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STRUCTURE OF IBERICIN

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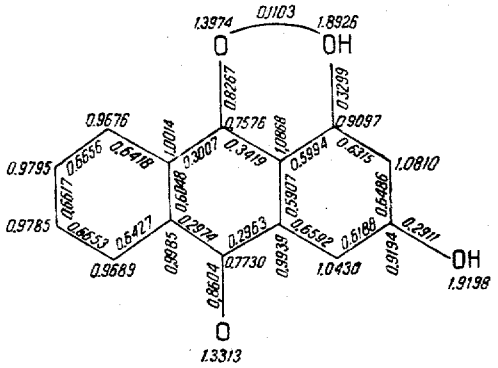
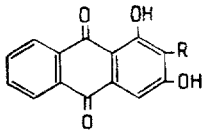
We have previously proposed for ibericin a structural formula in which the position of the side chain was established from the NMR spectrum [1].

A further study has shown that this structure is erroneous. In actual fact, in the NMR spectrum of 1, 3-dihydroxyanthraquinone (obtained by G. P. Syrova on a JNM-4H-100 instrument) in $CDCl_3$ the signals of the two aromatic protons are located at 6.58 ppm (J = 2 Hz) and 7.19 ppm (J = 2 Hz). It follows from the molecular diagram of 1, 3-dihydroxyanthraquinone (figure) obtained by calculation by the molecular orbital method in Hückel's approximation*, that the π-electron density at C-2 is greater than at C-4 (1.081 and 1.043, respectively). Consequently, the signal with δ = 6.58 relates to the proton in position 2 and



that with δ = 7.19 to the proton in position 4. The signal from the aromatic proton in the spectrum of ibericin in $CDCl_3$ is located at 7.17 ppm and is due to a proton in position 4.



I $R = CH_2OC_2H_5$

II $R = CH_2OH$

Thus, ibericin has the structure I. This conclusion was also confirmed by the results of a direct comparison of the IR spectra of ibericin and a compound of the same structure obtained and kindly given to us by Prof. R. H. Thomson (Dept. of Organic Chemistry, University of Aberdeen, Scotland) by heating lucidin II with ethanol containing traces of acid.

REFERENCES

1. V. A. Stikhin, A. I. Bankovskii, and M. E. Perel'son, KhPS [Chemistry of Natural Compounds], 12, 1966.
2. B. Pullman and A. Pullman, Rev. mod. phys., 32, 428, 1960.

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*The calculations were carried out with parameters taken from papers by the Pullmans [2]. The program for calculation was supplied by A. V. Tutkevich.