

ture of 4a (15.8 g, 0.06 mol), malononitrile (3.96 g, 0.06 mol), and powdered S (1.92 g, 0.06 g-atom) in 95% EtOH (70 ml) was treated dropwise with morpholine (4.5 ml), warmed to 50° (internal temperature) for 30 min, and stored in the cold until 5a crystallized out: yield 10.5 g (51%); mp 223–224° dec (95% EtOH, twice); ir (KCl) 3550, 3400, 3200, 2210 (C≡N), 1640, 1610 cm⁻¹.

Procedure 2. A well-stirred mixture of 4e (15.8 g, 0.039 mol), malononitrile (2.58 g, 0.039 mol), and powdered S (1.25 g, 0.039 g-atom) in 95% EtOH (100 ml) was treated dropwise with Et₂NH (4 ml) at 40°. When addition was complete the mixture was warmed to 55–60° (internal temperature) for 10 min, cooled, and poured into 0.1 N HCl (400 ml), yield 18.5 g (98%). This crude product, mp 95–110° dec, was used directly in the next step. Analytically pure 5e, mp 170–178° dec, was obtained after several recrystallizations from benzene–hexane: ir (KCl) 3400, 3200, 2200 (C≡N), 1600 cm⁻¹.

2,4-Diamino-6,8-diaryl-5,6,7,8-tetrahydro-7-methylpyrido[4',3':4,5]thieno[2,3-d]pyrimidines and 2,4-Diamino-6,8-diaryl-5,6-dihydro-8H-thiopyrano[4',3':4,5]thieno[2,3-d]pyrimidines (2a–e, Table I). **Procedure 1.** A finely ground mixture of 5a (8.6 g, 0.025 mol) and chloroformamide hydrochloride (8.6 g, 0.075 mol) was heated in an open pear-shaped flask by means of an oil bath kept at 175°. After 30 min at 175° (internal temperature) the mixture was cooled, transferred to a mortar, pulverized, and digested with hot 0.2 N HCl (2 × 600 ml). The digest was decolorized with charcoal, basified with concentrated NaOH, cooled, and filtered. The solid was washed with H₂O, dried, and chromatographed on silica gel (150 g). The fractions eluted with 10% MeOH–CHCl₃ (v/v) were combined and recrystallized from *i*-PrOH, yielding 1.3 g (12%) of 2a: almost colorless needles; mp 267–276° dec; ir (KCl) 3400, 1600, 1560, 1530, 1480, 1450 cm⁻¹.

Procedure 2. A mixture of 5e (9.1 g, 0.019 mol) and chloroformamide hydrochloride (9.1 g, 0.079 mol) was heated as in the preceding experiment. After 20 min at 180° (internal temperature) the melt was cooled, transferred to a mortar, pulverized, digested for 20 min with warm 0.5 N NaOH (300 ml), filtered, washed with H₂O, and dried. Chromatography of the tan solid (9.4 g) on silica gel (250 ml) with 5% MeOH–CHCl₃ (v/v) as the eluent yielded, after removal of the first few dark-colored fractions, 4.1 g (42%) of 2e as a cream-colored solid: mp 243–248° dec (MeCN); ir (KCl) 3400, 1610, 1550, 1520, 1430, 1410 cm⁻¹.

Oxidation of 2,4-Diamino-6,8-diaryl-5,6-dihydro-8H-thiopyrano[4',3':4,5]thieno[2,3-d]pyrimidines (2f–h, Table I). **Procedure 1.** A suspension of 2c (3.5 g, 0.0089 mol) in glacial AcOH (75 ml) and 30% H₂O₂ (23 ml, 0.2 mol) was stirred at room temperature for 1.25 hr, poured into cold H₂O (150 ml), basified with concentrated NH₄OH, and filtered. Pure 2f was obtained by boiling

the solid with THF (40 ml): yield 3.3 g (91%); mp 222–224°; ir (KCl) 3450, 3200, 1610, 1550, 1520, 1480, 1440, 1040 cm⁻¹ (broad, SO).

Procedure 2. A stirred mixture of 2c (0.5 g, 0.001 mol), glacial AcOH (6 ml), and 30% H₂O₂ (3.2 ml) was kept at room temperature for 22 hr, poured into ice-cold dilute NaOH, and filtered. The yield of 2h was 0.4 g (80%): mp 260–264° (THF); ir (KCl) 3400, 1620, 1590 (broad), 1550, 1520, 1480, 1450, 1320 (SO₂), 1130 cm⁻¹ (SO₂).

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2,4-Diaminothieno[2,3-d]pyrimidines as Antifolates and Antimalarials. 3. Synthesis of 5,6-Disubstituted Derivatives and Related Tetracyclic Analogs[†]

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A series of 15 2,4-diaminothieno[2,3-d]pyrimidines bearing alkyl, aralkyl, and aryl substituents at the 5 and/or 6 positions was synthesized from the corresponding 2-amino-3-cyanothiophenes and chloroformamide hydrochloride. Growth inhibition studies with *Streptococcus faecium* (ATCC 8043) revealed significant activity among the 5-alkyl-6-phenyl(or benzyl) derivatives but not the isomeric 6-alkyl-5-phenyl(or benzyl) analogs. Activity was not enhanced by bridging or halogen substituents. The 5-methyl-6-phenyl derivative was active against *Plasmodium berghei* in the mouse at 640 mg/kg, but none of the compounds were active against *P. gallinaceum* in chicks.

A number of 2,4-diamino-5,6,7,8-tetrahydrothianaphtheno[2,3-d]pyrimidines and related tricyclic compounds were synthesized in our laboratory as inhibitors of dihy-

drofolate reductase and as candidate antimalarials.^{1,2} Although several of these compounds displayed encouraging activity levels against the folate-requiring microorganism *Streptococcus faecium* (ATCC 8043), their antimalarial activity proved to be at best only marginal. Replacement of a ring carbon in the 5,6-cycloalkano moiety by nitrogen or sulfur resulted in even lower activity, and it was therefore concluded that hydrophobic binding must play a significant role in the formation of a strong

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Table I. Physical Constants of 2,4-Diaminothieno[2,3-*d*]pyrimidines

Compd	% yield	Mp, °C (anal sample)	Formula ^a
1a	82	239-242	C ₁₃ H ₁₂ N ₄ S
1b	45	270-273	C ₁₃ H ₁₀ Cl ₂ N ₄ S
1c	31	215-216	C ₁₄ H ₁₄ N ₄ S
1d	19	238-240	C ₁₄ H ₁₂ Cl ₂ N ₄ S
1e ^b	17	260-263	C ₁₄ H ₁₂ N ₄ S
1f	70	324-327	C ₁₄ H ₁₁ ClN ₄ S
1g	64	321-324	C ₁₄ H ₁₀ Cl ₂ N ₄ S
1h	9	336-339	C ₁₄ H ₉ ClN ₄ S
1i	64	247-248	C ₁₄ H ₁₄ N ₄ S
1j	36	252-255	C ₁₅ H ₁₆ N ₄ S
1k	52	268-272	C ₁₃ H ₁₁ ClN ₄ S
1l	69	210-212	C ₁₄ H ₁₃ ClN ₄ S
1m	55	234-236	C ₁₅ H ₁₄ N ₄ S
1n ^b	68	313-316	C ₁₄ H ₁₂ N ₄ S
1o	49	273-275	C ₁₄ H ₁₀ N ₄ S

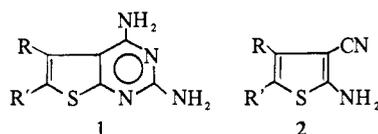
^aAll compounds were analyzed for C, H, N, and S and, where applicable, Cl. ^bSynthesized independently by Elslager, et al.: see ref 8.

Table II. Physical Constants of 2-Amino-3-cyanothiophenes

Compd	% yield	Mp, °C (anal sample)	Formula ^a
2a	17	150-154	C ₁₂ H ₁₀ N ₂ S
2b	18	203-204	C ₁₂ H ₈ Cl ₂ N ₂ S ^b
2c	29	131-132	C ₁₃ H ₁₂ N ₂ S
2d	24	169-172	C ₁₃ H ₁₀ Cl ₂ N ₂ S
2f	83	189-192	C ₁₃ H ₉ ClN ₂ S
2g	55	261-263	C ₁₃ H ₈ Cl ₂ N ₂ S
2i	34	151-153	C ₁₃ H ₁₂ N ₂ S
2j	98	140-142	C ₁₈ H ₁₄ N ₂ S
2k	95	157-158	C ₁₇ H ₉ ClN ₂ S
2l	86	198-202	C ₁₃ H ₁₁ ClN ₂ S
2m	95	194-196	C ₁₇ H ₁₂ N ₂ S
2n ^c	81	160-163	C ₁₃ H ₁₀ N ₂ S
3a	67	d	C ₁₃ H ₁₂ N ₂ S
3c	51	67-69	C ₁₂ H ₉ ClN ₂ S
3d	57	40-42	C ₁₃ H ₁₁ ClN ₂ S
3e	43	71-73	C ₁₇ H ₁₂ N ₂ S

^aAll compounds were analyzed for C, H, and N and, where applicable, Cl and S. ^bN: calcd, 25.04; found, 25.47. ^cSynthesized independently by Elslager, et al.: see ref 8. ^dBp 126-127° (0.005 mm).

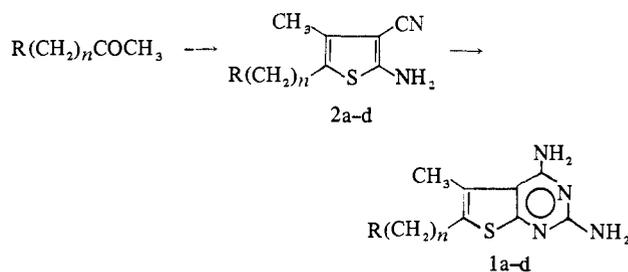
enzyme-inhibitor complex in this series. In order to explore this line of reasoning we undertook to prepare some additional 2,4-diaminothieno[2,3-*d*]pyrimidine derivatives 1 with bulky hydrophobic substituents rather than a simple cycloalkane moiety at positions 5 and 6. This paper describes the synthesis of 15 such compounds (Table I) by condensation of the corresponding 2-amino-3-cyanothiophene precursors 2 (Table II) with chloroformamide hydrochloride.



R and R' = alkyl, aryl, or aralkyl

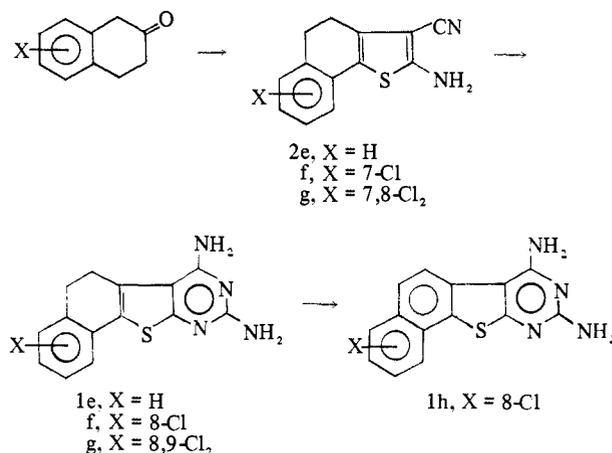
Reaction of 1-phenyl- and 1-(3',4'-dichlorophenyl)-2-propanone³ with malononitrile and sulfur in the presence of diethylamine or morpholine according to the general procedure of Gewald and coworkers⁴ gave the expected aminonitriles 2a and 2b; similarly, 1-phenyl- and 1-(3',4'-dichlorophenyl)-3-butanone afforded 2c and 2d, respectively. Further reaction of these aminonitriles with chloroformamide hydrochloride *via* the previously described

fusion technique^{1,2} provided the 6-aryl and 6-aralkyl derivatives 1a-d. Compound 1a has also been synthesized by Roth⁵ *via* a different approach involving the reaction of 2,4-diamino-6-mercaptopyrimidine with 3-bromo-4-phenyl-2-butanone.



2a, 1a, *n* = 1; R = Ph
 2b, 1b, *n* = 1; R = 3,4-Cl₂C₆H₃
 2c, 1c, *n* = 2; R = Ph
 2d, 1d, *n* = 2; R = 3,4-Cl₂C₆H₃

Condensation of 2-tetralone with malononitrile and sulfur gave exclusively the angular aminonitrile 2e, in accord with the earlier conclusion of Taylor and Berger.⁶ Similarly, 6-chloro- and 6,7-dichloro-2-tetralone⁷ underwent ring closure in a unidirectional manner, giving aminonitriles 2f and 2g, respectively. Further treatment of 2e-g with chloroformamide hydrochloride afforded the tetracyclic thienopyrimidines 1e,[‡] 1f, and 1g, and treatment of 1f with SeO₂ in refluxing glacial AcOH resulted in dehydrogenation to the fully aromatic analog 1h. Compounds 1e-h can be viewed as bridged analogs of 1a in which free rotation of the the phenyl ring is blocked.

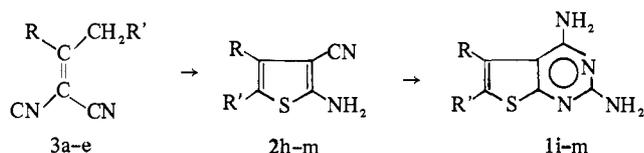


The angular structure 2e was favored by Taylor and Berger⁶ on the basis of nmr evidence. Additional support can be derived from the present work. The uv absorption spectrum of 1e in EtOH solution showed long wavelength maxima at 332 and 347 nm. Inasmuch as both the 6-benzyl-5-methyl analog 1c and the isomeric 5-benzyl-6-methyl analog 1h (*vide infra*) have their longest wavelength maximum at only 278 nm, whereas the 5-methyl-6-phenyl derivative 1a has a peak at 305 nm, it must be concluded that the phenyl ring in 1e is in direct conjugation with the thienopyrimidine moiety (which is possible only if 2e has the angular structure shown).

Not all the ketones used in this work could be converted into aminonitriles *via* the one-step reaction with malononi-

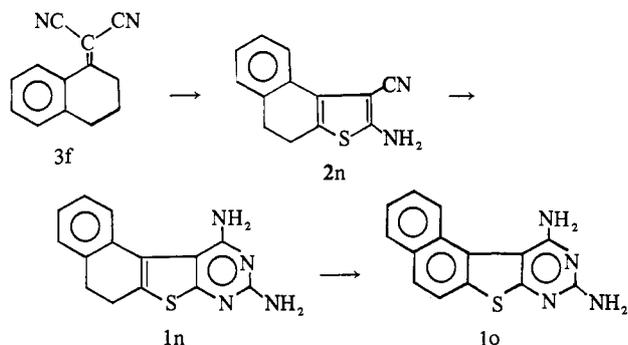
[‡]This compound was synthesized independently by Elslager and coworkers, Parke Davis and Co., Ann Arbor, Mich., as part of a synthetic program directed toward heteroanalogs of the 2,4-diaminoquinazoline antifolates; see ref 8.

trile and sulfur. In such instances it was necessary to first condense the ketone with malononitrile alone in the presence of NH_4OAc and then allow the resultant ylidene-malononitrile to react with sulfur and diethylamine in a separate step. Thus, 1-phenyl-2-butanone yielded ylidene-malononitrile **3a**, which was converted into a 1:1 mixture of aminonitriles **2h** and **2i**. That a mixture of **2h** and **2i** was formed instead of the expected **2h** alone was evidenced by the nmr spectrum in CDCl_3 solution, which showed both the Et group (τ 8.77, t; 7.38, q) and Ph group (τ 2.62, s) of **2h** and the Me group (τ 7.80, s) and PhCH_2 group (τ 6.17, s; 2.74, s) of **2i**. Two different NH_2 groups were likewise noted, at τ 5.55 and 5.15. Further reaction of chromatographically purified **2i** with chloroformamidine hydrochloride provided **1i**, which can be seen to be a position analog of **1a**. Another 5-benzyl analog, **1j**, was prepared similarly, *via* ylidene-malononitrile **3b**⁹ and aminonitrile **2j**. In the same manner, the 5-aryl-6-alkyl derivatives **1k** and **1l** and the 5,6-diphenyl derivative **1m** were synthesized *via* ylidene-malononitriles **3c-e** and aminonitriles **2k-m**.



- 3a, 2i, 1i**, R = PhCH_2 ; R' = Me
2h, R = Et; R' = Ph
3b, 2j, 1j, R = PhCH_2 ; R' = Ph
3c, 2k, 1k, R = 4- ClC_6H_4 ; R' = Me
3d, 2l, 1l, R = 4- ClC_6H_4 ; R' = Et
3e, 2m, 1m, R = R' = Ph

Lastly, 1-tetralone was converted *via* its ylidene-malononitrile derivative **3f**¹⁰ into aminonitrile **2n** and tetracyclic thienopyrimidine **1n**,^{†,8} which is isomeric with compound **1e** and can be viewed as a bridged analog of **1k** and **1l** wherein the phenyl ring cannot rotate freely. Further reaction of **1n** with SeO_2 in refluxing glacial AcOH resulted in dehydrogenation to the fully aromatic analog **1o**.



Biological Activity. Thienopyrimidines **1a-o** were assayed for antimetabolite activity against *Streptococcus faecium* (ATCC 8043) as previously described.¹¹ As indicated in Table III the 5-methyl-6-phenyl and 5-methyl-6-benzyl compounds **1a** and **1c** had ID_{50} values in the 0.001–0.01 $\mu\text{g}/\text{ml}$ range, and aromatic chlorine substitution (**1b,d**) did not affect the level of activity. Bridged 5-alkyl-6-aryl analogs **1e-g** were slightly less active than their open-chain counterparts, and in this series chloro substituents actually appeared to decrease activity. The 6-methyl-5-phenyl and 5-benzyl-6-methyl derivatives **1k** and **1i**, on the other hand, were relatively poor inhibitors, and neither replacement of the methyl group by ethyl (**1l**) nor bridging (**1n**) yielded active compounds. Aromatic substitution at the 5 and 6

Table III. Antibacterial and Antimalarial Activity of 2,4-Diaminothieno[2,3-d]pyrimidines

Compd	<i>S. faecium</i> (ATCC 8043) ID_{50} , $\mu\text{g}/\text{ml}^a$	<i>P. berghei</i> in mouse		
		Dose, mg/kg	T/C, days	Evaluation
1a	0.002	640	7.0/6.1	Active ^b
1b	0.002	640	6.4/6.1	
1c	0.002	640	13.6/6.1	
1d	0.01 ⁻	640	8.6/6.1	
1e	0.02			
1f	0.06	640	6.6/6.1	
1g	0.10	640	6.6/6.1	
1h	1.0 ⁺			
1i	1.0 ⁺	640	6.4/6.1	
1j	1.0 ⁺	640	6.4/6.1	
1k	1.0 ⁺	160	10.2/6.1 ^c	
1l	1.0 ⁺	640	6.2/6.1	
1m	1.0 ⁺	640	6.2/6.1	
1n	1.0			
1o	1.0 ⁺	160	9.0/6.1 ^c	

^aFolate concentration = 0.001 $\mu\text{g}/\text{ml}$. ^bActivity defined as 100% or greater increase in MST of five treated animals. ^cCompound not tested at higher dose.

positions simultaneously (**1j,m**) was likewise ineffectual, as was dehydrogenation to a fully aromatic tetracyclic ring system (**1h,o**).

Antimalarial assays against *Plasmodium berghei* in the mouse and *Plasmodium gallinaceum* in chicks were performed according to the method of Rane and coworkers.¹² In the *P. berghei* assay, ICR/Ha mice were infected with parasitized blood by intraperitoneal injection and were given a single subcutaneous dose of compound in oil 3 days after infection. In the *P. gallinaceum* assay, Leghorn chicks were given a single subcutaneous dose in oil immediately after infection *via* the intravenous route. Against *P. berghei* in the mouse (Table III), compound **1c** was active ($T/C > 6.1$ days) at a dose of 640 mg/kg. Compounds **1k** and **1o** likewise showed borderline activity at 320 mg/kg, the highest dose tested. Against *P. gallinaceum* in chicks, on the other hand, none of the compounds in this series exhibited significant activity.

One compound, **1a**, was tested *in vivo* against L1210 leukemia in BDF/1 hybrid mice and P1534 leukemia (ascitic form) in DBA/2 inbred mice. Injections were given intraperitoneally daily for 4 days beginning on the first day after tumor implantation. Although there was no activity against L1210, this compound at 62.5 mg/kg per day (four times) prolonged the life of P1534 leukemic mice by 23% beyond the survival time of untreated controls.

Experimental Section[§]

The following are specific representative procedures for the synthesis of compounds used in this study.

2,4-Diaminothieno[2,3-d]pyrimidines (1a-o, Table I). Chloroformamidine Hydrochloride Fusion Reactions. Procedure 1. An intimate mixture of **2i** (16 g, 0.07 mol) and chloroformamidine hydrochloride (16 g, 0.14 mol) was heated in an open pear-shaped flask immersed in an oil bath. Melting and foaming began at 80°

[§] Uv spectra were measured with Cary Model 11 and Model 15 spectrophotometers. Ir spectra were taken in KCl disks with a Perkin-Elmer Model 137B double-beam recording spectrophotometer. Nmr spectra were determined by means of a Varian A-60 instrument, with Me_4Si as the internal standard. Melting points were measured in Pyrex capillary tubes in a Mel-Temp apparatus (Laboratory Devices, Inc., Cambridge, Mass.) and are uncorrected. Microanalyses were performed by Galbraith Microanalytical Laboratories, Knoxville, Tenn., and Werby Laboratories, Boston, Mass., and are within $\pm 0.4\%$ of theory except where indicated.

(internal temperature); a homogeneous melt was obtained after 20 min, the temperature having risen to about 130°. Further heating led to a vigorously exothermic temperature increase to about 230° and complete resolidification of the melt. After cooling, the solid was triturated with 0.1 N NaOH, washed with H₂O, and then digested with several portions of boiling 0.1 N HCl (3 l. total). The combined digests were decolorized with charcoal and basified, and the precipitated crude 1i (20 g) was recrystallized (charcoal) from 95% EtOH (2.5 l.).

Procedure 2. A mixture of 2f (7.6 g, 0.029 mol), chloroformamidine hydrochloride (7.6 g, 0.066 mol), and dimethyl sulfone (34 g) was heated for 20 min in an open pear-shaped flask kept at 170° (bath temperature). The crude product was triturated with 0.5 N NaOH, filtered, washed with H₂O, and digested with a mixture of absolute EtOH (3 l.) and Et₂NH (50 ml) in several portions. A small amount of insoluble material was filtered off and the filtrate (charcoal) was stored at 0° until small yellow needles of 1f were deposited.

Procedure 3. A mixture of 2 (15 g, 0.057 mol) and chloroformamidine hydrochloride (15 g, 0.13 mol) was heated as above. Melting occurred above 120° (internal) and a mild exothermic effect was noted above 195°. After 30 min, during which time the internal temperature was not allowed to exceed 203°, the melt was cooled, transferred to a mortar, and pulverized. The crude solid was digested with 0.5 N NaOH (520 ml), washed with H₂O, and recrystallized from EtOH (charcoal), giving 1i in the form of pale yellow prisms.

SeO₂ Dehydrogenations. Procedure 4. A mixture of 1n (4.3 g, 0.016 mol) and SeO₂ (1.8 g, 0.016 mol) was stirred in refluxing AcOH (160 ml) for 18 hr. The hot mixture was filtered through Celite, the solvent was evaporated under reduced pressure, and the dark residue was triturated with boiling EtOH (500 ml) and filtered. The crude solid remaining after digestion was extracted with boiling 0.1 N HCl (360 ml) and then H₂O (240 ml), and the combined extracts were decolorized with charcoal. Basification with 10% NaOH gave 1o as a beige powder.

2-Amino-3-cyanothiophenes (2a-n, Table II). One-Step Synthesis. Procedure 1. A stirred mixture of 1-(3',4'-dichlorophenyl)-3-butanone (60 g, 0.28 mol), malononitrile (18 g, 0.28 mol), and powdered S (9.7 g, 0.3 g-atom) in 95% EtOH (150 ml) was treated dropwise with Et₂NH (27 ml). When the moderately exothermic reaction (50–60°) subsided, the mixture was refluxed for 5 min and then refrigerated overnight. The solid was collected and the mother liquor was concentrated under reduced pressure and diluted with H₂O. The combined crops of 2d were purified by recrystallization from 95% EtOH (75 ml/g, charcoal).

Procedure 2. A stirred mixture of 6,7-dichloro-2-tetralone⁷ (12 g, 0.054 mol), malononitrile (3.6 g, 0.054 mol), and powdered S (1.7 g, 0.054 g-atom) in 95% EtOH (120 ml) was warmed to 60° and treated with morpholine (3.9 ml) in one portion. After 15 min the solution was cooled at 0° until the product, 2g, precipitated out. Colorless needles were obtained after two recrystallizations from 95% EtOH (charcoal).

Two-Step Synthesis. Procedure 3. A stirred mixture of 3d (65 g, 0.28 mol) and powdered S (9.0 g, 0.28 g-atom) in 95% EtOH (100 ml) was treated dropwise with Et₂NH (25 ml). After the first 5 ml of Et₂NH had been added the internal temperature rose to 51°. When addition was complete the mixture was warmed at 50–60° for 1.5 hr and then cooled until crystallization of 2l occurred. Analytically pure material was obtained by recrystallization from 95% EtOH (charcoal).

Ylidenmalononitriles (3a-e, Table II). Procedure 1. A mixture of 1-phenyl-2-butanone (53 g, 0.36 mol), malononitrile (28 g, 0.43 mol), anhydrous NH₄OAc (5.8 g), and glacial AcOH (8.6 ml) in dry PhH (180 ml) was refluxed for 3 hr in a Dean-Stark apparatus. The solution was diluted with additional PhH, washed thoroughly with

H₂O, dried over Na₂SO₄, and evaporated to a dark amber-colored liquid under reduced pressure. Vacuum distillation gave 3a as a fraction, bp 121–127° (0.005 mm), which was sufficiently pure according to nmr for direct use in the next step. A center cut, bp 126–127° (0.005 mm), was analyzed.

Procedure 2. A mixture of *p*-chlorobutyrophenone (95 g, 0.52 mol), malononitrile (42 g, 0.63 mol), anhydrous NH₄OAc (10 g, 0.13 mol), and glacial AcOH (14 ml) in dry PhH (250 ml) was refluxed for 6 hr in a Dean-Stark apparatus. A viscous insoluble material was filtered off (Celite), and the filtrate was washed with H₂O and concentrated to dryness on the rotary evaporator. The residue was triturated with absolute EtOH, with cooling in a Dry Ice-acetone bath, until crystallization occurred. Filtration and recrystallization from EtOH containing a small amount of H₂O yielded analytically pure 3d.

1-(3',4'-Dichlorophenyl)-3-butanone. A mixture of 2,4-pentanedione (55 g, 0.55 mol), 3,4-dichlorobenzyl chloride (98 g, 0.5 mol), and K₂CO₃ (69 g) in anhydrous EtOH (500 ml, dried over Linde 3A molecular sieves) was refluxed for 16 hr.¹³ The volatile materials were removed on the rotary evaporator, and the residue (102 g) was distilled: yield 73 g (67%); bp 87–105° (0.001–0.05 mm). A redistilled sample, bp 85–90° (0.005 mm), was characterized as a crystalline semicarbazone derivative, mp 175–177° (EtOH). *Anal.* (C₁₁H₁₃Cl₂N₃O) C, H, Cl, N.

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