Crimson Publishers
Wings to the Research

Opinion

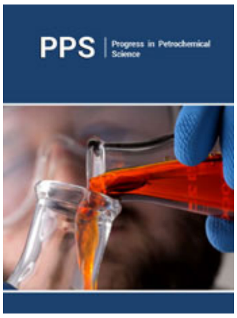
NMR Structural-Group Characteristics in Light, Heavy and Catalyzed Oils

Rakhmatullin IZ[1]*, Efimov SV[1], Tyurin VA[1], Klochkov AV[1], Varfolomeev MA[2] and Klochkov VV[1]

[1]Institute of Physics, Kazan Federal University, Russia

[2]Department of Petroleum Engineering, Kazan Federal University, Russia

ISSN: 2637-8035



***Corresponding author:** Ilfat Rakhmatullin, Institute of Physics, Kazan Federal University, Russia

Submission: July 28, 2022
Published: August 05, 2022

Volume 4 - Issue 3

How to cite this article: Rakhmatullin IZ, Efimov SV, Tyurin VA, Klochkov AV, Varfolomeev MA and Klochkov VV. NMR Structural-Group Characteristics in Light, Heavy and Catalyzed Oils. Progress Petrochem Sci. 4(3). PPS. 000590. 2022.
DOI: 10.31031/PPS.2022.04.000590

Opinion

^{13}C Nuclear Magnetic Resonance (NMR) spectroscopy has recently become increasingly popular as a tool for studying various petrochemical objects, the characteristics of natural raw materials and their individual organic compounds, expanding the possibilities for research in the field of geological and chemical problems [1].

The objective of this work is to carried out the comparison between light, heavy and catalyzed oil samples: obtaining their structural-group characteristics.

NMR experiments on studied oil samples were performed on a Bruker Advance III HD 700NMR spectrometer. The studied oil sample was diluted with deuterated chloroform. Field lock and shimming were achieved using the deuterium signal from $CDCl_3$ solvent.

Estimation of molar fractions C_p, C_{sq}, C_t, Car and the aromaticity factor (F_{CA}), and mean chain length (MCL) by integration of the corresponding areas of 13C NMR spectra was carried out in a way similar to our previous works [2-4] and presented in (Table 1).

Table 1: Molar fractions (%) of primary (C_p), secondary and quaternary (C_{sq}), tertiary (C_t), aromatic (C_{ar}) groups, aromaticity factor (F_{CA}) and mean chain length (MCL) of aliphatic hydrocarbons of light, heavy and catalyzed oil samples based on ^{13}C NMR spectra.

Group Type	Relative Molar Content, %		
	Light oil	Heavy oil	Catalyzed Oil (Ni-Co, Al2O3)
C_p	25.8	12	18.5
C_{sq}	53	46.2	55.4
C_t	10	12.6	10.8
C_{ar}	12.5	29.2	15.3
F_{CA}	0.123	0.292	0.155
MCL	6.9	11.8	7.5

(Table 1) Molar fractions (%) of primary (C_p), secondary and quaternary (C_{sq}), tertiary (C_t), aromatic (C_{ar}) groups, aromaticity factor (F_{CA}) and mean chain length (MCL) of aliphatic hydrocarbons of light, heavy and catalyzed oil samples based on ^{13}C NMR spectra.

Based on obtained data (Table 1), we can see that the highest percentage of primary and secondary/quaternary carbons is in light oil sample, which is however almost twice as low in the content of aromatic carbons. The twofold excess of the relative content of aromatic carbon in heavy oil sample compared with light oil sample is observed. The catalytic treatment of heavy oil leads to the fact that it approaches light oil in its structural-group characteristics. A decrease in the aromaticity factor (F_{CA}) and the average length of the hydrocarbon chain (MCL) also indicate about the success of the catalytic treatment of the studied heavy oil sample. Thus, there is a mutually inverse dependency for primary and aromatic carbons as the viscosity of the studied samples changes.

The ^{13}C NMR spectra showed a characteristic broader broadening in the aromatic area of the spectrum for heavy oil, but the number of separately distinguishable signals is already less than for the light oil sample. However, in this case, signals in the highly aromatic area related to the carboxy groups (COOH) of the carbon atom are clearly visible. Also, in the sample of heavy oil, signals from carbon atoms with a double bond in the presence of heteroatoms are observed. And their number is three times less compared to the light oil sample. For the catalyzed sample, we were able to clearly identify signals only for protonated carbon atoms. And it turned out that their number is two times less than for a sample of heavy oil and three times less than for a sample of light oil. It is also noticeable that a still rather strong broadening is retained in the aromatic region of the spectrum of the sample treated with the catalyst. Although the overall integration of this area and the structural group analysis show a noticeable decrease in the proportion of aromatic carbons for the catalyzed sample compared to the heavy oil sample (Table 1). Also, the signals in the NMR spectrum of catalyzed oil appear more clearly and are similar in shape to signals in a sample of light oil. There is a decrease in the signals of carbon CH_3 groups in the catalyzed oil sample. All these facts also prove that the use of a catalyst is very effective for upgrading oil and improving the quality of fuel.

Acknowledgement

This work was supported by the Ministry of Science and Higher Education of the Russian Federation under agreement No. 075-15-2020-931 within the framework of the development program for a world-class Research Center “Efficient developm

References

1. Edwards JC (2011) A review of applications of NMR spectroscopy in the petroleum industry. In: Nadkarni RA (Ed.), Spectroscopic analysis of petroleum products and lubricants, ASTM International, West Conshohocken, USA, pp: 423-473.
2. Rakhmatullin IZ, Efimov SV, Margulis B Y, Klochkov VV (2017) Qualitative and quantitative analysis of oil samples extracted from some Bashkortostan and Tatarstan oilfields based on NMR spectroscopy data. Journal of Petroleum Science and Engineering 156: 12-18.
3. Rakhmatullin IZ, Efimov SV, Tyurin VA, Al Muntaser AA, Klimovitskii AE, et al. (2018) Application of high resolution NMR (1H and 13C) and FTIR spectroscopy for characterization of light and heavy crude oils. Journal of Petroleum Science and Engineering 168: 256-262.
4. Rakhmatullin IZ, Efimov SV, Tyurin VA, Gafurov MR, Al Muntaser AA, et al. (2020) Qualitative and quantitative analysis of heavy crude oil samples and their SARA fractions with 13C nuclear magnetic resonance. Processes 8(8): 995.