances of 3·22 and 3·13 Å, respectively. The stacking of the hydroquinone groups in (I) is supported by an intermolecular O—H···O hydrogen bond with an O(1)···O(2)($-\frac{1}{2}$ + x, − y, z) distance of 2·730 (2) Å. As a result, infinite chains are constructed along the a axis as shown in Fig. 2(a). Crystals of (I) are deep blue and have π–π close contact. The color may be explained by an excimer fluorescence (Azumi & McGlynn, 1964; Azumi, Armstrong & McGlynn, 1964).
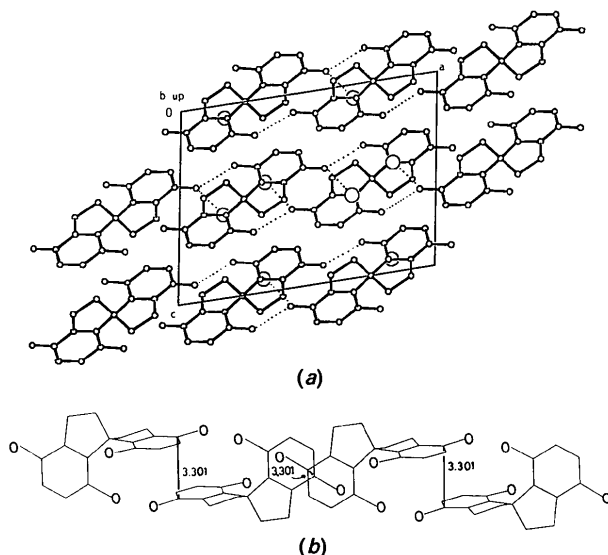
(a)

(b)

Fig. 2. (a) Projection of the crystal structure of (I) along the b axis. The larger circles represent water molecules. (b) Stacking diagram and interatomic distances (Å) of the hydroquinone groups in (I).

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