Table 2. *Selected bond lengths* (Å) *and angles* (°) *in* $C_{17}H_{14}NP$

Ring *A*		Ring *B*		Ring *C*	
P–C1	1·824 (2)	P–C7	1·824 (2)	P–C13	1·837 (3)
C1–C2	1·381 (4)	C7–C8	1·381 (4)	C13–C14	1·375 (4)
C2–C3	1·379 (5)	C8–C9	1·394 (4)	C14–C15	1·373 (5)
C3–C4	1·361 (7)	C9–C10	1·362 (7)	C15–C16	1·363 (5)
C4–C5	1·361 (6)	C10–C11	1·357 (7)	C16–C17	1·363 (6)
C5–C6	1·378 (5)	C11–C12	1·373 (5)	C17–N18	1·324 (5)
C6–C1	1·382 (4)	C12–C7	1·380 (4)	N18–C13	1·342 (3)
C1–C2–C3	120·9 (3)	C7–C8–C9	120·2 (3)	C13–C14–C15	119·5 (3)
C2–C3–C4	119·9 (3)	C8–C9–C10	120·5 (4)	C14–C15–C16	119·3 (3)
C3–C4–C5	120·5 (3)	C9–C10–C11	119·7 (3)	C15–C16–C17	117·7 (3)
C4–C5–C6	119·7 (4)	C10–C11–C12	120·3 (4)	C16–C17–N18	124·8 (3)
C5–C6–C1	121·1 (3)	C11–C12–C7	121·5 (4)	C17–N18–C13	116·8 (3)
C6–C1–C2	117·9 (3)	C12–C7–C8	117·8 (3)	N18–C13–C14	121·9 (3)
C2–C1–P	118·2 (2)	C8–C7–P	125·6 (2)	C14–C13–P	126·2 (2)
C6–C1–P	123·9 (2)	C12–C7–P	116·6 (2)	N18–C13–P	111·9 (2)
C1–P–C7	104·5 (1)	C7–P–C13	101·9 (1)	C13–P–C1	99·8 (1)

	Range	Average*
<C–H>	0·83 (3)–0·99 (3)	0·93[4]
<C–C–H>	115·7(2)–123·8(2)	120[3]

Shortest intermolecular contacts (excluding H···H)†

N18···C16′	3·627 (5)	N18···H16′	3·26 (3)

* Standard deviation on average value calculated as:
$\sigma(\bar{x}) = [\sum_{i=1}^{n} (x_i - \bar{x})^2/(n-1)]^{1/2}$.

† Atom $X(x, y, z) \rightarrow$ atom X' ($\frac{3}{2}-x, y-\frac{1}{2}, \frac{1}{2}-z$).

angles are given in Table 2.* The numbering scheme is given in Fig. 1.

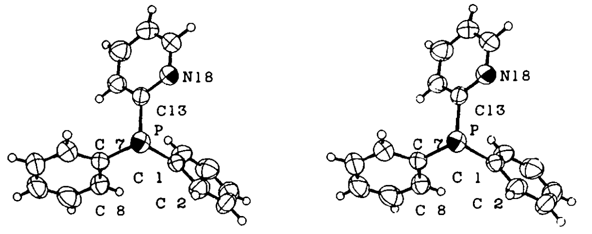

Fig. 1. Stereoview of $C_{17}H_{14}NP$ (50% boundary ellipses are shown).

Related literature. This study was aimed at providing structural data on the title compound, thus allowing for a comparison between the free ligand and its liganded states in which a Co/NO metallic fragment is attached to the N and/or P donor sites of the molecule (Roustan, Ansari & Ahmed, 1987).

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Structure of 5-Hydroxy-7,4′-dimethoxyflavanone

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Abstract. 5-Hydroxy-7-methoxy-2-(4-methoxyphenyl)chroman-4-one, $C_{17}H_{16}O_5$, $M_r = 300·3$, monoclinic, $C2/c$, $a = 17·38$ (2), $b = 5·321$ (4), $c = 30·74$ (3) Å, $\beta = 98·27$ (7)°, $V = 2814$ (4) Å^3, $Z = 8$, $D_x = 1·42$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0·7107$ Å, $\mu = 0·6$ cm^{-1}, $F(000) = 1264$, $T = 173$ K, $R = 0·0696$ for 1024 observed reflections with $I > 2\sigma(I)$. Lattice sites are occupied randomly by 2*R* or 2*S* isomers leading to partial disorder. The pyranone ring has a sofa conformation and the dihedral angle between the aromatic *A* and *B* rings is 70·8 (2)°. The hydrogen of the 5-hydroxy group is intramolecularly hydrogen-bonded to the carbonyl group.

Experimental. White needle-shaped crystals, m.p. 391 K, from an earlier study (Miles & Main, 1985), recrystallized from methanol. Space group defined by precession photography as *C*2/*c* or *Cc*, the former

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Table 1. *Final positional and equivalent isotropic thermal parameters for 5-hydroxy-7,4′-dimethoxyflavanone*

	x	y	z	U_{eq}(Å^2)*
O(1)	0·1461 (2)	0·0241 (9)	0·8358 (1)	0·058
C(2′)	0·1285 (7)	−0·196 (3)	0·8123 (4)	0·041
C(2″)	0·0890 (7)	−0·086 (3)	0·8055 (4)	0·034
C(3)	0·0563 (4)	−0·327 (1)	0·8184 (2)	0·047
C(4)	0·0361 (4)	−0·311 (1)	0·8635 (2)	0·044
O(4)	−0·0130 (2)	−0·4588 (9)	0·8754 (1)	0·060
C(5)	0·0572 (4)	−0·080 (1)	0·9351 (2)	0·049
O(5)	0·0047 (3)	−0·234 (1)	0·9507 (1)	0·063
C(6)	0·0918 (4)	0·105 (1)	0·9622 (2)	0·048
C(7)	0·1462 (4)	0·256 (1)	0·9453 (2)	0·047
O(7)	0·1850 (3)	0·4459 (9)	0·9694 (1)	0·062
C(71)	0·1679 (4)	0·493 (1)	1·0125 (2)	0·061
C(8)	0·1652 (4)	0·226 (1)	0·9035 (2)	0·048
C(9)	0·1284 (3)	0·042 (1)	0·8774 (2)	0·043
C(10)	0·0738 (3)	−0·118 (1)	0·8923 (2)	0·040
C(11)	0·1288 (5)	−0·120 (2)	0·7637 (2)	0·077
C(12)	0·1724 (4)	−0·298 (2)	0·7458 (2)	0·067
C(13)	0·1871 (4)	−0·277 (2)	0·7031 (2)	0·054
C(14)	0·1577 (3)	−0·076 (1)	0·6773 (2)	0·043
O(14)	0·1764 (2)	−0·0757 (9)	0·6358 (1)	0·060
C(141)	0·1495 (4)	0·133 (2)	0·6086 (2)	0·072
C(15)	0·1146 (4)	0·110 (2)	0·6935 (2)	0·055
C(16)	0·1014 (4)	0·083 (2)	0·7373 (3)	0·069
H(5)	−0·009 (3)	−0·40 (1)	0·921 (2)	0·060

* U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table 2. *Bond lengths* (Å) *and angles* (°) *for 5-hydroxy-7,4′-dimethoxyflavanone*

O(1)—C(2′)	1·39 (1)	C(7)—C(8)	1·380 (8)
O(1)—C(2′)	1·39 (1)	O(7)—C(71)	1·419 (7)
O(1)—C(9)	1·362 (7)	C(8)—C(9)	1·369 (8)
C(2′)—C(3)	1·47 (1)	C(9)—C(10)	1·399 (8)
C(2′)—C(11)	1·55 (1)	C(11)—C(12)	1·38 (1)
C(3)—C(4)	1·483 (8)	C(11)—C(16)	1·39 (1)
C(4)—O(4)	1·251 (7)	C(12)—C(13)	1·377 (9)
C(4)—C(10)	1·450 (8)	C(13)—C(14)	1·387 (9)
C(5)—O(5)	1·364 (7)	C(14)—O(14)	1·360 (6)
C(5)—C(6)	1·372 (8)	C(14)—C(15)	1·376 (9)
C(5)—C(10)	1·400 (8)	O(14)—C(141)	1·430 (7)
C(6)—C(7)	1·396 (8)	C(15)—C(16)	1·407 (9)
C(7)—O(7)	1·372 (7)	O(5)—H(5)	1·27 (6)
		O(4)—H(5)	1·42 (6)
C(2′)—O(1)—C(9)	118·9 (7)	C(8)—C(9)—C(10)	121·8 (6)
C(2′)—O(1)—C(9)	114·9 (6)	C(4)—C(10)—C(5)	122·6 (6)
C(2′)—C(3)—C(4)	114·4 (7)	C(4)—C(10)—C(9)	120·0 (6)
C(2′)—C(3)—C(4)	110·7 (7)	C(5)—C(10)—C(9)	117·4 (6)
C(3)—C(4)—O(4)	120·1 (6)	C(2)—C(11)—C(12)	106 (1)
C(3)—C(4)—C(10)	117·7 (6)	C(2)—C(11)—C(12)	138 (1)
O(4)—C(4)—C(10)	122·2 (6)	C(2)—C(11)—C(16)	135 (1)
O(5)—C(5)—C(6)	118·3 (6)	C(2)—C(11)—C(16)	103·6 (9)
O(5)—C(5)—C(10)	118·9 (6)	C(12)—C(11)—C(16)	117·7 (7)
C(6)—C(5)—C(10)	122·8 (6)	C(11)—C(12)—C(13)	120·9 (8)
C(5)—C(6)—C(7)	116·7 (6)	C(12)—C(13)—C(14)	120·3 (7)
C(6)—C(7)—O(7)	122·0 (6)	C(13)—C(14)—O(14)	114·7 (6)
C(6)—C(7)—C(8)	123·0 (6)	C(13)—C(14)—C(15)	121·4 (6)
O(7)—C(7)—C(8)	114·9 (6)	O(14)—C(14)—C(15)	123·8 (6)
C(7)—O(7)—C(71)	118·7 (5)	C(14)—O(14)—C(141)	116·5 (5)
C(7)—C(8)—C(9)	118·2 (6)	C(14)—C(15)—C(16)	116·6 (7)
O(1)—C(9)—C(8)	116·7 (6)	C(11)—C(16)—C(15)	123·1 (8)
O(1)—C(9)—C(10)	121·4 (6)	O(4)—H(5)—O(5)	148 (5)

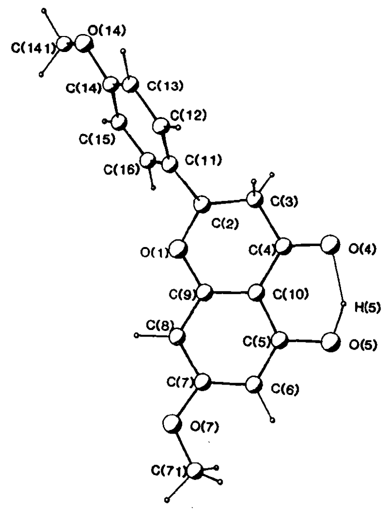
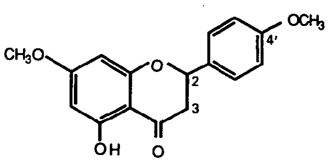


Fig. 1. *PLUTO* (Motherwell & Clegg, 1978) diagram of 5-hydroxy-7,4′-dimethoxyflavanone. Only one of the disordered [at C(2)] molecules is shown and the H atom on C(2) is not included.

being assigned on the basis of E statistics and the successful refinement. Cell constants (from 20 reflections, $\theta > 20°$) and data collection on a Nicolet XRD $P3$ four-circle diffractometer with graphite-monochromated Mo $K\alpha$ radiation. A total of 2044 reflections, 1755 unique ($R_{\rm int} = 0{\cdot}018$) using ω-scans, with $0 < h < 19$, $0 < k < 6$, $-36 < l < 34$, $3 < 2\theta < 45°$; 1024 data with $I > 2\sigma(I)$ used in the refinement. No crystal deterioration (three standards). No absorption correction. Structure solved by direct methods. C(2) would not refine as a single atom so was treated as two half-weighted carbon atoms, 0·91 (1) Å apart; the disorder arises through both enantiomers [differing in configuration at C(2)] randomly occupying each lattice site. The disorder had little effect on the rest of the molecule, being accommodated by a small rotation of the phenyl ring and a twisting of the CH_2 group at C(3) about the C(3)—C(4) vector. [Refinement was also attempted in space group Cc, with two independent molecules, but atoms converged to centrosymmetric positions without removing the disorder at C(2) so $C2/c$ was assumed to be correct.] Structure refined by full-matrix least squares (211 parameters), with all non-hydrogen atoms anisotropic except the disordered C(2). The hydroxyl hydrogen H(5) was clearly revealed as the highest peak in a penultimate difference map and was refined with a fixed temperature factor, while other hydrogen atoms were included in calculated positions with common isotropic temperature factors, except for those attached to C(2) and C(3) which were omitted because of disorder. Function minimized was $\sum w(\Delta F)^2$. At convergence $R = 0{\cdot}0696$, $wR = 0{\cdot}0711$ where $w^{-1} = [\sigma^2 F + 0{\cdot}0008F^2]$, max. Δ/σ 0·03, final ΔF map peaks $< | 0{\cdot}3 |$ e Å^{-3}. Scattering factors were those included in *SHELX*76 (Sheldrick, 1976), which was used for all calculations. Final refined atom coordinates and equivalent isotropic temperature factors are given in Table 1, bond parameters in Table 2 and the structure is illustrated for one enantiomer in Fig. 1.*



Related literature. The structure can be related to those of other flavanone derivatives (Narayanan, Zechmeister, Roehrl & Hoppe, 1971; Mariezcurrena, 1978; Hufford & Lasswell, 1979; Byrne, Cannon, Gawad, Joshi, Skelton, Toia & White, 1982; Cantrell & Hockstein, 1982). The intramolecular hydrogen bonding involving H(5), crystallographically located in the present study for the first time, has little effect on the geometry of the rest of the molecule.

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Structure of the Conducting Salt of Pyrazinoethylenedithiotetrathiafulvalene (PEDTTTF): α-(PEDTTTF)$_2$IBr$_2$, at 98 K

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Abstract. Bis{2-(dithiolo[4,5-*b*]dithiin-2-ylidene)dithiolo-[4,5-*b*]pyrazinium} dibromoiodide, $(C_{10}H_6N_2S_6)_2$-IBr_2, $M_r = 979\cdot86$, triclinic, $P\bar{1}$, $a = 8\cdot850\,(4)$, $b = 5\cdot691\,(2)$, $c = 15\cdot377\,(7)$ Å, $\alpha = 99\cdot04\,(4)$, $\beta = 87\cdot23\,(4)$, $\gamma = 108\cdot35\,(4)^\circ$, $V = 726\cdot0$ Å^3, $Z = 1$, $D_x = 2\cdot237$ g cm^{-3}, Mo $K\bar{\alpha}$, $\lambda = 0\cdot71069$ Å, $\mu = 48\cdot9$ cm^{-1}, $F(000) = 475$, $T = 98$ K. Final $R = 0\cdot077$ for 3879 observed reflections. Packing is similar to that of the room-temperature structure. The disorder of the ethylene group observed at room temperature (RT) has disappeared at 98 K. The planarity of the tetrathiafulvalene moiety is better in the low-temperature (LT) structure with the greatest deviation from the mean plane of this moiety being

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