SYNTHESIS OF PYRAZOLO[3,4-d]PYRIDAZINE AND IMIDAZO[4,5-d]PYRIDAZINE DERIVATIVES

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Novel synthesis of 1,3,5-trisustituted pyrazolo[3,4-d]pyridazin-4(5H)-ones by photolysis is reported.

5-(Benzylidene-1'-methylhydrazino)-4-chloro-2-methyl-3(2H)-pyridazinone underwent irradiation (in benzene, 100 w, hp) to yield 1,5-dimethyl-3-phenyl-pyrazolo[3,4-d] pyridazin-4(5H)-one (mp 141-142°, 85.5 % in yield, ir, cm⁻¹: 1645 (CON \langle), nmr (in CDC1₃) τ : 1.40-1.70(2H, m, arom. ortho-H), 1.95(1H, s, C⁷-H), 2.35-2.60(3H, m, arom. meta- and para-H), 5.99(3H, s, CH₃), 6.15(3H, s, CH₃)). The photolysis was successfully applied to the formation of 1-benzyl-5-methyl-(mp 136-137°, 84.8 %), 1-methyl-5-phenyl-(mp 199-200°, 75.5 %), 1-benzyl-5-phenyl-(mp 175-176°, 79.1 %), 1-methyl-5-benzyl-(mp 138-139°, 87.8 %), 1,5-dibenzyl-3-phenyl-pyrazolo[3,4-d] pyridazin-4(5H)-one (mp 146-147°, 86.7 %). The key intermediates, 5-(benzylidene-1'-alkylhydrazino)-4-chloro-2-sustituted 3(2H)-pyridazinones, were smoothly derived from the respective 2-substituted 4,5-dichloro-3(2H)-pyridazinones, by treatment with hydrazine, benzaldehyde, and the corresponding alkyl halides successively.

Synthesis and physico-chemical property of some imidazo[4,5-d]pyridazine derivatives are also discussed, to compare with those of the pyrazolo[3,4-d]pyridazine described above.