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LETTERS TO THE EDITOR

NOVEL BENZIMIDAZOLE DILITHIUM COMPOUND

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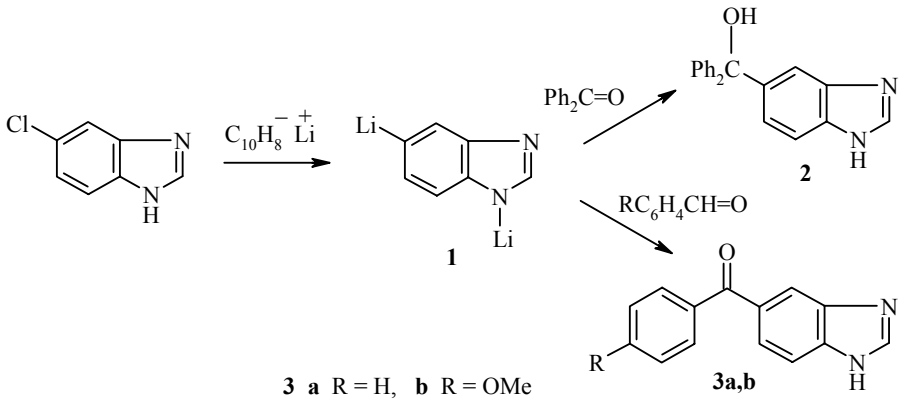
Keywords: 1,5-dilithium benzimidazole, 5-chlorobenzimidazole, lithium naphthalene, metallation.

We have established that when 5-chlorobenzimidazole reacts with lithium naphthalene at -15°C in THF, a novel benzimidazole dilithium compound is formed: 1,5-dilithium benzimidazole (**1**). The structure of compound **1** was determined by converting it to (5-benzimidazolyl)diphenylcarbinol (**2**).

Arylhetarylcarbinols are formed when active organometallic compounds of N-substituted azoles are reacted with aromatic aldehydes [1, 2]. However, when compound **1** is treated with aromatic aldehydes, instead of the expected aryl(5-benzimidazolyl)carbinols, we obtained aryl (5-benzimidazolyl) ketones **3a,b**.



The ^{1}H NMR spectra were taken on a Varian Unity 300 (300 MHz) in DMSO-d_6, internal standard TMS. The IR spectra were obtained on a Specord IR-75 spectrometer in nujol.

A solution of 5-chlorobenzimidazole (1.14 g, 7.5 mmol) in THF (10 ml) was added over a 5 min period, with stirring under an argon atmosphere at -15°C, to lithium naphthalene obtained from finely ground lithium (0.21 g, 30 mmol) and naphthalene (3.84 g, 30 mmol) in THF (20 ml). After 5 min, a solution of benzophenone or an aromatic aldehyde (35 mmol) in THF (10 ml) was added. The mixture was held for 1 h at -15°C and then for 2 h at 20-25°C, then a 20% aqueous solution of hydrochloric acid (15 ml) was added. The hydrochloric acid layer was separated, washed twice with 15 ml ether each time, and treated with a 22% aqueous solution of ammonia until pH > 7 was reached; the precipitate was filtered out, washed with water, and dried.

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(5-Benzimidazolyl)diphenylcarbinol (2). Yield 32%; mp 194°C (alcohol). IR spectrum, ν, cm^{-1}: 3210 (NH), 3400 (OH). ^1H NMR spectrum, δ, ppm (*J*, Hz): 6.15 (1H, s, OH); 7.05 (1H, d, *J* = 8.5, H-6(7)); 7.16-7.26 (10H, m, C_6H_5); 7.33 (1H, s, H-4); 7.41 (1H, d, *J* = 8.5, H-7(6)); 7.95 (1H, s, H-2); 12.13 (1H, br. s, NH). Found, %: C 79.89; H 5.45; N 9.43. $C_{20}H_{16}N_2O$. Calculated, %: C 79.98; H 5.37; N 9.33.

5-Benzoylbenzimidazole (3a). Yield 37%; mp 124-125°C (alcohol). IR spectrum, ν, cm^{-1}: 1650 (C=O), 2500-2800 (associated NH). ^1H NMR spectrum, δ, ppm (*J*, Hz): 7.48-7.75 (7H, m, H-6,7, C_6H_5); 7.96 (1H, s, H-4); 8.21 (1H, s, H-2); 12.58 (1H, br. s, NH). Found, %: C 75.53; H 4.64; N 12.65. $C_{14}H_{10}N_2O$. Calculated, %: C 75.66; H 4.54; N 12.60.

5-(*p*-Methoxybenzoyl)benzimidazole (3b). Yield 46%; mp 203-204°C (alcohol). IR spectrum, ν, cm^{-1}: 1640 (C=O), 3200 (NH). ^1H NMR spectrum, δ, ppm (*J*, Hz): 3.88 (3H, s, OCH_3); 6.99 (2H, d, *J* = 8.5, H-3',5'); 7.60 (2H, m, H-6,7); 7.75 (2H, d, *J* = 8.5, H-2',6'); 7.94 (1H, s, H-4); 8.20 (1H, s, H-2); 12.59 (1H, br. s, NH). Found, %: C 71.31; H 4.87; N 11.19. $C_{15}H_{12}N_2O_2$. Calculated, %: C 71.42; H 4.79; N 11.10.

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