The project "Qualitative and quantitative composition of oil and petroleum products" within the framework of the Strategic Academic Unit "Ecooil - Global Energy and Resources for the Materials of the Future".

The goal of the project is to adapt the methods of modern nuclear magnetic resonance (NMR) spectroscopy (one-dimensional NMR (1H, 13C) and two-dimensional NMR (COSY, HSQC, HMBC, TOCSY, HSQC-TOCSY, etc.) spectroscopy) to determining the qualitative and quantitative composition of oil and petroleum products, description in the NMR language of typical impurities present in these samples.
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RESEARCHES
The modern technic of NMR spectroscopy is not only increased sensitivity and high resolution, but also two-dimensional NMR spectroscopy methods that let us to extract additional information on the composition of oil and petroleum products samples from NMR spectra. In fact, NMR spectroscopy can be the main method of certification of any products of the oil industry. Taking into account the importance of products of processing hydrocarbon raw materials for the national economy, the task of applying modern NMR spectroscopy to determining the composition of oil and petroleum products is very important and relevant.

**Determination of the chemical composition, spatial structure and intramolecular mobility of organic and bioorganic compounds and complexes based on them in various solvents and in solid phase in such areas as organic and bioorganic chemistry, medicine and pharmacology.**

NMR spectroscopy can be used for qualitative and quantitative analysis of food products, isomeric products of organic compounds, polymeric substances, and natural products (oil, cellulose, etc.).

**WORK AND SERVICES**

1. **Analysis of samples in liquid phase and in solutions:**
   a) Determination of the chemical structure, the conformations of molecules in solutions, intermolecular interactions and equilibria, the purity of chemical compounds and the kinetics of the reactions;
   b) Analysis of the final and intermediate products of chemical reactions;
   c) Study of multiposition chemical exchange, structural analysis of proteins, enzymes, steroids, etc.

2. **Analysis of powdered and solid samples:****
   A) Structural analysis of compounds and complexes.
   B) Recording of high-resolution spectra, high-temperature spectra (up to 390 K), low-temperature spectra (down to 150 K).

**EQUIPMENT**

NMR spectrometer AVANCE - III-TM - HD – 700 “Bruker”
QCI CryoProbe sensor enables NMR measurements on cores - $^1$H, $^{13}$C, $^{15}$N, $^{31}$P; CP/MAS NMR - $^1$H, $^{13}$C, $^{15}$N; sensitivity of $^1$H $\sim 5600 : 1$ for 0.1% ethylbenzene solution.

The unit is located in room 104, Institute of Physics, KFU
$^1$H (500 MHz) and $^{13}$C (125.69 MHz), multicore, the ability to shoot two-dimensional NMR spectra (COSY, TOCSY, HSQC, NOESY), CP/MAS NMR on the $^{13}$C, $^{14}$N, $^{15}$N, $^{19}$F, $^{29}$Si; sensitivity of $^1$H - 200 : 1 for 0.1% ethylbenzene solution.

The unit is located in room 106, Institute of Physics, KFU

COFINANCING


EDUCATIONAL PROGRAMS

Lecture "NMR of crude oil"

PUBLICATIONS


Keywords: OpenLab, NMR, structure