Triazino[2,1-*b*]quinazolone, a New Ring System

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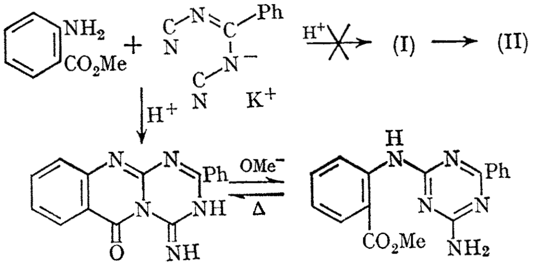
Summary The triazino[2,1-*b*]quinazolone ring system is formed by acid-catalysed cyclization of potassium dicyanobenzamidine with methyl anthranilate.

As part of an effort to prepare new fused *s*-triazino heterocycles with possible medicinal value, the preparation of a triazinoquinazolone system was investigated. Both triazine and quinazoline derivatives have each shown biological activity and so a fused heterocycle containing both ring systems was of interest.

The acid-catalysed cyclization† of potassium dicyanobenzamidine with methyl anthranilate could either give a triazino[1,2-*a*]-6-quinazolinone (II) or a triazino[2,1-*b*]-6-quinazolinone (III) system. That (III) was formed was shown by the fact that (i) treatment of the cyclized product with an excess of sodium methoxide gave 2-amino-4-(2-methoxycarbonylphenyl)amino-6-phenyl-*s*-triazine(IV); and that (ii) heating (IV) above its melting point gave (III). If (II) had been formed, treatment with an excess of sodium methoxide would have given 2,6-di-imino-1-(2-methoxycarbonylphenyl)-4-phenyl-1,2,3,6-tetrahydro-*s*-triazine (I), a possible intermediate from the cyclization[1] of the given starting materials. The synthesis of (III) by heating (IV) provides an alternative and potentially broad method for arriving at this new heterocyclic system. An unambiguous synthesis of (IV) was afforded by the reaction of 2-amino-4-chloro-6-phenyl-*s*-triazine with methyl anthranilate.



(III) (IV)

Only one of several tautomers of (III) is shown and the position of imino- and phenyl groups may be reversed. Since the reaction of mononitriles and anthranilate esters often yields substituted 2-amino-3,4-dihydro-4-quinazolinones,[2] [and since (II) was not formed] then the structure of (III) as shown, or a tautomer thereof, is quite likely. Compound (III) is a positional isomer of the riboflavin heterocyclic moiety.

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† Potassium dicyanobenzamidine[3] (0·06 mole), methyl anthranilate (0·063 mole), pyridine (0·054 mole), and anhydrous benzenesulphonic acid (0·12 mole) in anhydrous methanol (300 ml.) under reflux for 18 hr. Product (III) m.p. 342—343° (from dimethylformamide).

[1] J. T. Shaw, U.S.P. 3,215,693 (Nov. 2, 1965) (*Chem. Abs.*, 1966, **64**, 2110*e*).
[2] W. L. F. Armarego in "Fused Pyrimidines, Part I: Quinazolines," ed. D. J. Brown, Interscience, New York, 1967, p. 325.
[3] J. T. Shaw, *J. Org. Chem.*, 1962, **27**, 3890.