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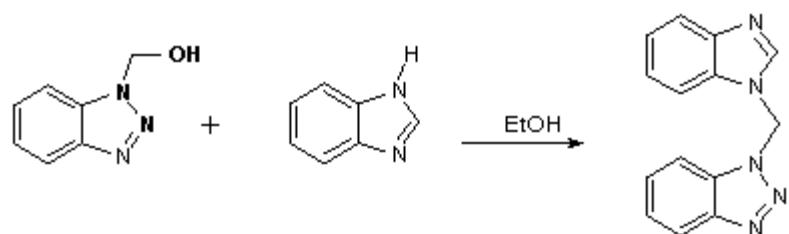
1-Benzimidazolyl-1-benztriazolylmethane

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Symmetrically substituted bis(azolyl)methanes are often prepared from azoles in dichloromethane under PTC conditions [1]. Unsymmetrically substituted 1-benztriazolylmethanes can be prepared from 1-hydroxymethylbenzotriazole [2] via nucleophilic substitution with secondary amines, in this case, benzimidazole.

1-Hydroxymethylbenzotriazole (2.98 g, 20 mmol) was dissolved in warm ethanol (50 ml). Benzimidazole (2.36 g, 20 mmol) was then added and the mixture was heated at reflux temperature. The reaction was monitored by TLC. After the reaction had ended the reaction mixture was set aside at 5 deg.C overnight. The crystalline product was then collected, washed with cold ether and recrystallized from ethanol. Yield 4.18 g (84.0 %) of a white crystalline powder.

M.p. 92-93 deg.C.

TLC (EtOAc): R_f 0.30.

¹H NMR (CDCl₃): 8.28 (s, 1H, -CH=), 7.00-8.13 (m, 8H, H_{arom}), 6.05 (s, 1H, CH₂), 5.63 (s, 1H, CH₂).

IR (cm⁻¹, KBr): 3179, 3115, 3096, 3063, 3001, 2965, 2863, 2797, 2741, 1458, 1408, 1306, 1273, 1246, 1235, 1159, 1076, 783, 768, 747, 619.

UV (λ_{max}/log e, methanol): 244/3.03, 250/3.05, 272/3.09, 279/3.06.

Anal. calc. for C₁₄H₁₁N₅ (249.0): C 67.47, H 4.42, N 28.10; found: C 67.17, H 4.30, N 27.84.

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References and Notes

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Sample Availability: Available from the author, 2g.

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