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A systematic investigation of the reactivity of 2,4,6-trichloropyrimidine with phenoxide nucleophiles has been conducted. Conditions have been described which lead to mono-, di-, and trisubstituted-pyrimidines. Unexpected product distributions for mono- and disubstituted products were observed and explanations for these results are offered.

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We have begun to explore the reactivity of 2,4,6-trichloropyrimidine **1** with a variety of nucleophiles with the goal of developing multisubstituted pyrimidines in which different substituents could be introduced sequentially. There is a significant body of literature that describes the reaction of **1** with neutral nucleophiles such as ammonia [1], methylamine [2], dimethylamine [3], and benzylamine [4] among others. Our initial report in this area described the reaction of **1** with ethanolamine and diethanolamine [5].

Replacement of the chlorine atoms by oxygen nucleophiles, however, is less extensive. Reactions involving **1** and a variety of alkoxides [6-8] proceeds quite readily.

We describe here our systematic investigations involving a variety of 4-substituted phenols under considerably milder conditions. A preliminary report included one example from this study [11].

Treatment of equimolar amounts of **1** with various 4-substituted phenols **2** in the presence of an equivalent amount of sodium hydroxide at room temperature afforded very good to excellent yields of monosubstituted products **3** and **4**, see Figure 1. While the formation of isomeric monosubstituted products was expected, the ratio of **3** to **4** was most surprising. Ratios ranging from 8:2 to 9:1 were initially isolated from the reaction. This assessment of the two isomers was based on ^1H nmr analysis of the mixture. Until

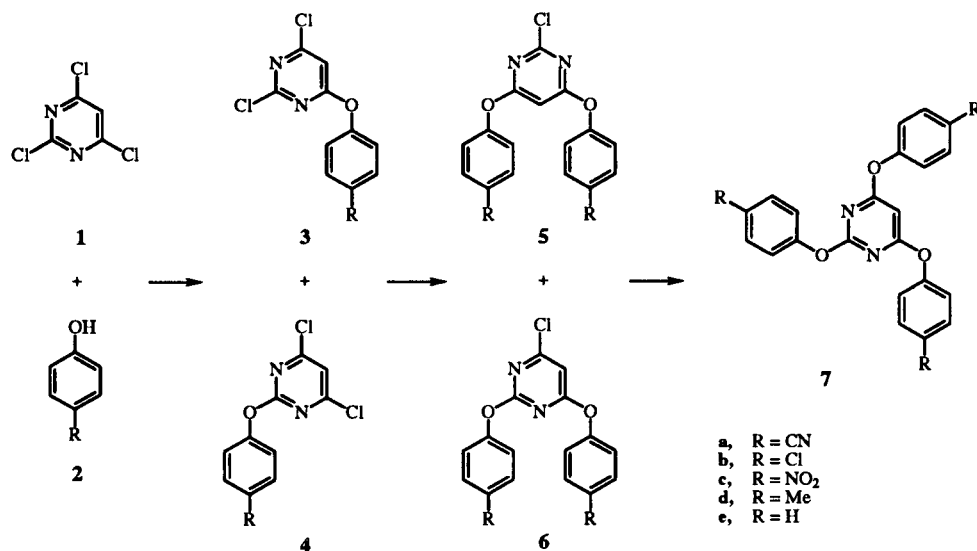


Figure 1

Since a suggested order of reactivity of nucleophiles places aryloxides considerably below alkoxides [9], we believed some selectivity could be achieved with substituted phenoxides as nucleophiles. Only one example involving phenols has been described [10]. In that case all three chlorine atoms of **1** were replaced by heating several phenols with potassium hydroxide at 215° for twenty minutes resulting in a 90% yield of the corresponding triaryloxy pyrimidines.

now the ratio of 4-substituted-pyrimidines to 2-substituted-pyrimidines arising from **1** has usually been in the order of 2:1 or 3:1 [2,3,5]. These previous observations have led to the assumption that there is little difference in reactivity for the C-Cl bond in either position 2 or 4. Statistically, a ratio of 2:1 should occur if both positions are equally reactive. However, these earlier reports all dealt with neutral nucleophiles. In the present circumstance the anionic nucleophile definitely favors substitution at the C-Cl bond of position 4.

One tempting explanation for these observations is found in a consideration of the mechanistic pathway. Most substitution reactions of this type follow a S_NAr (addition-elimination) process. However, it has been postulated that the intermediate Meisenheimer complex involving a *para*-quinoid structure is more favored than the corresponding *ortho*-quinoid structure [12-15], which is illustrated in Figure 2. Providing some support for this explanation is the observation that in the monochloropyridine series replacement of the chlorine by methoxide is in the order 4-Cl $\gg$ 2-Cl $>$ 3-Cl. It is postulated that the difference between 4-Cl and 2-Cl is attributable to the Meisenheimer intermediate where the ring nitrogen *para* to the tetrahedral carbon can bear the negative charge better than the *ortho* nitrogen [12,13]. There is parallel behavior with 4-Cl and 2-Cl pyrimidines [14]. In a study of thiophenoxide with tetrafluorophthalonitrile, reaction in methanol leads to an 8:1 ratio of two products. The major product is obtained by replacement of the two fluorine atoms *para* to the cyano groups. The minor product is derived from replacement of all four fluorine atoms. The formation of the major product is attributable to a *para*-quinoid intermediate [15].

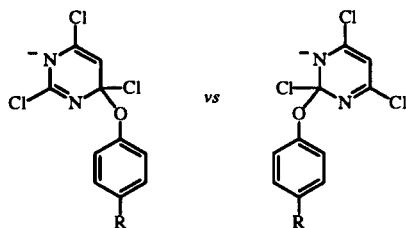


Figure 2

Purification of the crude product by recrystallization afforded only pure 3. The assignment of structure 3 is based on elemental analysis, mass spectral data, 1H nmr, and ^{13}C nmr. The 1H nmr spectrum is particularly useful for structural assignment because it displays a signal for the C-5 proton that is distinct from the aromatic ring protons. Furthermore, this signal is highly influenced by the electronic effects of neighboring groups. Thus, chlorine atoms in both positions 4 and 6 place the C-5 proton signal further downfield than the corresponding C-5 proton signal when the neighboring atoms are chlorine and oxygen.

When 1 was allowed to react with two equivalents of the phenols 2 in the presence of an excess of sodium carbonate, good yields of a mixture of isomeric disubstituted products 5 and 6 were obtained. The ratio of the two disubstituted products is approximately 1:1. This observation was even more unexpected than the results obtained during monosubstitution since the formation of 5 was not anticipated. To our knowledge no 4,6-disubstituted products

have ever arisen from similar reactions of 1 with other nucleophiles.

Compound 5 can only arise from 3 while 6 can come from either 3 or 4. Assuming that the ratio of ~9:1 for the 3/4 mixture obtained during the disubstitution process the rate of formation of 6 from 4 must be faster than either of the other rates, namely 3 $\rightarrow$ 5 and 3 $\rightarrow$ 6. It seems less probable that very much of 6 could be obtained from 3 due to the failure of position 2 to participate during the monosubstitution process.

It is possible that the argument offered to explain the preponderant formation of 3 over 4, namely enhanced stability of a *para*-quinoid intermediate, is appropriate here as well. Since the formation only of 5 would have been predicted using the *para*-substitution explanation, these results suggest a very strong competing factor that would decrease the yield of 5 by half.

We also considered that an alternative mechanism such as $S_{RN}1$ could be involved [16]. This process operates through a radical ion intermediate that would not necessarily follow the pattern exhibited by S_NAr processes in the past. To test this hypothesis, 1 was treated with 2b under the same conditions except that radical scavengers were added. No effect on either the ratio of 5 to 6 or the overall yield was observed which eliminated this pathway as a viable explanation.

Again, purification of the mixture was accomplished by recrystallization which yielded only 5 in pure form. Characterization by elemental analysis, mass spectra, 1H nmr, and ^{13}C nmr led to this assignment of the structure. Similar observations of the 1H nmr signal for the C-5 protons flanked by heteroatoms contributed to this assignment.

In order to ascertain less vigorous conditions sufficient to achieve trisubstitution as reported earlier [10], we subjected 1 to treatment with 2 as well as unsubstituted phenol. The triaryloxy pyrimidines 7 were obtained in high yields upon treatment of 1 with three equivalents of 2 and three equivalents of sodium hydroxide in dimethyl sulfoxide at 50°. Under these same conditions we also obtained the previously reported triphenoxy pyrimidine 7e in 92% yield. Even though 7b-e were previously described [10] we subjected these compounds to full characterization, in part because of differences between the literature melting points and those we obtained. Spectral data and elemental analysis supported these structural assignments.

EXPERIMENTAL

Melting points were determined using open capillary tubes in a Thomas-Hoover apparatus and are uncorrected. Infrared spectra were obtained in potassium bromide on a Perkin Elmer 1600 Series FTIR. The 1H and ^{13}C nmr spectra were recorded on a General Electric QE 300 instrument at 300 MHz and 75 MHz, respectively,

with tetramethylsilane as the internal standard. Relative integrals of peak areas are in agreement with the assigned structures. Ultraviolet spectra were recorded on a Cary 1 UV-Visible spectrophotometer. Mass spectra were measured on a Hewlett Packard 5995A GC/MS instrument using a direct insertion probe. Elemental analyses were performed by Galbraith Laboratories, Knoxville, TN.

2,6-Dichloro-4-(4'-cyanophenoxy)pyrimidine (3a).

2,4,6-Trichloropyrimidine (0.92 g, 5.0 mmoles) was dissolved in 10 ml of acetone and the solution cooled to 0° and stirred. Meanwhile a solution of 4-cyanophenoxide was prepared by dissolving 4-cyanophenol (0.595 g, 5.0 mmoles) and sodium hydroxide (0.205 g, 5.1 mmoles) in water (10 ml). The aqueous phenoxide solution was added slowly to the acetone solution. A white precipitate formed rapidly and the mixture was slowly warmed to room temperature and stirred for an additional 3 hours. After dilution with water (20 ml) the crude product was filtered to give 1.2 g (90%). The crude product contained the other isomer, 4,6-dichloro-2-(4'-cyanophenoxy)pyrimidine 4a, as a minor component in a ratio of 90:10.

This was recrystallized from methanol/ether to give pure 3a, mp 136-138°; ir (potassium bromide): ν 3113, 2220 (CN), 1547, 1493, 1402, 1338, 1270, 1195, 1109, 852, 543 cm^{-1} ; uv (methanol): λ max 207 nm (ϵ 22,300), 231 nm (ϵ 20,750), 256 nm (ϵ 11,000); ^1H nmr (dimethyl- d_6 sulfoxide): δ 7.54 (d, 2H, J = 8.4 Hz, aromatic), 7.62 (s, 1H, H-5), 8.00 (d, 2H, J = 8.4 Hz, aromatic); ^{13}C (dimethyl- d_6 sulfoxide): δ 171.0, 162.8, 158.9, 155.8, 135.4, 123.6, 119.1, 110.0, 108.6; ms: m/z 267 (21), 265 (35), 230 (100), 163 (25).

Anal. Calcd. For $\text{C}_{11}\text{H}_5\text{N}_3\text{Cl}_2\text{O}$: C, 49.62; H, 1.88; N, 15.79. Found: C, 49.60; H, 1.82; N, 15.61.

2,6-Dichloro-4-(4'-chlorophenoxy)pyrimidine (3b).

This compound was prepared using the procedure described for 3a. The crude product was obtained in 85% yield and contained the other isomer, 4,6-dichloro-2-(4'-chlorophenoxy)pyrimidine 4b, as a minor component in a ratio of 80:20.

This was recrystallized from hexane to give pure 3b, mp 78-80°; ir (potassium bromide): ν 3100, 1547, 1477, 1402, 1338, 1258, 1189, 1103, 970, 847 cm^{-1} ; uv (methanol): λ max 205 nm (ϵ 20,400), 258 nm (ϵ 8,100); ^1H nmr (deuteriochloroform): δ 6.86 (s, 1H, H-5), 7.10 (d, 2H, J = 9.0 Hz, aromatic), 7.40 (m, 2H, J = 8.7 Hz, aromatic); ^{13}C (deuteriochloroform): δ 163.2, 160.4, 150.4, 132.3, 130.4, 123.2, 106.6; ms: m/z 276 (27), 239 (100), 241 (70), 172 (34), 111 (29).

Anal. Calcd. For $\text{C}_{10}\text{H}_5\text{N}_2\text{Cl}_3\text{O}$: C, 43.56; H, 1.81; N, 10.16. Found: C, 43.73; H, 1.92; N, 10.30.

2,6-Dichloro-4-(4'-nitrophenoxy)pyrimidine (3c).

This compound was prepared using the procedure described for 3a. The crude product was obtained in 68% yield and contained the other isomer, 4,6-dichloro-2-(4'-nitrophenoxy)pyrimidine 4c, as a minor component in a ratio of 85:15.

This was recrystallized from chloroform/hexane to give pure 3c, mp 124-128°; ir (potassium bromide): ν 3091, 1552, 1488, 1397, 1199, 1109, 980, 852 cm^{-1} ; uv (methanol): λ max 204 nm (ϵ 26,500), 266 nm (ϵ 15,300); ^1H nmr (deuteriochloroform): δ 7.01 (s, 1H, H-5), 7.35 (d, 2H, J = 9.3 Hz, aromatic), 8.30 (d, 2H, J = 9.3 Hz, aromatic); ^{13}C (deuteriochloroform): δ 170.1, 163.7, 160.3, 156.5, 146.1, 126.0, 122.6, 107.3; ms: m/z 287 (28), 285 (40), 250 (100), 204 (19), 183 (12), 137 (3)

Anal. Calcd. For $\text{C}_{10}\text{H}_5\text{N}_3\text{Cl}_2\text{O}_3$: C, 41.96; H, 1.75; N, 14.69. Found: C, 41.86; H, 1.71; N, 14.56.

2,6-Dichloro-4-(4'-methylphenoxy)pyrimidine (3d).

This compound was prepared using the procedure described for 3a. The crude product was obtained in 85% yield and contained the other isomer, 4,6-dichloro-2-(4'-methylphenoxy)pyrimidine 4d, as a minor component in a ratio of 85:15.

This was recrystallized from methanol to give pure 3d, mp 49-52°; ir (potassium bromide): ν 3100, 1547, 1498, 1403, 1258, 1183, 1103, 980, 847 cm^{-1} ; uv (methanol): λ max 206 nm (ϵ 27,200), 251 nm (ϵ 12,000); ^1H nmr (deuteriochloroform): δ 2.38 (s, 3H, -CH₃), 6.75 (s, 1H, H-5), 7.02 (d, 2H, J = 8.4 Hz, aromatic), 7.23 (d, 2H, J = 8.4 Hz, aromatic); ^{13}C (deuteriochloroform): δ 171.6, 162.9, 160.3, 136.6, 130.9, 121.3, 106.2, 21.2; ms: m/z 256 (30), 254 (38), 221 (60), 219 (100), 183 (2), 152 (42), 91 (51).

Anal. Calcd. For $\text{C}_{11}\text{H}_8\text{N}_2\text{Cl}_2\text{O}$: C, 51.76; H, 3.14; N, 10.98. Found: C, 51.51; H, 3.14; N, 10.81.

2-Chloro-4,6-di-(4'-cyanophenoxy)pyrimidine (5a).

2,4,6-Trichloropyrimidine (0.92 g, 5.0 mmoles), 4-cyanophenol (1.19 g, 10.0 mmoles), and sodium carbonate (1.59 g, 15.0 mmoles) were taken up in ethanol (20 ml) and the mixture heated to reflux, with stirring, for 3 hours. After cooling to room temperature the mixture was diluted with water (100 ml) and the solid filtered, washed with water, and dried in air to give 1.57 g (90%) of a mixture of disubstituted products 5a and 6a in a ratio of 55:45.

This was recrystallized from acetonitrile to give pure 5a, mp 250-252°; ir (potassium bromide): ν 3070, 2215 (CN), 1579, 1493, 1413, 1263, 1210, 1012, 938, 836, 537 cm^{-1} ; uv (methanol): λ max 210 nm (ϵ 15,500), 234 nm (ϵ 19,800), 251 nm (ϵ 14,400); ^1H nmr (dimethyl- d_6 sulfoxide): δ 6.96 (s, 1H, H-5), 7.49 (d, 4H, J = 8.4 Hz, aromatic), 7.98 (d, 4H, J = 8.4 Hz, aromatic); ^{13}C (dimethyl- d_6 sulfoxide): δ 171.8, 158.8, 156.3, 135.3, 123.3, 118.9, 109.8, 94.1; ms: m/z 348 (23), 313 (78), 246 (22), 218 (29), 163 (97), 102 (100).

Anal. Calcd. For $\text{C}_{18}\text{H}_9\text{N}_4\text{ClO}_2$: C, 61.98; H, 2.58; N, 16.07. Found: C, 61.48; H, 2.54; N, 15.77.

2-Chloro-4,6-di-(4'-chlorophenoxy)pyrimidine (5b).

This compound was prepared using the procedure described for 5a. The crude product, 83%, consisted in a mixture of 5b and 6b in a ratio of 50:50.

This was recrystallized from hexane to give pure 5b, mp 160-161°; ir (potassium bromide): ν 3120, 1611, 1578, 1482, 1413, 1263, 1210, 1087, 1012, 943, 825, 670 cm^{-1} ; uv (methanol): λ max 204 nm (ϵ 23,400), 219 nm (ϵ 20,000), 249 nm (ϵ 8,400); ^1H nmr (deuteriochloroform): δ 6.21 (s, 1H, H-5), 7.10 (d, 4H, J = 8.7 Hz, aromatic), 7.40 (d, 4H, J = 8.7 Hz, aromatic); ^{13}C (deuteriochloroform): δ 172.8, 160.5, 151.8, 132.2, 130.0, 124.2, 91.5; ms: m/z 368 (27), 333 (36), 331 (66), 263 (19), 236 (12), 172 (63), 111 (100).

Anal. Calcd. For $\text{C}_{16}\text{H}_9\text{N}_2\text{Cl}_3\text{O}_2 \cdot 0.25\text{H}_2\text{O}$: C, 51.64; H, 2.57; N, 7.53. Found: C, 51.72; H, 2.32; N, 7.46.

2-Chloro-4,6-di-(4'-nitrophenoxy)pyrimidine (5c).

This compound was prepared using the procedure described for 5a. The crude product, 76%, consisted in a mixture of 5c and 6c in a ratio of 50:50.

This was recrystallized from chloroform to give pure **5c**, mp 248–52°; ir (potassium bromide): ν 3102, 1568, 1520, 1488, 1413, 1349, 1258, 1205, 852 cm^{-1} ; uv (methanol): λ max 204 nm (ϵ 41,000), 274 nm (ϵ 26,500), 249 nm (ϵ 8,400); ^1H nmr (dimethyl- d_6 sulfoxide): δ 7.05 (s, 1H, H-5), 7.55 (d, 4H, J = 8.7 Hz, aromatic), 8.35 (d, 4H, J = 8.7 Hz, aromatic); ^{13}C (dimethyl- d_6 sulfoxide): δ 171.8, 159.2, 157.6, 145.9, 126.6, 123.3, 94.4; ms: m/z 388 (48), 360 (100), 353 (796), 258 (18), 183 (70).

Anal. Calcd. For $\text{C}_{16}\text{H}_9\text{N}_4\text{ClO}_6 \cdot 0.25\text{H}_2\text{O}$: C, 48.87; H, 2.43; N, 14.25. Found: C, 48.81; H, 2.46; N, 14.48.

2-Chloro-4,6-di-(4'-methylphenoxy)pyrimidine (**5d**).

This compound was prepared using the procedure described for **5a**. The crude product, 87%, consisted in a mixture of **5d** and **6d** in a ratio of 55:45.

This was recrystallized from hexane to give pure **5d**, mp 105–108°; ir (potassium bromide): ν 3020–2920, 1616, 1584, 1552, 1498, 1413, 1263, 1210, 1016, 979, 940, 815 cm^{-1} ; uv (methanol): λ max 209 nm (ϵ 16,700), 243 nm (ϵ 9,050); ^1H nmr (deuteriochloroform): δ 2.45 (s, 6H, $-\text{CH}_3$), 6.05 (s, 1H, H-5), 7.05 (d, 4H, J = 8.7 Hz, aromatic), 7.21 (d, 4H, J = 9.0 Hz, aromatic); ^{13}C (deuteriochloroform): δ 172.8, 160.1, 150.4, 136.2, 130.8, 121.3, 90.2, 21.3; ms: m/z 326 (36), 298 (80), 291 (100), 223 (24), 152 (44), 91 (80).

Anal. Calcd. For $\text{C}_{18}\text{H}_{15}\text{N}_2\text{ClO}_2 \cdot 0.25\text{H}_2\text{O}$: C, 65.26; H, 4.72; N, 8.46. Found: C, 65.35; H, 4.55; N, 8.37.

2,4,6-Tri-(4'-cyanophenoxy)pyrimidine (**7a**).

2,4,6-Trichloropyrimidine (0.92 g, 5.0 mmoles), 4-cyanophenol (1.85 g, 15.5 mmoles), and powdered sodium hydroxide (0.62 g, 15.5 mmoles) were taken up in dimethyl sulfoxide (20 ml) and the mixture heated at -50° , with stirring, for 4 hours. After cooling to room temperature the mixture was diluted with water (100 ml) and the solid filtered, washed with water, and dried in air to give 88% of crude **7a**.

This was recrystallized from tetrahydrofuran/hexane to give pure **7a**, mp 202–205°; ir (potassium bromide): ν 3090, 2226 (CN), 1579, 1498, 1429, 1360, 1221, 1066, 1023, 836, 542 cm^{-1} ; uv (methanol): λ max 206 nm (ϵ 25,900), 233 nm (ϵ 21,900), 257 nm (ϵ 16,000); ^1H nmr (dimethyl- d_6 sulfoxide): δ 6.65 (s, 1H, H-5), 7.35 (d, 2H, J = 8.4 Hz, aromatic), 7.45 (d, 4H, J = 8.7 Hz, aromatic), 7.8 (d, 2H, J = 8.7 Hz, aromatic), 8.0 (d, 4H, J = 8.7 Hz, aromatic); ^{13}C (dimethyl- d_6 sulfoxide): δ 172.5, 163.4, 156.3, 156.2, 135.0, 134.6, 123.5, 119.1, 109.4, 108.9, 89.7; ms: m/z 431 (12), 313 (100), 246 (8), 213 (28), 169 (36), 102 (30).

Anal. Calcd. For $\text{C}_{25}\text{H}_{13}\text{N}_5\text{O}_3 \cdot 0.25\text{H}_2\text{O}$: C, 68.89; H, 3.02; N, 16.07. Found: C, 68.54; H, 2.97; N, 15.82.

2,4,6-Tri-(4'-chlorophenoxy)pyrimidine (**7b**).

This compound was prepared using the procedure described for **7a**. The crude product was obtained in 91% yield.

This was recrystallized from chloroform/hexane to give pure **7b**, mp 124–126° (lit. 107° [10]); ir (potassium bromide): ν 3080, 1600, 1573, 1482, 1424, 1349, 1215, 1087, 1010, 836, 804, 660 cm^{-1} ; uv (methanol): λ max 205 nm (ϵ 23,500), 221 nm (ϵ 21,800), 253 nm (ϵ 11,000); ^1H nmr (deuteriochloroform): δ 6.00 (s, 1H, H-5), 6.95–7.00 (m, 6H, aromatic), 7.20–7.40 (m, 6H, aromatic); ^{13}C (deuteriochloroform): δ 173.1, 164.4, 151.3, 130.0, 129.5, 123.3, 86.9; ms: m/z 460 (19), 331 (100), 305 (8), 222 (7), 178 (20), 111 (18).

Anal. Calcd. For $\text{C}_{22}\text{H}_{13}\text{N}_2\text{Cl}_3\text{O}_3$: C, 57.45; H, 2.83; N, 6.09. Found: C, 57.42; H, 2.92; N, 6.49.

2,4,6-Tri-(4'-nitrophenoxy)pyrimidine (**7c**).

This compound was prepared using the procedure described for **7a**. The crude product was obtained in 82% yield.

This was recrystallized from chloroform/hexane to give pure **7c**, mp 134–136°; ir (potassium bromide): ν 3091, 1568, 1520, 1482, 1434, 1328, 1221, 1109, 852 cm^{-1} ; uv (methanol): λ max 206 nm (ϵ 38,200), 274 nm (ϵ 26,500); ^1H nmr (deuteriochloroform): δ 6.3 (s, 1H, H-5), 7.20 (d, 2H, J = 8.7, aromatic), 7.30 (d, 4H, J = 9.0, aromatic), 8.10 (d, 2H, J = 9.3, aromatic), 8.30 (d, 4H, J = 8.7, aromatic); ^{13}C (deuteriochloroform): δ 172.4, 163.4, 157.2, 145.7, 145.4, 125.8, 125.4, 122.6, 89.2; ms: m/z 491 (20), 353 (100), 307 (22), 233 (60), 171 (80).

Anal. Calcd. for $\text{C}_{22}\text{H}_{13}\text{N}_5\text{O}_9$: C, 53.77; H, 2.65; N, 14.26. Found: C, 53.76; H, 2.75; N, 14.40.

2,4,6-Tri-(4'-methylphenoxy)pyrimidine (**7d**).

This compound was prepared using the procedure described for **7a**. The crude product was obtained in 85% yield.

This was recrystallized from chloroform/methanol to give pure **7d**, mp 125–127° (lit 118° [10]); ir (potassium bromide): ν 3027–2920, 1584, 1504, 1424, 1360, 1215, 1066, 1039, 1012, 809 cm^{-1} ; uv (methanol): λ max 206 nm (ϵ 41,000), 253 nm (ϵ 14,600); ^1H nmr (deuteriochloroform): δ 2.34 (s, 3H, $-\text{CH}_3$), 2.37 (s, 6H, $-\text{CH}_3$), 5.8 (s, 1H, H-5), 7.0–7.20 (m, 12H, aromatic); ^{13}C (deuteriochloroform): δ 173.6, 165.0, 150.6, 135.6, 134.9, 130.5, 130.0, 121.5, 85.8, 21.2; ms: m/z 398 (12), 291 (100), 197 (7), 158 (10), 135 (5), 91 (7).

Anal. Calcd. for $\text{C}_{25}\text{H}_{22}\text{N}_2\text{O}_3$: C, 75.38; H, 5.53; N, 7.04. Found: C, 75.16; H, 5.68; N, 7.41.

2,4,6-Tri-(phenoxy)pyrimidine (**7e**).

This compound was prepared using the procedure described for **7a**. The crude product was obtained in 92% yield.

This was recrystallized from methanol to give pure **7e**, mp 164–165° (lit 156° [10]); ir (potassium bromide): ν 3059, 1605, 1573, 1488, 1429, 1354, 1205, 1066, 1010, 810, 761, 667 cm^{-1} ; uv (methanol): λ max 207 nm (ϵ 33,600), 253 nm (ϵ 14,000); ^1H nmr (deuteriochloroform): δ 5.85 (s, 1H, H-5), 7.0–7.40 (m, 15H, aromatic); ^{13}C (deuteriochloroform): δ 173.5, 164.9, 152.8, 130.1, 129.6, 126.1, 125.5, 122.1, 121.8, 86.4 ppm; ms: m/z 356 (19), 279 (3), 263 (100), 237 (6), 169 (8), 77 (20).

Anal. Calcd. for $\text{C}_{22}\text{H}_{16}\text{N}_2\text{O}_3$: C, 74.14; H, 4.53; N, 7.86. Found: C, 73.83; H, 4.57; N, 7.77.

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