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3,5-Bis(trimethylsilyl)-1-methyl-4-thiophenoxypyridinium Iodide

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3,5-Bis(trimethylsilyl)-4-thiophenoxypyridine is readily converted to its pyridinium methiodide. The product is a precursor to "stunted" pyridylidene merocyanines that have bulky substituents at the 3- and 5-positions. Incorporation of such bulk is expected to afford chromophores with exceptionally high non-linear optical responses as a result of twisting between the donor and acceptor moieties [1].

A solution of 3,5-bis(trimethylsilyl)-4-thiophenoxypyridine [2] (1.0 g, 3.02 mmol) and methyl iodide (2.5 g, 17.6 mmol) in isopropanol (10 mL) was refluxed with stirring overnight, cooled and concentrated under vacuum to half its original volume. The resulting orange-yellow precipitate was recovered by filtration and washed with a little isopropanol to give a bright yellow solid (1.18 g, 83%) that was suitable for use without further purification. An analytical sample was prepared by recrystallisation from isopropanol to give the desired pyridinium iodide as bright yellow hairs.

M.p. 259-261 °C.

 1 H NMR (300 MHz, d_{6} -DMSO): 0.27, s, 18H; 4.42, s, 3H; 6.92-6.94, m, 2H; 7.20-7.25, m, 1H; 7.29-7.34, m, 2H.

¹³C NMR (75 MHz, *d*₆-DMSO): d 0.0 (CH₃), 48.2 (CH₃), 127.1 (CH), 127.2 (CH), 130.1 (CH), 137.5 (C_Q), 147.0 (C_Q), 151.0 (CH), 163.6 (C_Q).

Anal. Calc for C₁₈H₂₈INSSi₂ C 45.65, H 5.96, N 2.96. Found C 45.45, H 5.89, N 2.90.

IR (nujol): 1603, 1578, 1521, 1476, 1372, 1246, 924, 846, 774.

References

- 1. Albert, I. D. L.; Marks, T. J.; Ratner, M. A. J. Am. Chem. Soc. 1998, 120, 11174
- 2. Kay, A. J.; Woolhouse, A. D. *Molecules* **2001**, 6, M266.

Sample Availability: Available from the authors and from MDPI.

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