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FROM CHEMICAL SHIFTS TO ISOTOPE SHIFTS (50TH ANNIVERSARY OF THE NMR METHOD)

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In 50 years, the nuclear magnetic resonance method has become a solid part of the arsenal of techniques for establishment of the structure of organic compounds. Today it is already unthinkable to have a paper on synthesis of new organic compounds in which the structure has not been confirmed by NMR data. Furthermore, the method has been successfully used for establishing the spatial structure of synthesized compounds, studying tautomeric equilibrium, electronic effects, and substituent effects. This has been promoted by the improvement in NMR instruments and the development of new research techniques.

I well remember my own first PMR spectrum of the hydrosilylation products of 2-vinylfuran, taken in the 1950s on an instrument with operating frequency 19.7 MHz. How simple and how uninformative! Three years later, already operating at 60 MHz, we not only determined the structure of the isomers obtained, but also established the acceptor character of the silyl, germyl, and stannyl substituents bonded to the furan ring. The operating frequency of the instrument was changing: 90 MHz, then 360 MHz, expanding the range of nuclei. After five more years, we began to study intramolecular effects in cyclic organosilicon animoalcohols using ^{13}C and ^{29}Si NMR. Later, the development of new pulse techniques made it possible determine the silicon–nitrogen spin–spin coupling constants in bicyclic and tricyclic compounds with an intramolecular Si–N in both ^{15}N and ^{29}Si NMR spectra with the natural abundance of isotopes. For the first time, the ^{73}Gr NMR spectra were obtained for asymmetric compounds and heterocyclic compounds of six-coordinate germanium.

Development of the ultrahigh-resolution ^{29}Si NMR method (É. Kupce) allowed us to not only measure the long-range silicon–nitrogen spin–spin coupling constants, but also to obtain the isotope shifts from all the isotopes of all the elements of chloromethylsiloxane molecules.

With the introduction of new NMR investigation methods, the nature of the papers in the journal Khimiya Geterotsiklicheskikh Soedinenii changed accordingly. Noting the 50th anniversary of the NMR method, we decided to devote a special issue of this journal to the study of heterocyclic compounds by the nuclear magnetic resonance method. Many colleagues in different countries have positively responded to our proposal. As a result, we have put together an issue of the journal in which, after a brief historical essay by R. Freeman, we present reviews and regular papers on the NMR study of the tautomerism of mesoionic compounds and derivative of dihydropyridazino[3,4-b]quinoxalines, isomerization of spiro[1,3-oxazolidino-4,2′-[2H]chromenes), the configuration and conformation of derivatives of aziridine and 1,3,2-dioxaborins, chelates of hetarylformazans, and derivatives of natural with anolide steroids, the orientation of benzofuran in a magnetic field, and also on electronic substituent effects in derivatives of furna, thiophene, indazole, and indolizine. The presented papers describe the application of ^{1}H, ^{13}C, ^{14}N, ^{15}N, ^{17}O, ^{29}Si, ^{31}P, ^{77}Se, ^{113,111}Cd, ^{199}Hg NMR using COSY, HMBC, HMQC, HOHAHA, INEPT, INVGATE, INADEQUATE, and NOE techniques and also lanthanide shift reagents.

The editors of the journal thank all the authors who sent papers for this jubilee issue and hope that its publication will promote further application of the NMR method for investigation of heterocyclic compounds.

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