

Support Information for

Visbreaking of Heavy Oil in Supercritical Benzene

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Table S1. Chemical Shift of H Atoms Relating to Olefins Contained in Oil Samples

H atom type	chemical shift (ppm)	number of H atoms
-CR=CH ₂	4.5-4.7	2
-CH=CH ₂	4.7-5.0	3
-CR=CH-	5.0-5.2	1
-CH=CH-	5.2-5.5	2

Table S2. Equations Adopted in Modified Brown-Ladner Method for Determining Average Molecular Structure Parameters of Raw Heavy Oil or Liquid Products

parameter	equation	parameter	equation
M_n	from VPO	f	$12 \times n / (2 \times n + 1 - 2 \times r)$
β, γ	from $^1\text{H-NMR}$	BI	γ/β
H/C	$\text{H}\% \times 12 / \text{C}\%$	C_S	$f \times (\text{H}_\alpha + \text{H}_\beta + \text{H}_\gamma) \times \text{H}\% / 100$
n	$(\text{H}_\alpha + \text{H}_\beta + \text{H}_\gamma) / \text{H}_\alpha$	C_A	$\text{C}\% - C_S$
r	$(0.25 \times (\text{BI} + 4.12) - 1) / 2 \times (n - 1)$	C_1	$(12 \times \text{H}_{\text{aro}} + f \times \text{H}_\alpha) \times \text{H}\% / 100$
R_A	$(\#C_A - \#C_1) / 2 + 1$	$\#C_1$	$C_1 \times M_n / 1200$
R_N	$\%AS \times C_1 \times r / 100$	$\%AS$	$f \times \text{H}_\alpha \times \text{H}\% / C_1$
R_S	$\%AS \times \#C_1 / 100$	$\#C_A$	$C_A \times M_n / 1200$

Nomenclature

- M_n = number average molecular weight of oil samples, Da
- $\text{C}\%$ = weight percentage of carbon, wt%
- $\text{H}\%$ = weight percentage of hydrogen, wt%
- H_α = aliphatic hydrogen α to aromatic ring with chemical shift of 2.0-4.5 ppm
- H_β = aliphatic hydrogen β or further from aromatic ring with chemical shift of 1.05-2.0 ppm
- H_γ = methyl hydrogen γ or further from aromatic ring with chemical shift of 0.5-1.05 ppm
- H_{aro} = aromatic hydrogen with chemical shift of 6.0-9.0 ppm
- γ, β = peak height of H_γ or H_β from $^1\text{H-NMR}$
- BI = branchiness index.
- H/C = H/C atomic ratio
- n = average carbon number of alkyl substituents
- r = number of naphthene rings per substituent
- f = average C/H weight ratio of alkyl groups.
- C_S = fraction of non-aromatic C atoms in total C atoms contained in oil samples, %
- C_A = fraction of aromatic C atoms in total C atoms contained in oil samples, %
- C_1 = fraction of non-bridge aromatic ring carbons
- $\#C_1$ = average number of non-bridge aromatic ring carbon atoms per average molecule
- $\%AS$ = percent substitution of alkyl groups on non-bridge aromatic ring carbons
- $\#C_A$ = average number of aromatic ring carbon atoms per average molecule.
- R_A = average number of aromatic rings per average molecule
- R_N = average number of naphthenic rings per average molecule
- R_S = average number of alkyl substituents per average molecule