Correlation between the Stretching Vibrations of Aliphatic Groups and the Structural and Geochemical Properties of Crude Oils of the Same Genetic Type Using the Case of the Turija-Sever Oil Field, Pannonian Basin, Serbia

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SUPPLEMENTARY MATERIAL

Table A. Root-mean-square deviations (RMSD) and variances (Var.) of the peak maxima relative to mean values (Mean) for three parallel measurements of Tus-10, Tus-088, Tus-144 and Tus-083 samples covering the entire range of the CH₂/CH₃ branching factor

Sample	CH ₂ / CH ₃	CH ₃ asymmetric, cm ⁻¹				CH ₂ asymmetric, cm ⁻¹				CH ₂ symmetric, cm ⁻¹			
		Peak	Mean	RMSD	Var.	Peak	Mean.	RMSD	Var.	Peak	Mean.	RMSD	Var.
Tus-010	2.61	2952.63	2952.72	0.14	0.02	2920.90	2920.76	0.28	0.08	2851.69	2851.59	0.22	0.05
		2952.64				2920.44				2851.34			
		2952.88				2920.95				2851.75			
Tus-088	3.02	2952.72	2952.76	0.37	0.13	2919.56	2919.72	0.14	0.02	2850.51	2850.49	0.04	0.00
		2953.14				2919.78				2850.45			
		2952.41				2919.81				2850.52			
Tus-144	3.45	2952.90	2953.14	0.23	0.05	2918.70	2918.77	0.24	0.06	2849.57	2849.68	0.15	0.02
		2953.36				2918.57				2849.85			
		2953.16				2919.04				2849.61			
Tus-083	3.81	2952.85	2953.33	0.42	0.18	2917.19	2917.38	0.36	0.13	2848.98	2848.91	0.08	0.01
		2953.47				2917.15				2848.82			
		2953.66				2917.79				2848.94			

Table B. Test statistics of methylene stretching peak maxima

Samples	Vibrations	V_1 / V_2	$\bar{s}(x)$	$ \bar{x}_1 - \bar{x}_2 $	ξ
Tus-010 / Tus-088	asymmetric	0.08 / 0.02	0.224	1.04	5.69
	symmetric	0.05 / 0.00	0.118	1.10	8.53
Tus-088 / Tus-083	asymmetric	0.02 / 0.13	0.274	2.34	10.46
	symmetric	0.00 / 0.01	0.071	1.58	27.26
Tus-010 / Tus-083	asymmetric	0.08 / 0.13	0.324	3.38	12.78
	symmetric	0.05 / 0.01	0.173	2.68	18.98
Tus-010 / Tus-144	asymmetric	0.08 / 0.06	0.265	1.99	9.20
	symmetric	0.05 / 0.02	0.187	1.91	12.51

Tus-144 / Tus-083	asymmetric	0.06 / 0.13	0.308	1.39	5.53
	symmetric	0.02 / 0.01	0.122	0.77	7.73
Tus-088 / Tus-144	asymmetric	0.02 / 0.06	0.200	0.95	5.82
	symmetric	0.00 / 0.02	0.100	0.81	9.92

$$\bar{s}(x) = \sqrt{\frac{f_1 V_1 + f_2 V_2}{f_1 + f_2}} - \text{RMSD of two series of measurements;}$$

$$\xi = \frac{|\bar{x}_1 - \bar{x}_2|}{\bar{s}(x)} \sqrt{\frac{n_1 \cdot n_2}{n_1 + n_2}} - \text{test statistics;}$$

n_1 and n_2 – number of parallel measurements (3) for the calculation of $\bar{x}_1$ and $\bar{x}_2$ means;

f_1 и f_2 – degrees of freedom of series of measurements ($n - 1$);

V_1 и V_2 – variances of series of measurements;

The limiting value of ξ for $P = 0.9$ confidence probability is 2.92.