

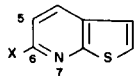
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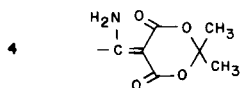
Ten derivatives of thieno[2,3-*b*]pyridine bearing substituents at the 6-position are obtained from transformations which start with 6-cyanothieno[2,3-*b*]pyridine (**2**). Treatment of **2** with sodium alkoxide-alkanol gives imidates (**3**) in ca. 85% yield. Methyl imidate **3a** reacts, in turn, with ammonium chloride to produce a carboxamidine (84%), with 1, $\omega$ -alkyldiamines to form cyclic amidines, and with Meldrum's acid to give an aminoester intermediate (**4**) (36%). Various reagents then convert **4** into the acetyl derivative (86%) (also obtained directly from **2**), an unsaturated aminoester (**6**) (80%), and a  $\beta$ -ketoester (**7**) (39%). Spectral data are reported for these compounds.

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In the preceding paper [2] we reported the direct substitution of the cyano group into the 6-position of thieno[2,3-*b*]pyridine (**1**) to give **2** and the successive transformations of this group into carbamoyl and thiocarbamoyl functions. The present paper concerns additional elaboration of the cyano group of **2** into a variety of other *C*-substituents at the 6-position of **1**, as shown in formulas **3-10**.



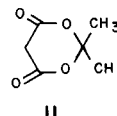
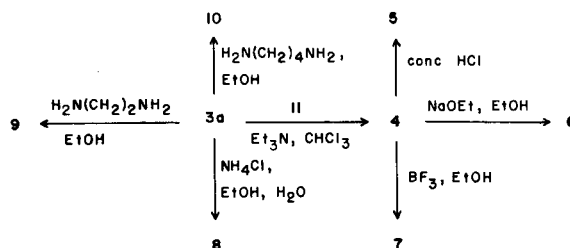
Compound	X - substituent	Compound	X - substituent
<b>1</b>	-H	<b>5</b>	-Ac
<b>2</b>	-CN	<b>6</b>	-C(=CHCO <sub>2</sub> Et)NH <sub>2</sub>
<b>3</b>	-C(=NH)OR	<b>7</b>	-C(=O)CH <sub>2</sub> CO <sub>2</sub> Et
<b>a</b> ,	R = Me	<b>8</b>	-C(=NH)NH <sub>2</sub>
<b>b</b> ,	R = Et	<b>9</b>	
<b>c</b> ,	R = n-Bu	<b>10</b>	



Methyl imidate **3a** readily resulted (87% yield) from stirring nitrile **2** with a solution of sodium methoxide in methanol at room temperature in the manner used by Schaefer and Peters on 2-cyanopyridine [3]. Other alkyl imidates **3b** and **3c** were obtained similarly from **2** and the corresponding solution of sodium alkoxide in alkanol. However, refluxing **2** with methanol and sodium borohydride, as used by Watanabe *et al.* on 2-cyanoquinoline [4], gave only a 46% yield of **3a** (plus unreacted nitrile).

Imidate **3a** served as an intermediate on the routes to compounds **4-10**, as summarized in Scheme 1. Thus, refluxing **3a** with Meldrum's acid (**11**) [5] in triethylamine/dichloroform [6] produced the enaminooester **4** (36%). Compound **4** was converted into 6-acetylthieno[2,3-*b*]pyridine

Scheme 1



(**5**) (86%) by refluxing with concentrated hydrochloric acid, into unsaturated aminoester **6** (80%) by refluxing with sodium ethoxide in ethanol, and into  $\beta$ -ketoester **7** (39%) by refluxing with boron trifluoride in ethanol [6]. Acetyl derivative **5** was also obtained (70%) from reaction of cyano compound **2** with methylmagnesium iodide, followed by acid hydrolysis. Amidine **8** (84%) resulted from refluxing **3a** with ammonium chloride in 80% ethanol [7]. The reaction failed when absolute ethanol was used, probably due to the low solubility of ammonium chloride in this solvent. However, the cyclic amidines **9** and **10** formed easily (59% and 85%, respectively) upon refluxing **3a** with the appropriate 1, $\omega$ -alkyldiamines in absolute ethanol [8].

## EXPERIMENTAL [9]

Methyl Thieno[2,3-*b*]pyridine-6-imidate (**3a**).

A mixture of 0.4 g (2.5 mmoles) of 6-cyanothieno[2,3-*b*]pyridine (**2**) [2], 0.25 mmole of sodium methoxide, and 2.5 ml of absolute methanol was stirred at room temperature for 12 hours. The yellow solution was neutralized with glacial acetic acid (0.25 mmole), rotoevaporated, and treated with a mixture of water (1 ml) and dichloromethane (10 ml). The organic layer, combined with further extracts of the aqueous layer with the same solvent, was dried (sodium sulfate) and evaporated. The residue sublimed at 50-60° (0.05 mm) to give 418 mg (87%) of white, shiny needles, mp

90-93°; ir: 3300 (NH), 1640  $\text{cm}^{-1}$  (C=N) [10]; pmr:  $\delta$  9.20 (broad s, NH), 8.12 (d,  $J_{4,5} = 8.2$  Hz, H-4), 7.85 (d, H-5), 7.63 (d,  $J_{2,3} = 6$  Hz, H-2), 7.29 (d, H-3), 4.04 (s, 3H,  $\text{CH}_3$ ); ms: (90°) 192 ( $M^+$ , 35), 161 ( $[\text{M} - \text{MeO}]^+$ , 50), 160 (52), 135 ( $I^+$ , 100), 134 ( $\text{TP}^+$ , 41), 63 (39), 45 ( $\text{CHS}^+$ , 43); uv:  $\lambda$  max 245 nm ( $\log \epsilon$  4.34), 289 (4.03).

Anal. Calcd. for  $\text{C}_9\text{H}_8\text{N}_2\text{O}_2$ : C, 56.2; H, 4.2; N, 14.6. Found: C, 56.2; H, 4.0; N, 14.3.

#### Ethyl Thieno[2,3-*b*]pyridine-6-imidate (3b):

In the manner used to prepare methyl imidate **3a**, except that sodium ethoxide in absolute ethanol replaced sodium methoxide in absolute methanol, there was obtained, after sublimation at 45-60° (0.02 mm), 424 mg (82%) of white, shiny needles, mp 72-74°; ir: 3290 (NH), 1640  $\text{cm}^{-1}$  (C=N) [10]; pmr:  $\delta$  9.20 (broad s, NH), 8.15 (d,  $J_{4,5} = 8.2$  Hz, H-4), 7.90 (d, H-5), 7.64 (d,  $J_{2,3} = 6$  Hz, H-2), 7.31 (d, H-3), 4.48 (q,  $J_{E} = 7$  Hz, 2H,  $\text{CH}_2\text{CH}_3$ ), 1.48 (t, 3H,  $\text{CH}_3$ ); ms: (60°) 206 ( $M^+$ , 43), 178 (39), 162 ( $\text{TPCO}^+$ , 22), 161 ( $[\text{M} - \text{EtO}]^+$ , 25), 136 (12), 135 ( $I^+$ , 100), 134 ( $\text{TP}^+$ , 38); 112\* (162-135); uv:  $\lambda$  max 245 nm ( $\log \epsilon$  4.37), 291 (3.98).

Anal. Calcd. for  $\text{C}_{10}\text{H}_{10}\text{N}_2\text{O}_2$ : C, 58.2; H, 4.9; N, 13.6. Found: C, 58.2; H, 4.7; N, 13.9.

#### *n*-Butyl Thieno[2,3-*b*]pyridine-6-imidate (3c):

In the foregoing manner was obtained from 403 mg of **2**, sodium 1-butoxide, and 1-butanol a crude brown solid which was evaporatively distilled at 80-85° (0.005 mm) to give 494 mg (84%) of **3c**, mp 67-69° (sintering at 63°); ir: 3280 (NH), 1640  $\text{cm}^{-1}$  (C=N) [10]; pmr:  $\delta$  9.17 (broad s, NH), 8.11 (d,  $J_{4,5} = 8.2$  Hz, H-4), 7.86 (d, H-5), 7.61 (d,  $J_{2,3} = 5.8$  Hz, H-2), 7.28 (d, H-3), 4.41 (t,  $J = 6.5$  Hz, 2H,  $\text{OCH}_2$ ), 2.0-1.3 (m, 4H,  $\text{OCH}_2\text{CH}_2\text{CH}_2$ )  $\ddagger$ ,  $\epsilon_{\infty}$ ,  $J_{E} = 7$  Hz, 3H,  $\text{CH}_3$ ); ms: (100°) 234 ( $M^+$ , 21), 179 (23), 178 ( $[\text{M} - \text{CH}_3\text{CH}_2\text{CH} = \text{CH}_2]^+$ , 63), 162 ( $\text{TPCO}^+$ , 31), 161 (26), 135 ( $I^+$ , 100), 134 ( $\text{TP}^+$ , 58); 147-148\* (178 - 162), 112-113\* (234 - 162), 102-103\* (178 - 135).

Anal. Calcd. for  $\text{C}_{12}\text{H}_{14}\text{N}_2\text{O}_2$ : C, 61.5; H, 6.0; N, 12.0. Found: C, 61.6; H, 5.9; N, 12.0.

#### 2,2-Dimethyl-5-[1-amino-1-(6-thieno[2,3-*b*]pyridyl)methylene]-1,3-dioxane-4,6-dione (4):

A mixture of 202 mg (1.05 mmoles) of imidate **3a**, 151.5 mg (equimolar amount) of Meldrum's acid (**11**) (Fluka), 16 mg (0.16 mmole) of triethylamine, and 12 ml of chloroform was refluxed for 12 hours. The residue from evaporation of the yellow solution was triturated with ether and recrystallized from ethanol to yield 116 mg (36%) of shiny, tan powder, mp 236-238° dec; ir: 3400, 3260 ( $\text{NH}_2$ ), 1710, 1670  $\text{cm}^{-1}$  (lactone C=O); pmr (hexadeuteriodimethylsulfoxide):  $\delta$  10.1 and 9.7 (2 broad s, both disappear on addition of deuterium oxide,  $\text{NH}_2$  group in rotamers), 8.34 (d,  $J_{4,5} = 8.2$  Hz, H-4), 8.02 (d,  $J_{2,3} = 6$  Hz, H-2), 7.55 (d, H-3) which overlaps 7.54 (d, 2H total, H-5), 1.72 (s, 6H,  $2\text{CH}_3$ ); ms: (240°) 304 ( $M^+$ , 5), 178 (25), 177 (20), 162 (18), 161 ( $[\text{TP} - \text{C} \equiv \text{NH}]^+$ , 55), 160 (51), 135 ( $I^+$ , 100), 134 ( $\text{TP}^+$ , 78); uv:  $\lambda$  max 231 nm ( $\log \epsilon$  4.42), 290 (4.26).

Anal. Calcd. for  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_4\text{S}$ : C, 55.3; H, 4.0; N, 9.2. Found: C, 55.2; H, 3.9; N, 9.1.

#### 6-Acetylthieno[2,3-*b*]pyridine (5). (a). From Enaminoester 4.

A mixture of 0.1 g of enaminoester **4** and 6 ml of concentrated hydrochloric acid was refluxed for 24 hours. Solid potassium carbonate was added to pH 7 and the mixture was extracted three times with chloroform. The residue from evaporation of dried (sodium sulfate), combined extracts was sublimed at 20-30° (0.005 mm) to yield 50.1 mg (86%) of powder, mp 80-82°; ir: 1685  $\text{cm}^{-1}$  (C=O); pmr:  $\delta$  8.17 and 8.05 (d of d,  $J_{4,5} = 8.2$  Hz, 2H, H-4 and H-5), 7.74 (d,  $J_{2,3} = 6$  Hz, H-2), 7.33 (d, H-3), 2.79 (s, 3H, Ac); ms: (70°) [11] 177 ( $M^+$ , 100), 162 ( $\text{TPCO}^+$ , 27), 149 (20), 135 ( $I^+$ , 82), 134 ( $\text{TP}^+$ , 99), 43 ( $\text{Ac}^+$ , 30); uv:  $\lambda$  max 247 nm ( $\log \epsilon$  4.26), 289 (4.16).

Anal. Calcd. for  $\text{C}_9\text{H}_7\text{NOS}$ : C, 61.0; H, 4.0; N, 7.9. Found: C, 61.1; H, 3.9; N, 7.7.

#### (b). From Cyano Compound 2.

To the Grignard reagent from 164 mg (6.75 mg-atoms) of magnesium,

0.42 ml of methyl iodide, and 5 ml of ether in a nitrogen atmosphere was added dropwise a solution of 0.9 g (5.63 mmoles) of **2** in 20 ml of benzene. The mixture was refluxed for 24 hours, cooled to 0°, treated with 15 ml of 6 *N* hydrochloric acid, and again refluxed for 6 hours. The aqueous layer was separated, neutralized with sodium bicarbonate, and extracted with chloroform. The benzene-ether layer was washed with aqueous sodium bicarbonate, added to the chloroform solution, dried (sodium sulfate), and evaporated. The brown residue was recrystallized from aqueous ethanol (charcoal) to give 0.7 g (70%) of tan powder, mp 82.5-84°, undepressed on admixture with product from part (a). Spectral data for products from (a) and (b) were also identical.

#### Ethyl 3-Amino-3-(6-thieno[2,3-*b*]pyridyl)-2-propenoate (6).

A mixture of 228 mg (0.75 mmole) of enaminoester **4**, 0.83 mmole of sodium ethoxide, and 10 ml of absolute ethanol was refluxed for 24 hours. The resultant gel was rotoevaporated, treated with 1.5 ml of water, adjusted to pH 14 by addition of 2 *M* sodium hydroxide, and extracted three times with 10-ml portions of chloroform. Evaporation of dried (sodium sulfate), combined chloroform extracts and slow sublimation at 60-65° (0.05 mm) gave 149 mg (80%) of slightly yellow powder, mp 79-82°, ir: 3470, 3340 ( $\text{NH}_2$ ), 1660  $\text{cm}^{-1}$  (C=O); pmr (hexadeuteriodimethylsulfoxide):  $\delta$  8.38 (d,  $J_{4,5} = 8.2$  Hz, H-4), 8.03 (d, H-2) which overlaps 8.02 (d, 2H total, H-5), 7.75 (broad s, disappears on addition of deuterium oxide,  $\text{NH}_2$ ), 7.54 (d,  $J_{2,3} = 6$  Hz, H-3), 5.47 (s, C=CH), 4.13 (q,  $J_{E} = 7$  Hz, 2H,  $\text{CH}_2\text{CH}_3$ ), 1.25 (t, 3H,  $\text{CH}_3$ ); ms: (150°) 248 ( $M^+$ , 16), 176 (42), 161 ( $\text{TPC} \equiv \text{NH}^+$ , 57), 135 ( $I^+$ , 71), 134 ( $\text{TP}^+$ , 100), 68 (52), 63 (43), 45 ( $\text{CHS}^+$ , 81), 43 (88); uv:  $\lambda$  max 244 nm ( $\log \epsilon$  4.28), 335 (4.28).

Anal. Calcd. for  $\text{C}_{12}\text{H}_{12}\text{N}_2\text{O}_2\text{S}$ : C, 58.0; H, 4.9; N, 11.3. Found: C, 58.0; H, 4.7; N, 11.1.

#### Ethyl 3-Oxo-3-(6-thieno[2,3-*b*]pyridyl)propanoate (7).

A solution of 165 mg (0.54 mmole) of enaminoester **4** and 310 mg (2.2 mmoles) of boron trifluoride etherate in 10 ml of absolute ethanol was refluxed for 48 hours and then rotoevaporated. The residue was treated with 1.1 ml of water and 10 ml of chloroform. The chloroform layer was combined with further chloroform extracts of the aqueous layer, dried (sodium sulfate), and evaporated. The residual liquid was chromatographed on a thick-layer plate (20 × 20 cm, 0.2 cm thick) of alumina with carbon tetrachloride as solvent to yield two zones: acetyl derivative **5**,  $R_f > 0$ ; ketoester **7**,  $R_f = 0$ . Acetone extraction of the latter zone gave a semisolid which was evaporatively distilled at 50-60° (0.03 mm) to yield 52 mg (39%) of a cream powder, mp 52-56°; ir: 3120 (chelated OH), 1735 (ester C=O), 1695  $\text{cm}^{-1}$  (keto C=O); pmr (hexadeuterioacetone):  $\delta$  8.44 (d,  $J_{4,5} = 8$  Hz, 1H, H-4 or H-5), 8.09 (d,  $J_{2,3} = 6$  Hz, H-2) which overlaps 8.07 (d, 2H total, H-5 or H-4), 7.56 (d, H-3), 4.21 (s, O=CCH<sub>2</sub>C=O) which overlaps 4.15 (q, 4H total,  $\text{CH}_2\text{CH}_3$ ), 1.20 (t,  $J_{E} = 7$  Hz, 3H,  $\text{CH}_3$ ); ms: (100°) 249 ( $M^+$ , 54), 204 (22), 177 ( $[\text{M} - (\text{CH}_2 = \text{CH}_2 + \text{CO}_2)]^+$ , 34), 162 ( $\text{TPCO}^+$ , 50), 135 ( $I^+$ , 69), 134 ( $\text{TP}^+$ , 100); 110-111\* (162 - 134); uv:  $\lambda$  max 235 nm ( $\log \epsilon$  4.24), 249 (4.29), 291 (4.23).

Anal. Calcd. for  $\text{C}_{12}\text{H}_{11}\text{NO}_3\text{S}$ : C, 57.8; H, 4.5; N, 5.6. Found: C, 58.0; H, 4.2; N, 5.9.

#### 6-Carbamidoylthieno[2,3-*b*]pyridine (8).

A mixture of 192 mg (1 mmole) of methyl imidate **3a**, 56.6 mg (1.06 mmoles) of ammonium chloride, and 10 ml of 80% ethanol was refluxed for 24 hours. The solution was concentrated *in vacuo*, treated with 10 ml of 1 *N* sodium hydroxide, and extracted three times with 20-ml portions of chloroform. Rotoevaporation of the dried (sodium sulfate) extract produced a solid which was sublimed at 75-80° (0.005 mm) to give 148 mg (84%) of powder, mp 119-121°; ir: 3470, 3310 ( $\text{HN} = \text{C-NH}_2$ ), 1630  $\text{cm}^{-1}$  (N-C=N stretch) [12]; pmr:  $\delta$  8.16 (s, 2H, H-4 and H-5), 7.62 (d,  $J_{2,3} = 6$  Hz, H-2), 7.31 (d, H-3), 5.1 (broad s, 3H,  $\text{HN} = \text{C-NH}_2$ ); pmr (hexadeuterioacetone):  $\delta$  8.28 (s, 2H, H-4 and H-5), 7.87 (d,  $J_{2,3} = 6$  Hz, H-2), 7.48 (d, H-3), 6.57 (broad s); ms: (110°) 178 (34), 177 ( $M^+$ , 100), 161 ( $\text{TPC} \equiv \text{NH}^+$ , 77), 160 (42), 135 ( $I^+$ , 78), 134 ( $\text{TP}^+$ , 44), 91 (27); uv:  $\lambda$  max 245 nm ( $\log \epsilon$  4.41), 291 (4.19).

*Anal.* Calcd for  $C_8H_7N_3S$ : C, 54.2; H, 4.0; N, 23.7. Found: C, 54.4; H, 3.8; N, 23.8.

6-(4,5-Dihydroimidazol-2-yl)thieno[2,3-*b*]pyridine (**9**).

To a solution of 0.17 ml (2.5 mmoles) of ethylene diamine in 2.5 ml of absolute ethanol was added a solution of 478 mg (equimolar amount) of methyl imidate **3a** in 3 ml of the same solvent. The mixture was refluxed for two days, until a test by thin-layer chromatography with alumina/chloroform showed that all **3a** ( $R_f > 0$ ) had reacted (product  $R_f = 0$ ), and then rotoevaporated. The residue was dissolved in ether and filtered. Evaporation of the solvent plus sublimation of the residue at 90-95° (0.005 mm) gave 302 mg (59%) of shiny powder, mp 134-137°; ir: 3240 (NH), 1600  $cm^{-1}$  (N-C=N stretch) [12]; pmr (hexadeuterioacetone):  $\delta$  8.29 and 8.17 (2 d,  $J_{4,5} = 8.5$  Hz, H-4 and H-5), 7.85 (d,  $J_{2,3} = 6$  Hz, H-2), 7.46 (d, H-3), 3.77 (s, 4H,  $CH_2CH_2$ ), 3.34 (broad s, disappears on addition of deuterium oxide, NH); ms (160°): 204 (15), 203 ( $M^+$ , 100), 202 (30), 175 ( $[M - C_2H_4]^+$ , 18), 174 (84), 161 (TPC  $\equiv NH^+$ , 26), 134 (TP $^+$ , 85); uv:  $\lambda$  max 241 nm ( $\log \epsilon$  4.41), 292 (4.16).

*Anal.* Calcd. for  $C_{10}H_9N_3S$ : C, 59.09; H, 4.46; N, 20.67. Found: C, 59.12; H, 4.50; N, 20.74.

6-(4,5,6,7-Tetrahydro-1,3-diazepin-2-yl)thieno[2,3-*b*]pyridine (**10**).

In the same manner used to synthesize **9** there was reacted 0.25 ml (2.5 mmoles) of 1,4-diaminobutane with 489 mg (equimolar amount) of **3a** over a period of 36 hours. The crude product was evaporatively distilled at 100-110° (0.005 mm) to give a yellow liquid which solidified on standing to yield 491 mg (85%) of **10**, mp 86-89° (sintering at 82°). Recrystallization from acetone gave tan shiny polygons, mp 89-92° (sintering at 87°); ir: 3340 (NH), 1645  $cm^{-1}$  (N-C=N stretch) [12]; pmr:  $\delta$  8.29 (d,  $J_{4,5} = 8.2$  Hz, H-4), 8.05 (d, H-5), 7.53 (d,  $J_{2,3} = 6$  Hz, H-2), 7.25 (d, H-3) 3.1-4.0 (broad s, 4H), 1.7-2.1 (m, 4-5H); ms: (100°) 231 ( $M^+$ , 100), 230 (92), 203 (29), 174 (58), 161 (TPC  $\equiv NH^+$ , 37), 134 (TP $^+$ , 69), 91 (28); uv:  $\lambda$  max 247 nm ( $\log \epsilon$  4.50), 291 (4.29).

*Anal.* Calcd. for  $C_{12}H_{13}N_3S$ : C, 62.3; H, 5.7; N, 18.2. Found: C, 62.2; H, 5.4; N, 18.1.

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[9] Unless otherwise noted, infrared spectra were determined on potassium bromide pellets by means of a Beckman IR-10 instrument; ultraviolet spectra, on solutions in 95% ethanol by means of a Cary model 15 spectrophotometer; and pmr spectra, on deuteriochloroform solutions with tetramethylsilane as internal reference by means of a Varian XL-100 instrument. Dr. Richard Wielesek determined mass spectra by means of a CEC model 21-110 double focusing instrument, operated at 70 eV. In general, the ms data presented for each compound consist of the temperature of the ion source (°C), the m/e value for every peak  $\geq 134$  and of relative abundance  $\geq$  the minimal percentage shown in the various parentheses, and any apparent metastable peak (indicated by an asterisk) plus the corresponding ion decomposition pathway. For some compounds significant peaks at m/e < 134 are also shown. For compound **4** the molecular ion is included despite its lower abundance (5%) than for its congeneric reported ions. The symbol TP refers to the 6-thieno[2,3-*b*]pyridyl group. Elemental analyses were also obtained by Dr. Wielesek or by Guelph Chem. Labs., Guelph, Ont., Canada.

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