

The cyclopropyliminium rearrangement of cyclopropylthiazoles

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2-Cyclopropyl-4-methylthiazole 3a. Yield 83%. IR (CHCl₃, ν/cm^{-1}): 3088, 3008, 2952, 2924, 1680, 1528; EI-MS, m/z : 139 (72) [M]⁺, 138 (100) [M-H]⁺, 113 (32), 72 (52), 71 (66). ¹H NMR (200 MHz, CDCl₃), δ : 1.14 (m, 4H, CH₂CH₂), 2.22 (m, 1H, CH), 2.36 (s, 3H, Me), 6.59 (s, 1H, H(5)). ¹³C NMR (50 MHz, CDCl₃), δ : 10.9 (CH₂CH₂), 14.5 (CH), 17.2 (Me), 110.8 (C(5)), 152.1 (C(4)), 172.4 (C(2)). Anal. Calcd. for C₇H₉NS (%): C, 60.39; H, 6.52; N, 10.06. Found (%): C, 60.29; H, 6.56; N, 10.01.

4-Cyclopropyl-2-methylthiazole 4a was synthesized by a reported procedure.⁷ ¹H NMR (200 MHz, CDCl₃) δ 0.99 (m, 4H), 1.90–2.10 (m, 1H), 2.64 (s, 3H), 6.63 (s, 1H); ¹³C NMR (50 MHz, CDCl₃) δ 7.8 (CH₂CH₂), 12.2 (CH), 19.3 (Me), 110.1 (C(5)), 158.5 (C(4)), 165.4 (C(2)). The other physical data have been reported previously.⁷

4-Cyclopropyl-2-phenylthiazole 4b. Yield 95%; IR (CHCl₃, ν/cm^{-1}): 3412, 3108, 3087, 3008, 1525, 1501, 1463; EI-MS, m/z : 201 (100) [M]⁺, 200 (81) [M-H]⁺, 175 (10), 121 (49). ¹H NMR (300 MHz, CDCl₃), δ : 0.95 (m, 4H, CH₂CH₂), 2.08 (m, 1H, CH), 6.79 (s, 1H, H(5)), 7.39 (m, 3H, *m*- and *p*-CH), 7.90 (m, 2H, *o*-CH). ¹³C NMR (75 MHz, CDCl₃), δ : 8.2 (CH₂CH₂), 12.3 (CH), 110.6 (C(5)), 126.5 and 128.9 (*o*- and *m*-CH), 129.8 (*p*-CH), 133.9 (*i*-C), 159.9 (C(4)), 167.4 (C(2)). Anal. Calcd. for C₁₂H₁₁NS (%): C, 71.60; H, 5.51; N, 6.96. Found (%): C, 71.69; H, 5.48; N, 6.90.

3-Phenyl-6,7-dihydro-5H-pyrrolo[2,1-b]thiazol-4-ium bromide 5b. Yield 85%, mp 224–226 °C. IR (KBr, ν/cm^{-1}): 2996, 2936, 1628, 1500. EI-MS, m/z : 283 (2) and 281 (2) [M]⁺, 202 (4) [M-Br]⁺, 175 (63), 89 (100). ¹H NMR (200 MHz, DMSO-d₆), δ : 2.72 (m, 2H, H₂C(6)), 3.57 (t, 2H, H₂C(7), $J = 7.4$), 4.56 (t, 2H, H₂C(5), $J = 7.5$), 7.56–7.76 (m, 5H, Ph), 8.21 (s, 1H, H(2)). ¹³C NMR (50 MHz, DMSO-d₆), δ : 25.5 (C(6)), 30.5 (C(7)), 53.1 (C(5)), 124.4 (C(2)), 126.8 and 128.7 (*o*- and *m*-CH), 127.9 (*p*-CH), 130.0 (*i*-C), 141.8 (C(3)), 176.9 (C(7a)). Anal. Calcd. for C₁₂H₁₂BrNS (%): C, 51.07; H, 4.29; Br, 28.31; N, 4.96; S, 11.36. Found (%): C, 51.16; H, 4.32; N, 4.90.

3-Phenyl-6,7-dihydro-5H-pyrrolo[1,2-c]thiazol-4-ium iodide 6b. Yield 68%, heating for 2 h, mp 170–172 °C. IR (KBr, ν/cm^{-1}): 3443, 3114, 3101, 1584, 1470, 1446. EI-MS, m/z : 329 (2) [M]⁺,

202 (46) [M-I]⁺, 175 (100), 121 (15). ¹H NMR (300 MHz, DMSO-d₆), δ: 2.69 (m, 2H, H₂C(6)), 3.16 (t, 2H, H₂C(7), *J* = 7.5), 4.63 (t, 2H, H₂C(5), *J* = 7.2), 7.74 (m, 3H, *m*- and *p*-CH), 7.95 (d, 2H, *J* = 7.2, *o*-CH), 8.02 (s, 1H, H(1)). ¹³C NMR (75 MHz, DMSO-d₆), δ: 24.7 (C(6)), 27.5 (C(7)), 52.3 (C(5)), 114.5 (C(1)), 124.9 (*i*-C), 128.3 and 129.2(*o*- and *m*-CH), 132.6 (*p*-C), 153.5 (C(7a)), 163.7 (C(3)). Anal. Calcd. for C₁₂H₁₂INS (%): C, 43.78; H, 3.67; N, 4.25. Found (%): C, 43.62; H, 3.69; N, 4.30.