

ALL-UNION SCHOOL FOR INSTRUCTION IN PHYSICAL
METHODS FOR THE STUDY OF HETEROCYCLIC
COMPOUNDS

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An all-union school for instruction in physical methods for the study of heterocyclic compounds was organized by the Institute of Organic Synthesis of the Academy of Sciences of the Latvian SSR (AS of the Latvian SSR), the Division of Chemical and Biological Sciences of the AS of the Latvian SSR, and the Latvian Branch of the D. I. Mendeleev All-Union Chemical Society, with the support of the Division of General and Technical Chemistry of the Academy of Sciences of the USSR. The task facing the school was to raise the methodological level of research in the chemistry of heterocyclic compounds. Its aim was to give an accurate presentation of the possibilities of various instrumental (physical and physicochemical) and computational methods used for the interpretation of molecular structures and for the evaluation of the reactivities of heterocyclic compounds and to give an accurate presentation of the use of computer techniques for the treatment of data from physicochemical experiments.

The participants in the school were chemists from academic and applied-science institutes, problem laboratories, and the chairs of higher educational institutions (VUZ) of 18 cities that are chemical centers of the country (Moscow, Leningrad, Novosibirsk, Kiev, Sverdlovsk, Minsk, Rostov-on-Don, Kazan', Irkutsk, Saratov, Yaroslavl, Khar'kov, Ufa Krasnodar, Riga, as well as Angarsk, Shchelkovo, and Olaine). More than 200 participants (70 of whom were from other cities), representing almost all of the scientific organizations in which the problems of the heterocyclic chemistry are being worked out, were present. Ten two-hour lectures and four one-hour lectures were given at the school; in addition, the school consisted of seminar-consultations and a survey of modern instrumental technique and computers.

The opening lecture by the director of the Institute of Organic Synthesis, Academician of the Latvian SSR S. A. Giller, was devoted to the problems involved in the use of modern physical methods and computers in the chemistry of heterocyclic compounds. He compared the possibilities of the various methods and especially emphasized the achievements of modern mass spectrometry, NMR and ESR spectrometry, automated x-ray diffraction analysis, and gas-liquid chromatography. The revolutionizing effect of computers on concrete examples was demonstrated, and some problems for future development (electron microscopy of molecules and holography) were characterized.

Professor V. T. Aleksanyan (Moscow) examined the modern state of Raman spectroscopy with laser excitation and its possibilities for the investigation of organic molecules, noting that in many respects the method is superior to IR spectroscopy.

Master of Chemical Sciences V. A. Pestunovich (Irkutsk) illuminated his lecture with new aspects of the application of NMR for the study of fine-structure effects of heterocyclic compounds, touching upon the possibilities of both static and dynamic NMR spectroscopy for the quantitative evaluation of electronic effects, rates of rotation and inversion, and other conformational transitions.

The lecture by V. K. Voronov (Irkutsk) on the use of paramagnetic complexes for the investigation of complex heterocyclic systems (the so-called "shift method") and the lecture by A. E. Shvets (Riga) on mathematical programs for the simulation of NMR spectra useful for the interpretation of complex spectra were also devoted to NMR spectroscopy.

Translated from *Khimiya Geterotsiklicheskikh Soedinenii*, No. 4, pp. 572-573, April, 1973.

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Associate Member of the AS of the Latvian SSR Ya. P. Stradyn' (Riga) explained the principles and methods for the development of polarography and demonstrated the possibilities of this method for obtaining the physicochemical characteristics and reactivity indexes of heterocyclic molecules.

Master of Chemical Sciences R. A. Gavar (Riga) presented a lecture on the ESR spectra of anion radicals of heterocyclic systems obtained by electrochemical generation of these particles directly in the spectrometer resonator. The lecture by I. V. Turovskii (Riga) dealt with potentiometric and spectrophotometric methods for the determination of protolysis (ionization) constants of nitrogen-containing heterocycles.

Master of Chemical Sciences I. B. Mazheika (Riga) delivered a lecture on the dipole moments and structures of heterocyclic compounds in which he stressed the problems of vector calculation of group dipole moments of complex heterocycles composed of molecules of several heteroatoms.

Master of Chemical Sciences A. A. Anderson (Riga) examined the regularities of the behavior of heterocyclic compounds under the conditions of gas-liquid chromatography, particularly the interrelationship between the retention indexes and the molecular structures.

Master of Chemical Sciences Ya. Ya. Bleidelis (Riga) set forth the fundamentals of x-ray diffraction analysis, presented interesting examples of the interpretation of the complete structures of heterocyclic compounds, and touched upon the advances in automation of x-ray diffraction experiments.

The lecture by Master of Technical Sciences A. B. Rozenblit (Riga) on the use of computer technique in the treatment and analysis of data from physicochemical experiments was comprehensive. He not only discussed the basic fundamentals of the use of computers for the automation of physicochemical experiments but also presented examples of the usefulness of this method for the treatment of chromatographic, spectral, polarographic, and mass-spectrometric data.

Two lectures were devoted to computational methods. Professor V. I. Minkin (Rostov-on-Don) gave an interesting comparison of methods of quantum-chemical calculation that are currently in use and made a critical examination of the inadequacies of each of them as applied to the calculation of a given physicochemical parameter. Doctor of Chemical Sciences G. V. Bykov (Moscow) presented a lecture on a model of electronic charges of bonds and its application in organic chemistry.

The lectures and seminars as well as the exchange of ideas among the participants in the school gave a great deal of useful knowledge and stimulation for further research. In this connection, at the last session of the school - the first of its kind - there was a statement of a desire for periodic conducting of similar schools in various centers of the USSR that are engaged in the study of the chemistry of heterocyclic compounds.