0·051, $S = 1·72$; $w = 1/\sigma^2(F)$ was calculated from $\sigma^2(I) = \sigma^2(I_c) + (0·04I)^2$, where $\sigma(I_c)$ is the standard deviation in I based on counting statistics alone. $(\Delta/\sigma)_{max}$ in the final cycle was 0·06. $(\Delta\rho)_{max} = 0·17$, $(\Delta\rho)_{min} = -0·13$ e Å^{-3}. The four highest peaks in the final difference Fourier map are near the CH_3 groups suggesting that there is some disorder in their orientations. Atomic scattering factors and anomalous-dispersion corrections for all atoms were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). The computer programs used were from *TEXSAN* (Molecular Structure Corporation, 1985).

Atomic coordinates are given in Table 1 and interatomic distances and angles in Table 2.* The atomic labelling and thermal ellipsoids are shown in Fig. 1.

Related literature. Sen (1969) reported the same space group and unit cell for the title compound, dmp.$\frac{1}{2}H_2O$, although he did not recognize the presence of the water molecule. His experimental density, 1·27 g cm^{-3}, is in excellent agreement with our calculated value. Watson, Galloy, Vögtle & Müller (1984) have reported the structure of the 1/1 complex of dmp with resorcinol. The only other reported structure involving free dmp is that of Zn(dmp)$(CN)_2$.dmp.$3H_2O$ (Monge, Martínez-Ripoll & García-Blanco, 1978). The structure of the dmpH$^+$ ion has been reported in the $FeCl_4^-$ salt (Veidis, Witten, Reiff, Brennan & Garafalo, 1981).

There are also about two dozen structures reported where dmp is a ligand in a metal complex. The most recent of these are Cu(dmp)$(CH_3CN)^+$ (Munakata, Maekawa, Kitagama, Matsuyama & Masuda, 1989), Ru(dmp)$(o\text{-phen})_2^{2+}$ (Ichida, Tachigashiki & Sasaki, 1989) and Cu(dmp)$(CN)_2^-$ (Ogura, Shemish, Scott, Pyrka & Fernando, 1988).

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* Lists of anisotropic thermal parameters, H-atom parameters, intermolecular distances, least-squares planes, and observed and calculated structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53642 (27 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of 7-Methoxy-2-(2-methoxyphenyl)-4*H*-1-benzopyran-4-one (2′,7-Dimethoxyflavone)

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Abstract. $C_{17}H_{14}O_4$, $M_r = 282·30$, monoclinic, $P2_1/c$, $a = 12·498$ (4), $b = 9·490$ (2), $c = 12·184$ (2) Å, $\beta = 107·87$ (2)°, $V = 1375·4$ (6) Å^3, $Z = 4$, $D_x = 1·36$ g cm^{-3}, Cu $K\alpha$, $\lambda = 1·54178$ Å, $\mu = 7·98$ cm^{-1}, $F(000) = 592$, $T = 291$ K, $R = 0·042$ for 1848 observed reflections. The benzopyran heterocycle is

0108-2701/91/051103-03$03.00

Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* (Å^2)

$$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
O1	2914 (1)	2343 (2)	2683 (1)	3·24 (2)
C2	2134 (2)	2379 (2)	1613 (2)	2·94 (3)
C3	2301 (2)	1703 (2)	709 (2)	3·47 (3)
C4	3317 (2)	917 (2)	807 (2)	3·43 (3)
C5	5203 (2)	298 (2)	2183 (2)	3·75 (4)
C6	5964 (2)	378 (2)	3252 (2)	3·96 (4)
C7	5707 (2)	1112 (2)	4139 (2)	3·46 (3)
C8	4675 (2)	1769 (2)	3935 (2)	3·37 (3)
C9	3915 (2)	1666 (2)	2833 (2)	2·99 (3)
C10	4145 (2)	939 (2)	1945 (2)	3·18 (3)
O11	3472 (1)	286 (2)	−18 (1)	5·13 (3)
O12	6532 (1)	1134 (2)	5163 (1)	4·43 (3)
C13	6371 (2)	1977 (3)	6065 (2)	4·74 (5)
C1′	1176 (2)	3276 (2)	1627 (2)	3·03 (3)
C2′	104 (2)	3145 (2)	811 (2)	3·33 (3)
C3′	−745 (2)	4066 (3)	849 (2)	4·10 (4)
C4′	−551 (2)	5102 (3)	1670 (2)	4·93 (5)
C5′	485 (2)	5235 (3)	2482 (2)	4·85 (5)
C6′	1341 (2)	4319 (3)	2466 (2)	3·77 (4)
O7′	−49 (1)	2088 (2)	34 (1)	4·62 (3)
C8′	−1149 (2)	1859 (4)	−732 (3)	5·85 (6)

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

C2—O1	1·368 (2)	C9—O1	1·368 (2)
C3—C2	1·345 (3)	C1′—C2	1·474 (3)
C4—C3	1·445 (3)	C10—C4	1·454 (3)
O11—C4	1·236 (3)	C6—C5	1·360 (3)
C10—C5	1·403 (3)	C7—C6	1·404 (3)
C8—C7	1·385 (3)	O12—C7	1·352 (2)
C9—C8	1·390 (3)	C10—C9	1·385 (3)
C13—O12	1·423 (3)	C2′—C1′	1·407 (3)
C6′—C1′	1·392 (3)	C3′—C2′	1·386 (3)
O7′—C2′	1·352 (3)	C4′—C3′	1·370 (4)
C5′—C4′	1·373 (4)	C6′—C5′	1·383 (3)
C8′—O7′	1·421 (3)		

C9—O1—C2	119·6 (1)	C3—C2—O1	121·6 (2)
C1′—C2—O1	110·3 (2)	C1′—C2—C3	128·0 (2)
C4—C3—C2	122·1 (2)	C10—C4—C3	114·9 (2)
O11—C4—C3	122·5 (2)	O11—C4—C10	122·6 (2)
C10—C5—C6	120·8 (2)	C7—C6—C5	120·5 (2)
C8—C7—C6	120·4 (2)	O12—C7—C6	115·3 (2)
O12—C7—C8	124·3 (2)	C9—C8—C7	117·7 (2)
C8—C9—O1	114·9 (2)	C10—C9—O1	122·0 (2)
C10—C9—C8	123·1 (2)	C5—C10—C4	122·7 (2)
C9—C10—C4	119·6 (2)	C9—C10—C5	117·6 (2)
C13—O12—C7	118·2 (2)	C2′—C1′—C2	122·8 (2)
C6′—C1′—C2	118·8 (2)	C6′—C1′—C2′	118·4 (2)
C3′—C2′—C1′	119·5 (2)	O7′—C2′—C1′	117·4 (2)
O7′—C2′—C3′	123·1 (2)	C4′—C3′—C2′	120·7 (2)
C5′—C4′—C3′	120·6 (2)	C6′—C5′—C4′	119·6 (2)
C5′—C6′—C1′	121·1 (2)	C8′—O7′—C2′	118·3 (2)

planar within experimental errors (max. deviation from the best mean plane through the ten atoms 0·031 Å). The dihedral angle between the heterocycle and the phenyl ring is 23·5 (5)°. The methoxy groups are nearly coplanar with their aromatic rings (torsion angles about C_{arom}—O are 4–6°).

Experimental. Crystals obtained by evaporation from ethanol. D_m not measured. Parallelepiped crystal with approximate dimensions 0·12 × 0·14 × 0·28 mm. Lattice parameters refined using 15 reflections in the range $3 \leq 2\theta \leq 30°$. Huber four-circle diffractometer, graphite-monochromated Cu $K\alpha$ radiation. 2483 h, k, $\pm l$ measured reflections with $(\sin\theta)/\lambda \leq 0{\cdot}60$ Å^{-1}; $0 \leq h \leq 14$, $0 \leq k \leq 11$, $-14 \leq l \leq 13$, 1848 with $I \geq 2{\cdot}5\sigma(I)$. Standard reflection $0\bar{1}2$ checked every 50 reflections: no significant deviation. Structure solved by *SHELXS*86 (Sheldrick, 1985). All H atoms from difference Fourier map. Anisotropic least-squares refinement (*SHELX*76; Sheldrick, 1976) using F; H atoms isotropic with common refined temperature factor. $w = 1/(\sigma^2 + 0{\cdot}00583F^2)$, $R = 0{\cdot}042$, $wR = 0{\cdot}053$ for 1848 observed reflections. Final maximum $\Delta/\sigma = 0{\cdot}04$. $S = 0{\cdot}85$. Maximum and minimum heights in final difference Fourier synthesis = 0·15 and −0·24 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). The atomic parameters are given in Table 1.[*] Fig. 1 is a stereoscopic view of the molecule, showing the numbering of the atoms (program *PLUTO*; Motherwell & Clegg, 1978). Bond distances and angles are given in Table 2.

Related literature. This structure analysis forms part of our work on flavones which are sterically hindered around the bond linking the phenyl ring and the benzopyrone moiety (Wallet, Gaydou, Tinant, Declercq, Baldy & Bonifassi, 1990). Although 2′-methoxyflavone is nearly planar, the 2′,4′,5,7-tetramethoxy derivative displays a dihedral angle between the phenyl and the heterocycle planes of 25·1° (Wallet, Gaydou, Jaud & Baldy, 1990). This value is quite similar to that observed for the title compound.

Related structures reported by other authors are 5-hydroxy-6′,8-dimethoxy-2′,5′,7-triethoxyflavone (Kimura, Okuda, Taira, Shoji, Takemoto & Arichi, 1984), 3′,5-dihydroxy-2′,4′,5′,6,7,8-hexamethoxyfla-

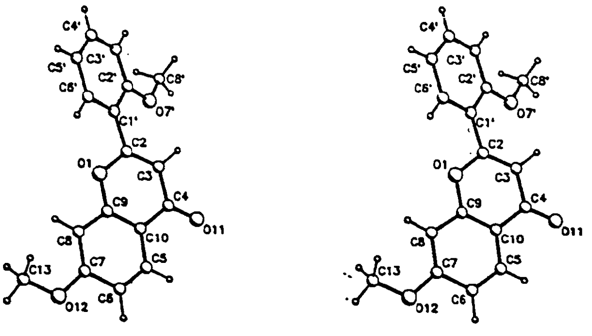

Fig. 1. Stereoscopic view of the molecule.

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[*] Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53576 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

vone (Quijano, Calderon, Gomez, Escobar & Rios, 1985) and 3′,5-dihydroxy-2′,4′,5′,6,7-pentamethoxyflavone (Al-Yahya, Hifnawy, Mossa, El-Feraly, McPhail & McPhail, 1987).

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Structure of 5-Benzoyl-1-methyl-4-phenylpyrimidine-2-thione

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Abstract. (I) $C_{18}H_{14}N_2SO$, $M_r = 306{\cdot}4$, monoclinic, $P2_1/n$, $a = 9{\cdot}724\,(4)$, $b = 15{\cdot}991\,(3)$, $c = 10{\cdot}408\,(3)$ Å, $\beta = 106{\cdot}18\,(3)°$, $V = 1554$ Å^3, $Z = 4$, $D_x = 1{\cdot}309$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 18{\cdot}2$ cm^{-1}, $F(000) = 640$, $T = 293$ K, final $R = 0{\cdot}053$, $wR = 0{\cdot}042$, for 2735 unique reflections. In the pyrimidine ring, the S—C(1) bond distance of 1·656 (3) Å is longer than 1·61 Å, the distance expected for an S—C double bond [Pauling (1963). *The Nature of the Chemical Bond*, 3rd edition. New York: Cornell Univ. Press]. The bond lengths of N(2)—C(1) and N(6)—C(1) are 1·385 (4) and 1·378 (4) Å respectively. The distance between N(2) and C(2), which is the C atom of methyl group, is longer than the N—C distances mentioned above, 1·482 (4) Å.

Experimental. Data collection on a crystal with dimensions 0·3 × 0·1 × 0·1 mm was carried out using a Nonius CAD-4 diffractometer with monochromated Cu $K\alpha$ radiation in the Department of Crystallography and Mineralogy, University of Frankfurt. The unit-cell dimensions were determined from the angular settings of 25 reflections with $6 < \theta < 20°$. The space group was determined from systematic extinctions. 5683 reflections were measured ($-11 \le h \le 11$, $0 \le k \le 18$, $-12 \le l \le 12$) using ω–2θ scans with a scan angle of 1·4°. Symmetry equivalent reflections were averaged, $R_{\rm int} = 0{\cdot}020$ for the observed reflections only, resulting in 2735 unique reflections of which 2105 were observed with $F > 4\sigma(F)$. The structure was solved by direct methods using *SHELXS86* (Sheldrick, 1986) and refined anisotropically using *SHELX76* (Sheldrick, 1976). The H atoms were refined isotropically with fixed temperature factors, approximately equal to the isotropic equivalent of the parent C-atom temperature factors. The final agreement factors were $R = 0{\cdot}053$ and $wR = 0{\cdot}042$ for 241 variables. The function

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