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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(*Received* 29 *May* 1990; *accepted* 10 *October* 1990)

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, $R_{int} = 0{\cdot}020$ 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 *SHELXS*86 (Sheldrick, 1986) and refined anisotropically using *SHELX*76 (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

0108-2701/91/051105-02$03.00

Table 1. *Fractional positional and equivalent isotropic thermal parameters with e.s.d.'s in parentheses*

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

	x	y	z	U_{eq}(Å^2 × 10^2)
S	0·2615 (1)	0·5418 (1)	0·5643 (1)	7·64 (4)
C(1)	0·3548 (3)	0·4538 (2)	0·5838 (3)	5·01 (12)
N(2)	0·3733 (2)	0·4105 (2)	0·4746 (2)	4·93 (10)
C(3)	0·4543 (3)	0·3412 (2)	0·4890 (3)	4·83 (12)
C(4)	0·5198 (3)	0·3081 (2)	0·6130 (3)	4·12 (11)
C(5)	0·4906 (3)	0·3502 (2)	0·7218 (3)	4·29 (11)
N(6)	0·4157 (2)	0·4197 (2)	0·7083 (2)	4·82 (10)
C(2)	0·3067 (4)	0·4420 (3)	0·3373 (4)	6·84 (16)
C(11)	0·5384 (3)	0·3166 (2)	0·8613 (3)	4·62 (12)
C(12)	0·5907 (3)	0·3715 (2)	0·9672 (3)	5·59 (13)
C(13)	0·6314 (4)	0·3407 (3)	1·0977 (4)	7·27 (17)
C(14)	0·6176 (4)	0·2579 (3)	1·1214 (4)	8·07 (18)
C(15)	0·5626 (4)	0·2032 (3)	1·0180 (4)	7·78 (17)
C(16)	0·5242 (4)	0·2329 (2)	0·8867 (4)	6·08 (14)
O(40)	0·7401 (2)	0·2443 (2)	0·7164 (2)	6·47 (9)
C(40)	0·6291 (3)	0·2416 (2)	0·6242 (3)	4·82 (12)
C(41)	0·6042 (3)	0·1754 (2)	0·5219 (3)	4·37 (11)
C(42)	0·4668 (3)	0·1496 (2)	0·4547 (4)	7·04 (16)
C(43)	0·4493 (4)	0·0869 (3)	0·3616 (5)	10·73 (23)
C(44)	0·5623 (5)	0·0506 (3)	0·3321 (4)	9·02 (20)
C(45)	0·6994 (4)	0·0757 (2)	0·3977 (4)	6·64 (15)
C(46)	0·7188 (3)	0·1374 (2)	0·4912 (3)	5·26 (13)

Table 2. *Bond lengths* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

S—C(1)	1·656 (3)	C(13)—C(12)	1·395 (5)
N(2)—C(1)	1·385 (4)	C(14)—C(13)	1·361 (6)
N(6)—C(1)	1·378 (4)	C(15)—C(14)	1·374 (5)
C(3)—N(2)	1·343 (4)	C(16)—C(15)	1·396 (5)
C(2)—N(2)	1·482 (4)	O(40)—C(40)	1·229 (3)
C(4)—C(3)	1·376 (4)	C(41)—C(40)	1·473 (4)
C(5)—C(4)	1·412 (4)	C(42)—C(41)	1·387 (4)
C(40)—C(4)	1·485 (4)	C(46)—C(41)	1·382 (4)
C(11)—C(5)	1·496 (4)	C(43)—C(42)	1·372 (5)
C(5)—N(6)	1·316 (4)	C(44)—C(43)	1·351 (6)
C(12)—C(11)	1·390 (4)	C(45)—C(44)	1·378 (5)
C(16)—C(11)	1·378 (4)	C(46)—C(45)	1·362 (4)

N(2)—C(1)—S	121·1 (2)	C(13)—C(12)—C(11)	119·4 (4)
N(6)—C(1)—S	121·9 (3)	C(14)—C(13)—C(12)	120·4 (4)
N(6)—C(1)—N(2)	117·0 (3)	C(15)—C(14)—C(13)	120·9 (4)
C(3)—N(2)—C(1)	121·8 (3)	C(16)—C(15)—C(14)	119·4 (4)
C(2)—N(2)—C(1)	119·9 (3)	C(15)—C(16)—C(11)	120·3 (4)
C(2)—N(2)—C(3)	118·3 (3)	O(40)—C(40)—C(4)	119·3 (3)
C(4)—C(3)—N(2)	121·7 (3)	C(41)—C(40)—C(4)	119·3 (2)
C(5)—C(4)—C(3)	115·1 (3)	C(41)—C(40)—O(40)	121·4 (3)
C(40)—C(4)—C(3)	118·9 (3)	C(42)—C(41)—C(40)	121·2 (3)
C(40)—C(4)—C(5)	125·3 (3)	C(46)—C(41)—C(40)	120·2 (3)
N(6)—C(5)—C(4)	123·1 (3)	C(46)—C(41)—C(42)	118·6 (3)
C(11)—C(5)—C(4)	122·0 (3)	C(43)—C(42)—C(41)	119·0 (3)
C(11)—C(5)—N(6)	114·9 (3)	C(44)—C(43)—C(42)	121·8 (4)
C(5)—N(6)—C(1)	121·0 (3)	C(45)—C(44)—C(43)	119·9 (4)
C(12)—C(11)—C(5)	119·3 (3)	C(46)—C(45)—C(44)	119·1 (4)
C(16)—C(11)—C(5)	120·9 (3)	C(45)—C(46)—C(41)	121·6 (3)
C(16)—C(11)—C(12)	119·7 (3)		

minimized was $\sum w(F_o - F_c)^2$ with $w = 1/\sigma^2(F_o)$ and $\sigma(F_o)$ from counting statistics; final $(\Delta/\sigma)_{max} = 0{\cdot}09$ and $\Delta\rho_{max} = 0{\cdot}39$ e Å^{-3}. The scattering factors used were those from *International Tables for X-ray Crystallography* (1974, Vol. IV). The figure was prepared with *ORTEP* (Johnson, 1976).

Final positional and thermal parameters are given in Table 1, the bond lengths and angles in Table 2. A view of the molecule and numbering scheme is given in Fig. 1.*

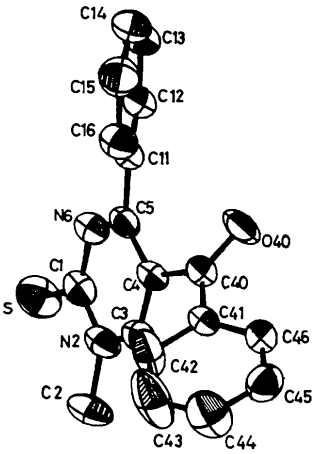

Fig. 1. Crystallographic numbering scheme.

Related literature. The title molecule, 5-benzoyl-1-methyl-4-phenylpyrimidine-2-thione, is a pyrimidine derivative. Various analogues of thiopyrimidine possess effective antibacterial, antifungal, insecticidal, antivirial and miticidal activities (Brown, 1984).

Details of the source and chemical background of (I) are given in Altural, Akçamur, Sarıpınar, Yıldırım & Kollenz (1989).

The observed bond distances are entirely consistent with 5-benzoyl-1-(diphenylmethylenamino)-4-phenyl-1*H*-pyrimidine-2-thione (Akçamur, Altural, Sarıpınar, Kollenz, Kappe, Peters, Peters & Schnering, 1988).

* 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 53645 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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