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NMR Analysis of ^{13}C -Enriched Hydrocarbons

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^1H and ^{13}C nuclear magnetic resonance (NMR) spectra deliver information on the electronic structure of hydrocarbons. However, the natural abundance of ^{13}C nuclei is small ($\sim 1.1\%$) what is good for any fast analysis, as it simplifies the ^1H and ^{13}C spectra, but not so good for detail investigations. Using the fast ^1H and ^{13}C measurements many valuable NMR parameters are omitted, especially the variety of spin-spin coupling constants between magnetically active hydrogen and carbon-13 nuclei. It is possible to recover all the lost pieces of information when ^{13}C -enriched compounds are applied for NMR analysis. In such a case, the ^1H and ^{13}C spectra are much complex and their analysis requires more time though with computers all problems can be solved, as it is illustrated by the NMR spectra of ^{13}C -enriched hydrocarbons: acetylene- $^{13}\text{C}_2$, ethylene- $^{13}\text{C}_2$, ethane- $^{13}\text{C}_2$ and benzene- ^{13}C . For the above compounds, all the spin-spin coupling constants were determined and compared with the results of quantum-chemical calculations. It gives us more information on the electronic structure of investigated hydrocarbons what is important for precise analytical applications. The new NMR parameters can partially be observed also for ordinary hydrocarbons, i.e. without enrichment in ^{13}C , but their presence is marked so weakly that one should know their values before the analysis starts. Let us note that the fast and faultless recognition of gaseous mixtures in our atmosphere is the important problem of safety for all of us.

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Biography:

Dr. Karol Jackowski is employed at the Faculty of Chemistry, the University of Warsaw (Poland). He worked as a postdoctoral fellow at the University of Sheffield (Great Britain) in 1976-1977 and as a Visiting Assistant Professor at the University of Illinois at Chicago Circle (USA) in 1983-1985. At present, he is a Full Professor of Physical Chemistry at the University of Warsaw. Professor Dr. Karol Jackowski pioneered a new method of standardization of NMR spectra based on the direct measurements of absolute shielding. Since 2007 he is a member of ISMAR and Editorial Board of the International Journal of Spectroscopy.