unserer Meinung auch das Vorkommen des 1-Phenyl-1,2-propandions (**4**) im aetherischen Öl von *Catha edulis*, indem sein quantitativer Anteil proportional mit der Verminderung des Cathinonanteils im betreffenden Gewebe abnimmt[9]. Im Gegensatz zum 3,6-Dimethyl-2,5-diphenylpyrazin (**5**) bezw. seinen Dihydroverbindungen, die alle als Isolationsartefakte angesehen werden müssen, konnte **4** auch in frischem Pflanzenmaterial aufgefunden werden[9].

Physikalische und spektroskopische Daten. Cathinonoxalat: M.p. 172–175 °C; $[\alpha]_D^{21} = -34{,}4°$ (Methanol); UV (Wasser), λ_{max} ($\log\varepsilon$): 249 nm (4,08), 281 nm (3,40); ^{1}H-NMR (DMSO, Natriumtrimethylsilylpropansulfonat): 1,48 ppm (d, J = 7 Hz, Methyl), 5,13 ppm (q, J = 7,5 Hz, Methin), 7,57–7,75 ppm (m, Aromat, 3 Protonen), 8,1 ppm (dd, J_{ortho} = 7,5 Hz, J_{meta} = 2,5 Hz, Aromat, 2 Protonen); CD (Wasser), λ_{max} (θ): 285 nm (−2445), 248 nm (+9009).

N-Acetylcathinon: Farblose, visköse Masse; ^{1}H-NMR (Deuterochloroform, TMS): 1,42 ppm (d, J = 7 Hz, Methyl), 2,05 ppm (s, Acetyl), 5,57 ppm (p, J = 7 Hz, Methin), 6,6–6,8 ppm (b, Amin), 7,46–7,64 ppm (m, Aromat, 3 Protonen), 7,9 ppm (dd, J_{ortho} = 8 Hz, J_{meta} = 2 Hz, Aromat, 2 Protonen); MS, m/e (%): 191 (M^+, 23), 122 (15), 105 (88), 86 (100), 77 (70), 51 (20), 44 (82), 43 (48).

Cathine (**2** und **3** im Verhältnis 4:1): Base, M.p. 62–73 °C; $[\alpha]_D^{22} = +23°$ (Methanol); UV (0,01 n HCl-Lösung), λ_{max} ($\log\varepsilon$): 251 nm (2,20), 257 nm (2,28), 263 nm (2,20); ^{1}H-NMR (Deuterochloroform, TMS): 0,92 ppm (d, J = 7 Hz, Methyl), 2,56 ppm (b, Amin und Hydroxyl), 2,94 ppm (p, J = 7 Hz, Methin von **2**), 3,44 ppm (q, J = 6–7 Hz, Methin von **3**), 4,2 ppm (d, J = 7 Hz, Methin von **2**), 4,45 ppm (d, J = 5 Hz, Methin von **3**), 7,3 ppm (s, Aromat); MS, m/e (%): 152 (M + 1, 3,75), 151 (M^+, 1,25), 132 (10), 118 (11), 117 (10), 107 (29), 105 (18), 91 (15), 79 (61), 77 (80), 51 (30), 45 (51), 44 (100); CD (0,01 n HCl-Lösung), λ_{max} (θ): multipler negativer Cottoneffekt im Bereich von 270–240 nm, 266 nm (−110); für **2**: $\theta_{266} = -221$; für **3**: $\theta_{266} = +370$.

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Novel synthesis of 2,4-diphenylpyrimido [4,5-b] quinoline

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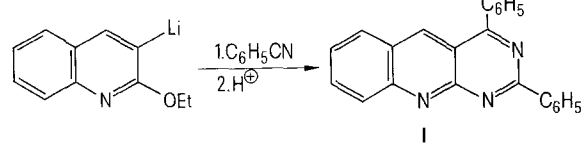
Summary. Reaction of n-butyllithium in ether with 2-ethoxyquinoline and further reaction with benzonitrile gives 2,4-diphenylpyrimido [4,5-b] quinoline (**I**). With the use of lithium di-isopropylamide, compound **I** is obtained in better yield without side products.

The pyrimido [4,5-b] quinoline ring system is of interest because of its structural similarity to the pyrimido [4,5-b] quinoxaline ring system of the naturally-occurring flavins. Conrad and Reinbach[2] reported the synthesis of the dihydroxy derivative by the condensation of o-aminobenzaldehyde and barbituric acid. King et al.[3] have extended this reaction for the synthesis of dialkylaminoalkyl derivatives. This route, which uses a preformed pyrimidine, lacks flexibility and versatility. Subsequently Taylor and Kalenda[4] described 4 elegant and versatile synthetic routes which allowed the preparation of many derivatives of this ring system. 1 of these routes involves the cyclisation of 2-aminoquinoline-3-carboxamide with reagents such as formamide.

In connection with a project of developing new chemotherapeutic agents, we needed a sample of 2,4-diphenylpyrimido [4,5-b] quinoline. To the best of our knowledge the above-mentioned routes do not afford the title compound. Now a novel and general single step synthesis of the pyrimido [4,5-b] quinoline ring system is reported.

2-Ethoxyquinoline was lithiated using n-butyllithium[5]. The metalation mixture was treated with excess of benzonitrile in ether at −20 °C, the cooling bath was removed and the reaction mixture was stirred overnight. Subsequent work-up afforded 2,4-diphenylpyrimido [4,5-b] quinoline (**I**) $C_{23}H_{15}N_3$, m.p. 225 °C. The compound **I** gave satisfactory elemental and spectral analysis. When lithium di-isopropyl amide was used for lithiation, compound **I** was obtained in 20% yield without side products.



I

This synthesis is reminiscent of the synthesis of a pyrimido [5,4-c] quinoline reported by us recently[6].

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