Analysis of oil from Guafita fields (Venezuela) by uses two infrared analysis techniques: conventional transmission spectroscopy and attenuated total reflection (ATR) spectroscopy

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ABSTRACT

Oils from Guafita field (Barinas basin) were studied using two common spectroscopic techniques for liquid or viscous samples: transmission and attenuated total reflection (ATR). The obtained spectra were similar and there was an excellent correlation between compositional indexes calculated for oils analyzed by both techniques. When areas are integrated a large variability appears, related to band intensity and overlap. Oils from Guafita field show similar aromaticities, but present differences in the aliphaticity and branching, which could reflect secondary processes that took place in the reservoir.

Key words: FTIR, ATR, oils, Guafita, Barinas-Apure basin

EXPERIMENTAL

Five oil samples from the Guafita field, Barinas basin, Venezuela, were studied using two infrared analysis techniques, conventional transmission spectroscopy and attenuated total reflection (ATR) spectroscopy using a Varian 640 Model operated in Fourier Transform. For transmission spectra thin films of oil were laid on a potassium bromide (KBr) thin plate in the spectral range of 4000-400 cm^{-1}. For the ATR spectra a drop of oil was introduced in a simple bounce model MIRacle™ Pike technologies using the spectral range of 4000-650 cm^{-1}; spectra were subsequently corrected using the ATR correction algorithm for the Resolution Pro ™ software. Triplicate spectra were made for each sample using absorbance scale and 4 cm^{-1} resolution. Spectra were processed and areas for each band were calculated using the OMNIC software.

RESULTS AND DISCUSSION

Reproducibility of results

The absorption bands in the IR for the five oil samples are similar, regardless of the technique used. Each spectrum consists of two groups of bands associated with aliphatic and aromatic hydrocarbons, described and identified by Lamontagne et al. (2001). Each identified band area was integrated from valley to valley and data were normalized to compare the different spectra. With the normalized data we calculated the relative standard deviation percentage (RSD%) in order to determine the reproducibility of the integration methodology used. An example for two of the five samples used can be seen in Table 1.

Table 1 Integrated band areas and relative standard deviation percentage for two samples

	GF-7		RSD%		GF-24		RSD%	
	KBr	ATR	KBr	ATR	KBr	ATR	KBr	ATR
A_{724}	0.989	1.198	3.897	8.137	0.866	1.250	2.119	10.068
A_{743}	1.204	1.778	5.194	11.131	1.230	1.650	2.267	2.979
A_{814}	0.869	1.025	3.364	1.617	0.799	1.030	4.066	3.434
A_{864}	0.729	0.863	3.086	4.922	0.712	0.832	4.118	8.506
A_{1030}	0.697	0.561	18.912	6.273	0.629	0.646	7.252	10.922
A_{1376}	4.972	5.378	5.096	2.110	5.283	5.690	2.140	3.753
A_{1460}	13.008	13.261	3.740	0.683	13.877	13.835	2.414	3.232
A_{1600}	1.506	1.996	2.086	21.762	1.424	1.300	3.410	0.251
A_{1700}	0.428	0.645	10.069	19.993	0.461	0.405	10.800	8.587
$A_{(2872, 2962, 2953, 2926)}$	75.600	73.293	1.194	0.705	74.719	73.362	0.833	1.357

Areas measured for different bands by the two methods show variable reproducibility. The strongest signals and those that do not overlap ($A_{(2872, 2962, 2953, 2926)}$, A_{1376}, A_{1460}) have the lowest RSD%, while the signals associated with sulfoxide, carbonyl and aromatic groups (bending and stretching), with low intensities and a high overlap, show high and variable RSD%. For example, A_{864} and A_{814} are the signals that have the highest overlap and A_{1030}, A_{1600}, A_{1700} are the less intense.

Correlation between the spectrometric techniques used

The area values obtained were used to calculate indexes that characterize oils according to their chemical composition (Permanyer et al., 2002). Plots of the indexes calculated for both techniques show an excellent correlation (R^2 between 0.9686 and 0.9889 for all samples). As an example figure 1a shows the correlation obtained for sample GF-7.

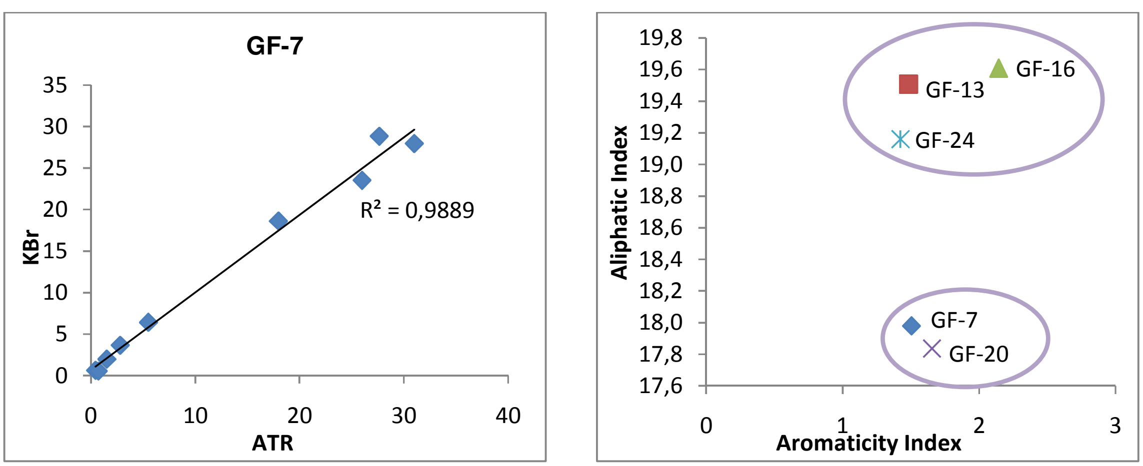

Figure 1 Correlation plots between a) indexes that describe the chemical composition of oil samples from Guafita field. b) aromaticity index vs. aliphatic index.

This shows that the correction algorithm used for the ATR data is entirely appropriate and makes possible the direct comparison of the ATR signals to those obtained by conventional transmission. Similarly high correlations validate both techniques for determining the chemical composition of oils.

Molecular characterization of oils

Although the oils studied belong to the same field, there are differences in their aliphatic index, separating them into two groups (figure 1b). Oils GF-7 and 20 are less aliphatic than GF-13, 16 and 24; a similar feature is observed with the branching index. These differences may be caused by secondary processes occurring within the reservoir. However, regarding the aromaticity and aromatic rings, the oils from Guafita field conform one group of samples, as shown by the indexes of aromaticity, substitution 1 and 2.

CONCLUSIONS

The spectra obtained by both techniques are similar, with two groups of bands associated to aliphatic and aromatic hydrocarbons; there is also a high correlation between the compositional indexes for oils calculated from both techniques of analysis.

The band areas were integrated from valley to valley, giving a variable reproducibility of the data that is associated with the intensity and the overlap of signals.

Oils from Guafita field are equally aromatic, but aliphatic compositional differences were found and may be associated with secondary processes occurring within the reservoir.

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