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High-resolution NMR study of some light and heavy crude oils

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Petroleum as a natural object contains hundreds of substances mainly belonging to the three homologous series of hydrocarbons (alkanes, cycloalkanes, and aromatic hydrocarbons), as well as heteroatomic compounds (particularly, asphaltene-resinous substances) containing non-metals (sulfur, oxygen, nitrogen). Trace elements such as V, Ni, Fe, Zn, etc. are also present. In contrast to other physical-chemical methods, nuclear magnetic resonance (NMR) spectroscopy allows obtaining both qualitative and quantitative information on a mixture of organic compounds: types of molecules and their relative content [1]. Taking into account the importance of oil to the economy, there is a very important and urgent task for adaptation of modern 1D NMR (^1H , ^{13}C) and 2D NMR (COSY, HSQC experiments) spectroscopy to determination of oil composition.

The NMR methods can determine aromatic and aliphatic hydrogens and carbons in oil samples. In our previous work both ^1H and ^{13}C NMR have been applied to the study of some Bashkortostan and Tatarstan oils [2]. It was shown that the information on content of general functional groups (tertiary and primary carbon atoms, aromatic cores) and possible presence of olefins or water impurity can be obtained by NMR spectroscopy.

The aim of this study was to determine the qualitative and quantitative composition of four different samples of oils: two of which are low viscosity oils (less than 8 cP) from Middle-Nazym oilfield (one of which was subjected to heat treatment), and the other two are highly viscous oils (more than 25 cP) from Ashal'cha field (Republic of Tatarstan) and Vishanskoe deposit (Republic of Belarus) by means of the modern methods of NMR spectroscopy. ^1H , ^{13}C NMR, APT ^{13}C spectroscopy, two-dimensional ^1H , ^1H -COSY, ^1H , ^{13}C -HSQC NMR experiments were applied to provide detailed information on the hydrocarbon chemistry of the studied petroleum objects and to carry out comparative analysis between oil samples of different density and different origin.

[1] G. Kalabin, L. Kanitskaya, D. Kushnaryov, "Quantitative NMR spectroscopy of natural organic raw materials and products of its processing", Moscow: Chemistry, (2000), 408 p.

[2] I. Rakhmatullin, S. Efimov, B. Margulis, V. Klochkov, J. Petrol. Sci. Eng., (2017), accepted.