Novel Synthesis of Di-imines by the Transformation of 1-Aryl-4,6-disubstituted Pyrimidin-2(1*H*)-ones

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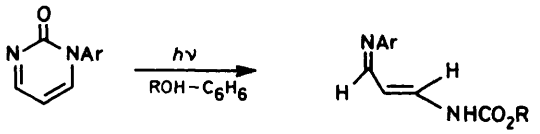
The di-imines (4), which are versatile starting materials for the synthesis of heterocycles, are obtained in fair yields when the 1-aryl-4,6-disubstituted pyrimidin-2(1*H*)-ones (3) are treated with alkoxide, both photochemically and thermally. The di-imines (4) thus obtained, when treated with carbon disulphide, give the 1,3-thiazine-2-thiones (8) and/or the 1-arylpyrimidine-2(1*H*)-thiones (9).

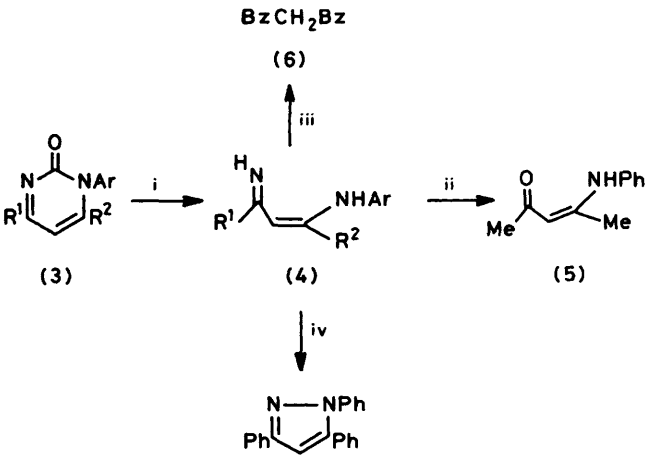
THE di-imine compounds (4) may be considered as 1-azabutadiene derivatives and used as intermediates in the synthesis of various heterocycles that contain one or two nitrogen atoms in the ring, such as the pyridines,[1] pyrimidines,[2] and pyrazoles.[3] It has been reported that the di-imines (4) can be prepared by the reaction of Schiff bases with saturated nitriles in the presence of aluminium trichloride as a catalyst.[4] We report herein a new method for the synthesis of the di-imines (4) by the transformation of 1-aryl-4,6-disubstituted pyrimidin-2-(1*H*)-ones (3).

RESULTS AND DISCUSSION

Transformation of 1-*Aryl*-4,6-*disubstituted Pyrimidin*-2-(1H)-*ones* (3) *to the Di-imines* (4).—We reported previously the photochemical ring-opening of 1-arylpyrimidin-2(1*H*)-ones (1) to 1-alkoxycarbonylamino-3-aryliminoprop-1-enes (2).[5] In order to elucidate the mechanism of formation of compounds (2), we investigated the photochemical reactions of the 1-arylpyrimidin-2(1*H*)-ones (1) and (3) in the presence of alkoxide. Irradiation of 1-phenylpyrimidin-2(1*H*)-one (1; Ar = Ph) in methanol–benzene (1 : 20) in the presence of sodium methoxide gave an intractable mixture. However, a solution of the pyrimidin-2(1*H*)-one (3a) in methanol–benzene (1 : 20) in the presence of sodium methoxide was irradiated with a high-pressure mercury lamp at room temperature for 12 h and then purified by a silica gel column chromatography to give the di-imine (4a) in 86% yield. On the other hand, irradiation of compound (3a) in methanol in the absence of sodium methoxide gave 3,4,6-triphenyl-2-oxo-1,3-diazabicyclo[2.2.0]hex-5-ene.[6] The di-imine (4a) was also obtained in 76% yield when the arylpyrimidin-2(1*H*)-one (3a) was refluxed † in methanol–benzene (1 : 20) in the presence of sodium methoxide for 10 h. The structure of di-imine (4a) was confirmed on the basis of physical properties and elemental analysis (see Experimental section). As expected, the di-imine (4a), when treated with hydrochloric acid in ethanol, gave dibenzoylmethane (6) in nearly quantitative yield. Furthermore, treatment of the di-imine (4a) with thionyl chloride in pyridine at 90 °C for 3 h[3] gave 1,3,5-triphenylpyrazole (7) in 91% yield (Scheme 1).



(1) (2)



(6) (3) (4) (5) (7)

	Ar	R¹	R²
a;	Ph	Ph	Ph
b;	C_6H_4Me-*p*	Ph	Ph
c;	C_6H_4Me-*m*	Ph	Ph
d;	C_6H_4OMe-*p*	Ph	Ph
e;	Ph	C_6H_4Me-*p*	C_6H_4Me-*p*
f;	Ph	Ph	C_6H_4Me-*p*
g;	Ph	Ph	Me
h;	Ph	Me	Me

SCHEME 1 i, *hν* or heat, alkoxide; ii, silica gel [(3h) only]; iii, HCl–EtOH [(4a) only]; iv, 90 °C, $SOCl_2$–C_5H_5N [(4a) only]

The di-imine (4a) was also obtained in fair yields by the treatment of the pyrimidin-2(1*H*)-one (3a) with sodium ethoxide or potassium t-butoxide. Similarly, the other 1-aryl-4,6-disubstituted pyrimidin-2(1*H*)-ones (3b)—(3g) were treated with alkoxide to afford the di-imines (4b)—(4g). In case of the pyrimidin-2(1*H*)-one (3 h), 4-anilinopent-3-en-2-one (5) was obtained *via* hydrolysis of the imine functional group of the di-imine (4 h), presumably formed initially from the reaction of compound (3h) with alkoxide. The results are summarized in Table 1.

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† When compound (3a) was treated with sodium methoxide in methanol–benzene (1 : 20) at room temperature, no products were obtained and compound (3a) was recovered quantitatively.

Reaction of Di-imines (4) *with Carbon Disulphide.*—The versatility of di-imines (4) in the synthesis of various heterocycles that contain nitrogen atoms has been reported.[7] We examined the reaction of the di-imine (4) with carbon disulphide * and found that the 1,3-thiazine-2-thiones (8) and/or 1-arylpyrimidine-2(1*H*)-thiones (9) were formed. A solution of the di-imine (4a) in carbon disulphide was heated at 70 °C for 5 h to give the 1,3-thiazine-2-thione (8a) and pyrimidine-2(1*H*)-thione (9a) in 31% and trace yields, respectively. The structure of the 1,3-thiazine-2-thione (8a) was confirmed by spectroscopic data and elemental analyses. Similarly, other di-imines [(4b), (4d), (4g), and (4i)] reacted with carbon disulphide to give the 1,3-thiazine-2-thiones (8a) and (8i) and the pyrimidine-2(1*H*)-thiones (9d), (9g), and (9i) (see Table 2).

TABLE 1

The di-imines (4) obtained from the 1-aryl-4,6-disubstituted pyrimidin-2(1*H*)-ones (3)

Compd.	Conditions	Alkoxide	Solvent	Yield of (4) (%) [a]
(3a)	$h\nu$, 12 h	NaOMe	MeOH–C_6H_6	86
	reflux, 10 h	NaOMe	MeOH–C_6H_6	76
	$h\nu$, 12 h	NaOEt	EtOH–C_6H_6	75
	reflux, 5 h	KOBu^t	C_6H_6	71
(3b)	$h\nu$, 12 h	NaOMe	MeOH–C_6H_6	80
	reflux, 5 h	KOBu^t	C_6H_6	57
(3c)	$h\nu$, 12 h	NaOMe	MeOH–C_6H_6	81
(3d)	$h\nu$, 10 h	NaOMe	MeOH–C_6H_6	70
	reflux, 5 h	KOBu^t	C_6H_6	65
(3e)	$h\nu$, 12 h	NaOMe	MeOH–C_6H_6	56
(3f)	$h\nu$, 12 h	NaOMe	MeOH–C_6H_6	63
(3g)	$h\nu$, 12 h	NaOMe	MeOH–C_6H_6	40
	reflux, 5 h	KOBu^t	C_6H_6	10
(3h)	$h\nu$, 15 h	NaOMe	MeOH–C_6H_6	43 [b]

[a] Isolated yield. [b] The yield of 4-anilinopent-3-en-2-one (5).

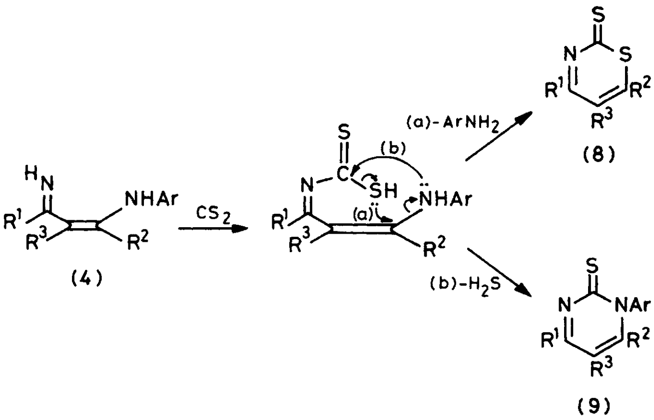
TABLE 2

1,3-Thiazine-2-thiones (8) and 1-arylpyrimidine-2(1*H*)-thiones (9) obtained from the di-imines (4) and carbon disulphide

Compound	Yield (%) (8)	Yield (%) (9)
(4a)	31	trace
(4b)	38	trace
(4d)	30	36
(4g)	trace	24
(4i) [a]	36	64

[a] The di-imine (4i) was independently prepared according to a method described previously (ref. 4).

The formation of 1,3-thiazine-2-thiones (8) and pyrimidine-1(2*H*)-thiones (9) can be explained easily by two alternative reaction paths, (a) and (b) (see Scheme 2). In all cases, the formation of aniline derivatives was detected by gas chromatography.



SCHEME 2 For compounds (4a), (4b), (4d), (4g), and (4i). [R^3 = H for (4a), (4b), (4d), and (4g); compound (4i), prepared using a method described in ref. 4, has Ar = R^1 = R^2 = Ph, R^3 = Me]

EXPERIMENTAL

Starting Materials.—The pyrimidin-2(1*H*)-ones (3a)—(3g) were prepared by a modification of a method described previously [9,10] and compound (3h) was prepared as described in reference 10. The properties of, and data for, compounds (3a)—(3h) are listed below.

1,4,6-*Triphenylpyrimidin*-2(1*H*)-*one* (3a) had m.p. 247.5—249 °C; λ(EtOH) 208 (ε 3.61 × 10^4), 277 (1.97 × 10^4), and 340 nm (1.28 × 10^4); ν (KBr) 1 670 cm^{-1}; δ($CDCl_3$) 6.93 (1 H, s), 7.1—7.7 (13 H, m), and 8.15—8.35 (2 H, m) (Found: C, 81.2; H, 4.85; N, 8.65. $C_{22}H_{16}N_2O$ requires C, 81.45; H, 4.95; N, 8.45%).

4,6-*Diphenyl*-1-p-*tolylpyrimidin*-2-(1H)-*one* (3b) had m.p. 245—246.5 °C; λ(EtOH) 207 (ε 3.79 × 10^4), 277 (1.84 × 10^4), and 340 nm (1.25 × 10^4); ν(KBr) 1 650 cm^{-1}; δ($CDCl_3$) 2.27 (3 H, s), 6.89 (1 H, s), 7.05—7.70 (12 H, m), and 8.15—8.35 (2 H, m) (Found: C, 81.5; H, 5.2; N, 8.3. $C_{23}H_{18}N_2O$ requires C, 81.65; H, 5.35; N, 8.3%).

4,6-*Diphenyl*-1-m-*tolylpyrimidin*-2(1H)-*one* (3c) had m.p. 206—207 °C; ν(KBr) 1 675 cm^{-1}; δ($CDCl_3$) 2.26 (3 H, s), 6.87 (1 H, s), 6.9—7.3 (10 H, m), 7.43—7.57 (2 H, m), and 8.15—8.20 (2 H, m) (Found: C, 81.35; H, 5.15; N, 8.35. $C_{23}H_{18}N_2O$ requires C, 81.65; H, 5.35; N, 8.3%).

1-p-*Methoxyphenyl*-4,6-*diphenylpyrimidin*-2(1H)-*one* (3d) had m.p 283—284 °C; λ(EtOH) 207 (ε 3.82 × 10^4), 227sh (2.20 × 10^4), 277 (2.01 × 10^4), and 339 nm (1.30 × 10^4); ν(KBr) 1 655 cm^{-1}; δ($CDCl_3$) 3.77 (3 H, s), 6.80—7.65 (13 H, m), and 8.15—8.35 (2 H, m) (Found: C, 77.75; H, 5.0; N, 8.1. $C_{23}H_{18}N_2O_2$ requires C, 77.95; H, 5.1; N, 7.9%).

1-*Phenyl*-4,6-*di*-p-*tolylpyrimidin*-2(1H)-*one* (3e) had m.p. 205—206 °C; ν(KBr) 1 670 cm^{-1}; δ($CDCl_3$) 2.28 (3 H, s), 2.43 (3 H, s), 6.85 (1 H, s), 7.00—7.25 (11 H, m), and 8.11 (2 H, d, *J* 8.3 Hz) (Found: C, 81.45; H, 5.65; N, 7.9. $C_{24}H_{20}N_2O$ requires C, 81.8; H, 5.7; N, 7.9%).

1,4-*Diphenyl*-6-p-*tolylpyrimidin*-2(1H)-*one* (3f) had m.p. 173 °C (decomp.); ν(KBr) 1 665 cm^{-1}; δ($CDCl_3$–CD_3OD) 2.30 (3 H, s), 6.94 (1 H, s), 7.00—7.58 (12 H, m), and 8.10—8.20 (2 H, m) (Found: C, 81.35; H, 5.35; N, 8.35. $C_{23}H_{18}N_2O$ requires C, 81.65; H, 5.35; N, 8.3%).

6-*Methyl*-1,4-*diphenylpyrimidin*-2(1H)-*one* (3g) had m.p. 271—272 °C; ν(KBr) 1 645 cm^{-1}; δ($CDCl_3$) 2.07 (3 H, d, *J* 0.7 Hz), 6.77 (1 H, d, *J* 0.7 Hz), 7.20—7.55 (8 H, m), and 8.10—8.20 (2 H, m) (Found: C, 77.7; H, 5.4; N, 10.85. $C_{17}H_{12}N_2O$ requires C, 77.85; H, 5.35; N, 10.65%).

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* Burluenga and his co-workers have reported that di-imines, prepared by the reaction of Schiff bases with saturated nitriles in the presence of aluminium trichloride,[4] reacted with carbon disulphide to afford pyrimidine-2(1*H*)-thiones in high yields.[8] In the experimental conditions described herein, 1,3-thiazine-2-thiones (8), in addition to pyrimidine-2(1*H*)-thiones, were obtained.

4,6-*Dimethyl*-1-*phenylpyrimidin*-2(1H)-*one* (3 h) had m.p. 243—244 °C (lit.,[10] m.p. 245—246 °C; λ(EtOH) 210 (ε 2.23×10^4) and 304 nm (9.5×10^3); ν(KBr) 1 650 cm^{-1}; δ(CDCl$_3$) 1.97 (3 H, d, *J* 0.7 Hz), 2.40 (3 H, s), 6.20 (1 H, d, *J* 0.7 Hz), 7.14—7.31 (2 H, m), and 7.40—7.57 (3 H, m).

General Procedure for the Photochemical Reactions of the Pyrimidin-2(1H)-*ones* (3) *in the Presence of Alkoxide*.—A solution of the pyrimidin-2(1*H*)-one (3) (200 mg) in benzene (40 ml) in the presence of alkoxide [prepared from sodium (1 mol equiv.) and alcohol (2 ml)] was irradiated with a high-pressure mercury lamp for 10—15 h under argon at room temperature. After removal of the solvent, the residue was chromatographed on a silica gel column with benzene–ethyl acetate (10 : 1) to give the di-imine (4) [Note: Compound (3h) gave the product (5)]. The data for compounds (4a)—(4g) and (5) are given below.

General Procedure for Thermal Reactions of the Pyrimidin-2(1H)-*ones* (3) *in the Presence of Alkoxide*.—A solution of the pyrimidin-2(1*H*)-one (3) (200 mg) and alkoxide (1 mol equiv.) in benzene (40 ml) was refluxed under argon for 5—10 h. After removal of the solvent, the residue was chromatographed on a silica gel column. Elution with benzene–ethyl acetate (10 : 1) yielded the di-imine (4).

3-*Anilino*-1,3-*diphenylprop*-2-*enimine* (4a) had m.p. 129.5—130.5 °C (from chloroform–hexane); λ(EtOH) 205 (ε 3.34×10^4), 238 (1.82×10^4), and 363 nm (1.75×10^4); ν(KBr) 3 455, 1 615, and 1 600 cm^{-1}; δ(CDCl$_3$) 5.39 (1 H, s) and 6.67—7.66 (17 H, m); δ_C (CDCl$_3$) 96.3 (d), 156.6 (s), and 168.0 p.p.m. (s), in addition to aromatic carbon peaks (Found: C, 84.4; H, 6.05; N, 9.5. $C_{21}H_{18}N_2$ requires C, 84.55; H, 6.05; N, 9.4%).

1,3-*Diphenyl*-3-p-*toluidinoprop*-2-*enimine* (4b) had m.p. 164—165 °C (from chloroform–hexane); λ(EtOH) 207 (ε 2.90×10^4), 239 (1.85×10^4), and 365 nm (1.65×10^4); ν(KBr) 3 455, 1 620, and 1 600 cm^{-1}; δ(CDCl$_3$) 2.22 (3 H, s), 5.38 (1 H, s), 6.62 (2 H, d, *J* 7.8 Hz), 6.90 (2 H, d, *J* 7.8 Hz), and 7.13—7.66 (12 H, m) (Found: C, 84.35; H, 6.4; N, 8.95. $C_{22}H_{20}N_2$ requires C, 84.6; H, 6.45; N, 8.95%).

1,3-*Diphenyl*-3-m-*toluidinoprop*-2-*enimine* (4c) had m.p. 86—87 °C (from chloroform–hexane); ν(KBr) 3 450, 1 615, and 1 575 cm^{-1}; δ(CDCl$_3$) 2.20 (3 H, s), 5.38 (1 H, s), and 6.42—7.66 (16 H, m) (Found: C, 84.45; H, 6.45; N, 8.7. $C_{22}H_{20}N_2$ requires C, 84.6; H, 6.45; N, 8.95%).

3-p-*Anisidino*-1,3-*diphenylprop*-2-*enimine* (4d) had m.p. 134.5—135 °C (from chloroform–hexane); λ(EtOH) 206 (ε 3.01×10^4), 238 (1.85×10^4), and 369 nm (1.55×10^4); ν(KBr) 3 460, 1 610, and 1 600 cm^{-1}; δ(CDCl$_3$) 3.70 (3 H, s), 5.37 (1 H, s), 6.65 (4 H, s), and 7.21—7.66 (12 H, m) (Found: C, 80.4; H, 6.1; N, 8.65. $C_{22}H_{20}N_2O$ requires C, 80.45; H, 6.15; N, 8.55%).

3-*Anilino*-1,3-*di*-p-*tolylprop*-2-*enimine* (4e) had m.p. 127—128 °C (from chloroform–hexane); λ(EtOH) 206 (ε 3.96×10^4), 244 (1.85×10^4), and 363 nm (1.89×10^4); ν(KBr) 3 455, 1 615, and 1 595 cm^{-1}; δ(CDCl$_3$) 2.27 (3 H, s), 2.38 (3 H, s), 5.38 (1 H, s), 6.68—7.20 (13 H, m), and 7.51 (2 H, d, *J* 8.3 Hz) (Found: C, 84.55; H, 6.7; N, 8.5. $C_{23}H_{22}N_2$ requires C, 84.6; H, 6.8; N, 8.6%).

3-*Anilino*-1-*phenyl*-3-p-*tolylprop*-2-*enimine* (4f) had m.p. 124.5—125.5 °C (from chloroform–hexane); λ(EtOH) 205 (ε 3.56×10^4), 236 (1.82×10^4), and 360 nm (1.71×10^4); ν(KBr) 3 470, 1 610, and 1 520 cm^{-1}; δ(CDCl$_3$) 2.26 (3 H, s), 5.39 (1 H, s), and 6.69—7.66 (16 H, m) (Found: C, 84.55; H, 6.45; N, 8.9. $C_{22}H_{20}N_2$ requires C, 84.6; H, 6.45; N, 8.95%).

3-*Anilino*-1-*phenylbut*-2-*enimine* (4g) had m.p. 82.5—83.5 °C (from chloroform–hexane); λ(EtOH) 204 (ε 3.36×10^4), 229 (1.78×10^4), and 339 nm (1.89×10^4); ν(KBr) 3 450, 1 615, and 1 590 cm^{-1}; δ(CDCl$_3$) 1.95 (3 H, s), 5.16 (1 H, s), and 6.79—7.63 (12 H, m) (Found: C, 81.2; H, 6.8; N, 11.55. $C_{16}H_{16}N_2$ requires C, 81.3; H, 6.8; N, 11.85%).

4-*Anilinopent*-3-*en*-2-*one* (5) had m.p. 101.5—103 °C (lit.,[11] m.p. 103 °C); ν(KBr) 1 660 and 1 565 cm^{-1}; δ(CDCl$_3$) 1.99 (3 H, s), 2.10 (3 H, s), 5.19 (1 H, s), 7.05—7.43 (5 H, m), and 12.47br (1 H, s).

Reaction of the Di-imine (4a) *with Hydrochloric Acid*.—A solution of the di-imine (4a) (100 mg) and hydrochloric acid (1 ml) in ethanol (10 ml) was refluxed for 1 h. The reaction mixture was poured into water and extracted with dichloromethane. The extract was washed with aqueous sodium hydrogencarbonate, water, and then dried (anhydrous MgSO$_4$). After removal of the solvent, the residue was recrystallized from benzene–hexane to yield dibenzoylmethane (6) in quantitative yield.

Reaction of the Di-imine (4a) *with Thionyl Chloride in Pyridine*.—To a solution of the di-imine (4a) (100 mg) in pyridine (5 ml) was added thionyl chloride (50 mg) at 0 °C (ice-bath). The mixture was stirred while being warmed to room temperature and then heated at 90 °C for 8 h. The reaction mixture was poured into ice–water and extracted with dichloromethane. The extract was washed with aqueous sodium hydrogencarbonate, water, and then dried (anhydrous MgSO$_4$). After removal of the solvent, the residue was recrystallized from hexane to yield 1,3,5-tripyrazole (7) (91% yield), m.p. 139 °C (lit.,[3] m.p. 138—139 °C); ν(BKr) 1 595, 1 560, 1 505, 1 485, 1 320, 1 310, 1 125, 765, 710, and 690 cm^{-1}; δ(CDCl$_3$) 6.96 (1 H, s), 7.16—7.58 (13 H, m), and 8.09—8.19 (2 H, m).

Reaction of the Di-imines (4a), (4b), (4d), (4g), *and* (4i)* *with Carbon Disulphide*.—A solution of the di-imine (4) (100 mg) in carbon disulphide (5 ml) in a sealed tube was heated at 70 °C for 5—10 h. After the carbon disulphide had been evaporated off under reduced pressure, the residual oil was chromatographed with benzene–ethyl acetate (10 : 1) to give the 1,3-thiazine-2(1*H*)-thione (8) and/or pyrimidine-2(1*H*)-thione (9). Data for compounds (8a), (8i), (9d), (9g), and (9i) are given below.

4,6-*Diphenyl*-1,3-*thiazine*-2-*thione* (8a) had m.p. 152—153 °C (from chloroform–hexane); λ(EtOH) 205 (ε 2.67×10^4), 242 (1.51×10^4), 321 (3.51×10^4), and 479 nm (5.1×10^3); ν(KBr) 1 580, 1 560, 1 455, 1 240, 1 060, 760, and 690 cm^{-1}; δ_H (CDCl$_3$) 7.40—7.75 (9 H, m) and 8.15—8.30 (2 H, m); δ_C (CDCl$_3$) 111.4 (d), 136.7 (s), 164.3 (s), and 168.3 p.p.m. (s), in addition to aromatic carbon peaks (Found: C, 68.0; H, 3.9; N, 4.95. $C_{16}H_{11}NS_2$ requires C, 68.3; H, 3.95; N, 5.0%).

5-*Methyl*-4,6-*diphenyl*-1,3-*thiazine*-2-*thione* (8i) had m.p. 134—135 °C (from chloroform–hexane); λ(EtOH) 206 (ε 2.93×10^4), 234 (1.60×10^4), 315 (2.61×10^4), and 459 nm (4.9×10^3); ν(KBr) 1 595, 1 545, 1 445, 1 250, 1 045, 755, and 690 cm^{-1}; δ_H (CDCl$_3$) 2.10 (3 H, s), 7.41—7.51 (8 H, m), and 7.68—7.78 (2 H, m); δ_C (CDCl$_3$) 19.0 (q), 122.2 (s), 138.2 (s), 163.8 (s), and 169.1 p.p.m. (s), in addition to aromatic carbon peaks (Found C, 69.15; H, 4.4; N, 4.7. $C_{17}H_{13}NS_2$ requires C, 69.1; H, 4.45; N, 4.75%).

1-p-*Methoxyphenyl*-4,6-*diphenylpyrimidine*-2(1H)-*thione* (9d) had m.p. 245 °C (decomp.) (from chloroform–hexane);

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* The di-imine (4i) was independently prepared according to a method described previously (ref. 4).

λ(EtOH) 209 (ε 3.38 × 10^4), 298 (4.44 × 10^4), and 409 nm (4.0 × 10^3); ν(KBr) 1 605, 1 590, 1 570, 1 510, 1 355, and 1 240 cm^{-1}; δ(CDCl$_3$) 3.74 (3 H, s), 6.66—7.54 (13 H, m), and 8.18—8.28 (2 H, m) (Found: C, 74.65; H, 4.85; H, 4.85; N, 7.45. $C_{23}H_{18}N_2OS$ requires C, 74.6; H, 4.85; N, 7.55%).

6-*Methyl*-1,4-*diphenylpyrimidine*-2(1H)-*thione* (9g) had m.p. 210—211 °C (decomp.) (from chloroform–hexane); ν(KBr) 1 605, 1 590, 1 515, 1 350, and 1 240 cm^{-1}; δ(CDCl$_3$) 2.12 (3 H, d, J 0.6 Hz), 7.10 (1 H, d, J 0.6 Hz), 7.19—7.30 (2 H, m), 7.42—7.64 (6 H, m), and 8.14—8.24 (2 H, m) (Found: C, 73.1; H, 5.0; N, 10.0. $C_{17}H_{14}N_2S$ requires C, 73.35; H, 5.0; N, 10.05%).

5-Methyl-1,4,6-triphenylpyrimidine-2(1*H*)-thione (9i) had m.p. 297—298 °C (lit.,[8] m.p. 298—299 °C); ν(KBr) 1 605, 1 580, 1 570, 1 500, 1 355, and 1 240 cm^{-1}; δ_H (CDCl$_3$) 1.89 (3 H, s), 6.99—7.30 (11 H, m), 7.43—7.50 (2 H, m), and 7.67—7.78 (2 H, m); δ_C (CDCl$_3$) 16.9 (q), 116.2 (s), 158.9 (s), 169.1 (s), and 182.2 p.p.m. (s), in addition to aromatic carbon peaks.

[2/114 *Received*, 20*th January*, 1982]

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