Research of Eastern Siberia Oils with the Use of Infrared Spectroscopy Method

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Abstract. Oil is a multicomponent mixture and infrared spectroscopy may be one of the most instant methods for determining the classes of hydrocarbon compounds. Oil consists of organic and mineral compounds. It is found in all types of rocks and can be met in the most unexpected places. The rate and volume of oil and gas production depends on many factors involving natural and man-made ones. The forecast for the development of fluid systems of various types and for their regimes plays an important part in assessing water resources, their management conditions, and for designing and developing hydrocarbon deposits. Currently, Eastern Siberia is one of the most attractive regions for investors [1-3]. There is one of the largest Russian oil and gas basins belonging to the Siberian platform in the Irkutsk region [4-6]. This work presents the study of Eastern Siberia oils with the use of infrared spectroscopy in order to determine the chemical group composition and spectral indices of oils.

1. Introduction
The use of infrared (IR) spectroscopy is based on the fact that each separate organic compound possesses only its inherent absorption spectrum, that is, it is its unique property. The absorption of infrared radiation by a substance is conditioned by natural vibrations of the molecules as well as of individual structural groups in the molecule. The possibility of using IR spectra in petroleum chemistry is limited by the complexity of researched objects, nevertheless, it is possible to obtain useful results conducting a comparative study of systematically selected samples.

The infrared spectrometry method is very sensitive and to analyze a sample one needs a sufficiently small amount of a substance of any molecular weight under various aggregative conditions. When obtaining the spectrum, the recording time may be less than a minute, moreover, a significant value of signal-to-noise ratio allows working with low-transparency samples, such as natural oils [7,8].

Certain structural groups and bonds correspond to characteristic absorption bands. Identical structural groups or bonds can be part of the molecules of various compounds having various absorption spectra, but each of them will have one or more identical frequencies that are characteristic of a given structural group or bond. To define the belonging of frequencies in the spectra of the analyzed compounds to the groups of atoms or bonds the researchers use spectral atlases of infrared spectroscopy or tables with characteristic absorption frequencies of substances with known structure [9,10].
The method of determining the oil type using IR spectra was proposed by G. Brandens and S. Bhattacharyya; it corresponds to the generally accepted chemical classification of the three main classes of hydrocarbons and is based on a directly proportional relationship between the content of aromatic and methane structures of oil. The identification is carried out by measuring the relative intensities at the maxima of the analyzed characteristic absorption bands. According to the basic law of absorption, the band intensity is related to the number of absorbed groups in a specific layer of the substance. The research of oils, resins and petroleum products is carried out in the near, middle and far ranges of the IR spectrum [11-16].

2. Materials and methods
This work presents the study of Eastern Siberia oils with the use of infrared radiation spectra. Physical and chemical properties of oils are presented in Table 1.

Table 1. Physical and chemical properties of Eastern Siberia oils.

| Characteristics | Danilovsky | Ichyodinsky | Machchobinsky | Yarakta |
|-----------------|------------|-------------|---------------|---------|
| Density at 20°C, kg/m³ | 849.0 | 808.0 | 859.0 | 829.4 |
| Congelation temperature, °C | -38.0 | -53.0 | -47.0 | -38.0 |
| Molecular mass, a.m.u. | 245 | 185 | 281 | 224 |
| Content, % wt hard paraffins | 2.10 | 1.22 | 1.35 | 2.15 |

IR spectra were obtained using a Bruker IFS-25 spectrometer in a thin layer in the wavelength range of 600-4000 cm⁻¹. The interpretation of the spectra is shown in Table 2.

The chemical group composition was calculated on the base of the IR spectra [17]:

\[
\% A_l = \frac{D_{725}}{\Sigma D} \cdot 100 \text{ (alkane structures)} \quad (1.1)
\]

\[
\% H = \frac{D_{1035} + D_{1660}}{\Sigma D} \cdot 100 \text{ (naphthenic structures)} \quad (1.2)
\]

\[
\% A = \left( \frac{D_{1610}}{\Sigma D} \right) \cdot 100 \text{ (arene structures)} \quad (1.3)
\]

The spectral indices were calculated according to the values of the absorption bands of the IR spectra; the ratio of optical densities at the maxima of the absorption bands allowed obtaining spectral indices:

\[
C_{ar} = \frac{D_{1610}}{D_{725}} \quad (1.4)
\]

\[
C_{al} = \frac{D_{725} + D_{1380}}{D_{1610}} \quad (1.5)
\]

\[
C_b = \frac{D_{725}}{D_{1464}} \quad (1.6)
\]

where \(C_{ar}\) – aromaticity index; \(C_{al}\) – aliphatic index (characterizes the ratio of aromatic and n-paraffin hydrocarbons in oils); \(C_b\) – branching index which characterizes the structure of paraffin fragments.
5. The method can be used in comprehensive research of objects. Thus, the obtained spectral evidences of naphthenic oils are characterized by the calculation of the aromaticity index, which allows identifying high-aliphatic branched structures and the lowest aliphatic index as it is characteristic of the aromatic structures [18]. The band of 725 cm\(^{-1}\) is identified at 1380 cm\(^{-1}\) according to the absorption band. The intense band in the range of 1464 cm\(^{-1}\) is caused by scissor-like deformation vibrations of C–H bonds in methylene (CH\(_2\)) groups in the molecules of aliphatic hydrocarbons and in the side chains of naphthenic aromatic hydrocarbons as well as their derivatives, such as resins and asphaltenes.

The calculated indices presented in Table 2 reflect the ratio of substituted bi- and tricyclic aromatic structures to the total content of aromatic structures (C\(_{870/1610}\)) and the ratio of the sum of aliphatic fragments (C\(_{1464/1610}\)) to aromatic molecules (C\(_{1464/1610}\)).

The researched oils of Eastern Siberia do not differ much in their spectral indices; the oil of the Ichyodinsky field has the highest aromaticity and branching (C\(_b\)) indices [19]. The alkane chains of this oil have branched structures and the lowest aliphatic index (1.5). The low content of hard paraffins and molecular mass conditions the low congelation temperature (-53). The oil from the Machchobinsky field has the lowest aromaticity index and the highest aliphatic index (1.858). The branching index (1.335) indicates mainly that there are normal paraffin hydrocarbons in it.

The aromaticity index allows determining the type of oil as follows: methane – C\(_{ar} > 0.35\); naphthenic – 0.6 < C\(_{ar} < 1.2\); aromatic – C\(_{ar} > 2\) [20].

The analysis of spectral indices of aromaticity shows that the studied oils can be classified as naphthenic oils (Tabl 2).

Naphthenic oils are characterized by the predominant content of naphthenic hydrocarbons, as evidenced by the calculation of the oils’ chemical group composition by the IR spectra.

4. Conclusion

Thus, the obtained spectral indices allow characterizing the functional properties of oil more comprehensively. Taking into account the minimum time of spectra recording and processing of researched objects one can identify the type of oil without a chemical analysis. The IR spectroscopy method can be used in monitoring of oil production and oil refining at the molecular level.

5. References

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