A New Approach to Ring Expansion of Keto-Aziridines to 2,5-diaryl Oxazoles

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General Procedure for Preparation of 2,5-Diaryl oxazoles (2a-h). I$_2$ (1.0 mmole) was added to a solution of the aziridines (1) (1.0 mmole) and dicyclohexylcarbodiimide (1.0 mmole) in CH$_3$CN (10 mL). The mixture was refluxed for 2-12 h. The crude product was purified by column chromatography (silica gel, EtOAc/Hexane: 2/5) to provide the desired 2,5-diaryl oxazole 2 (77-90%).

2-(3-Nitrophenyl)-5-phenyloxazole (2b). Yellow Solid, m.p. 140-143°C; IR (KBr): $\nu$ (cm$^{-1}$) 3060, 1522, 1351, 1133, 766, 692; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ = 8.85 (t, $J$ = 2.1 Hz, 1H), 8.36 (dt, $J$ = 7.6, 1.2 Hz, 1H), 8.23 (ddd, $J$ = 8.2, 2.2, 1.2 Hz, 1H), 7.67-7.70 (m, 2H), 7.60 (t, $J$ = 8.0 Hz, 1H), 7.38-7.43 (m, 3H), 7.30-7.34 (tt, $J$ = 7.9, 1.2 Hz, 1H), ppm; $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 161.7, 153.2, 148.4, 129.3, 129.1, 128.9, 128.7, 128.6, 128.3, 127.7, 126.8, 125.7, 123.2 ppm. Anal. Calcd for C$_{15}$H$_{10}$N$_2$O$_3$: C, 67.68; H, 3.80; N, 10.52%. Found: C, 67.54; H, 3.67; N, 10.12%.

2-(2,4-Dichlorophenyl)-5-phenyloxazole (2c). Yellow Solid, m.p. 90-92°C; IR (KBr): $\nu$ (cm$^{-1}$) 3064, 1662, 1590, 1482, 1101, 867, 828, 756, 685; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.25-7.31 (m, 1H), 7.34-7.39 (m, 2H), 7.42 (s, 1H), 7.47 (d, $J$ = 2.0 Hz, 1H), 7.65 (d, $J$ = 8.1 Hz, 2H), 7.97 (d, $J$ = 8.1 Hz, 2H) ppm; $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 121.1, 123.8, 124.5, 124.6, 127.4, 129.0, 129.1, 129.2, 130.0, 131.8, 148.7, 152.4, 158.8 ppm. Anal. Calcd for C$_{15}$H$_{9}$Cl$_2$NO: C, 62.09; H, 3.13; N, 4.83%. Found: C, 62.11; H, 3.05; N, 4.77%.

2-(4-Chlorophenyl)-5-phenyloxazole (2g). Yellow Solid, m.p. 100-102°C; IR (KBr): $\nu$ (cm$^{-1}$) 3062, 2991, 1655, 1585, 821, 754, 691; $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.1 (d, $J$ = 7.5, 2H), 7.84-7.61 (m, 3H), 7.51-7.32 (m, 5H) ppm; $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 160.2, 151.5, 136.4, 130.1, 129.1, 128.9, 127.8, 127.5.
125.9, 124.2, 123.5 ppm. Anal. Calcd for C₁₅H₁₀ClNO: C, 70.46; H, 3.94; N, 5.48%. Found: C, 70.04; H, 3.90; N, 5.18%.

5-(2-Naphthalyl)-2-phenyloxazole (2h)
Yellow Solid, m.p. 98-100°C; IR (KBr): ν (cm⁻¹) 3066, 3054, 2986, 1661, 1657, 1587, 1112, 821, 741, 677; ¹H NMR (400 MHz) (CDCl₃) δ 8.19-8.10 (m, 3H), 7.91-7.80 (m, 2H), 7.83 (d, J = 7.2 Hz, 1H), 7.77 (d, J = 7.2 Hz, 1H), 7.55 (s, 1H), 7.53-7.47 (m, 5H); ¹³C NMR (100 MHz) (CDCl₃) δ 161.4, 151.4, 133.4, 133.1, 130.4, 128.8, 128.7, 128.2, 127.9, 127.4, 126.8, 126.5, 126.4, 125.3, 123.9, 122.9, 122.1. Anal. Calcd for C₁₉H₁₃NO: C, 84.11; H, 4.83; N, 5.16%. Found: C, 84.27; H, 4.42; N, 5.22%.
2,5- diphenyl oxazole (2a)
2-(3-nitro-phenyl)-5-phenyl oxazole (2b)
2-(2,4-dichlorophenyl)-5-phenyl oxazole (2c)
5-(4-methoxy-phenyl)-2-phenyl-oxazole (2d)

5-(4-bromo-phenyl)-2-phenyl-oxazole (2e)
2-(4-Metoxephenyl)-5-phenyl oxazole (2f)
5-(2-naphthalen)-2-phenyl-oxazole (2h)