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Mechanistic Approach to Thermal Production of New Materials from Asphaltenes of Castilla Crude Oil

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Supplementary Figures:

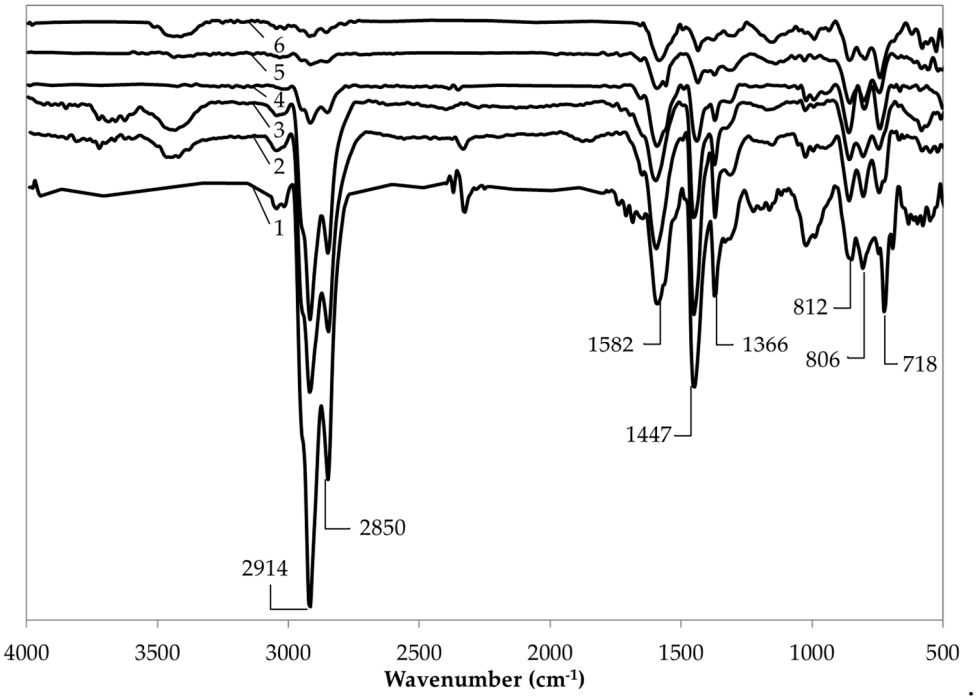

Figure S1. FTIR spectra of the original (1) and pyrolyzed asphaltenes at temperatures (°C): (2) 330, (3) 360, (4) 390, (5) 420, (6) 450.

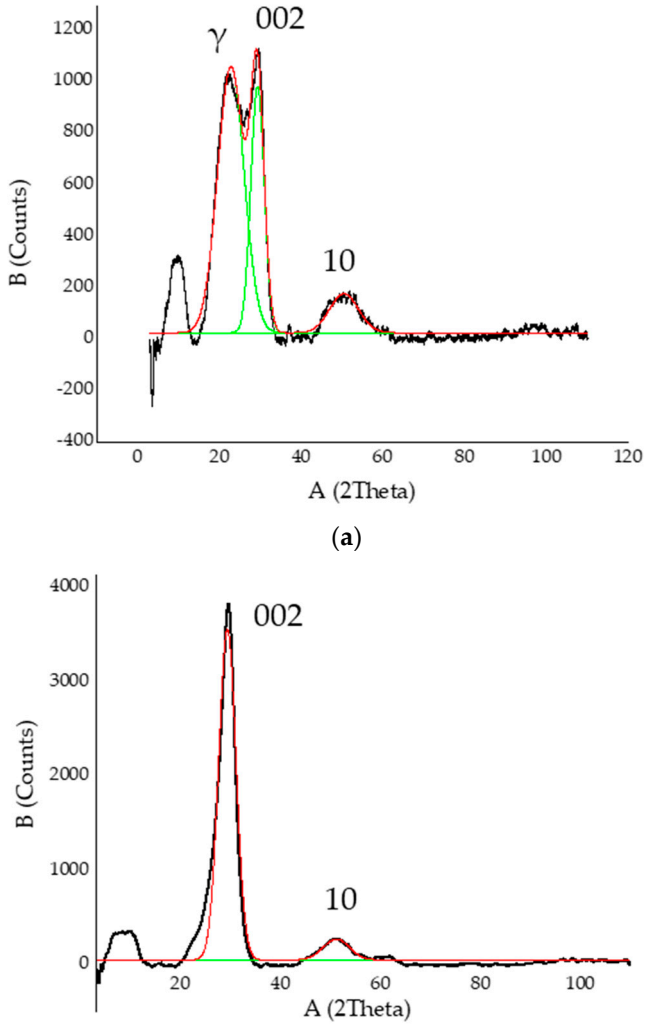

Figure S2. Diffractogram of the (**a**) original asphaltenes and; (**b**) coke obtained at 390 °C. .

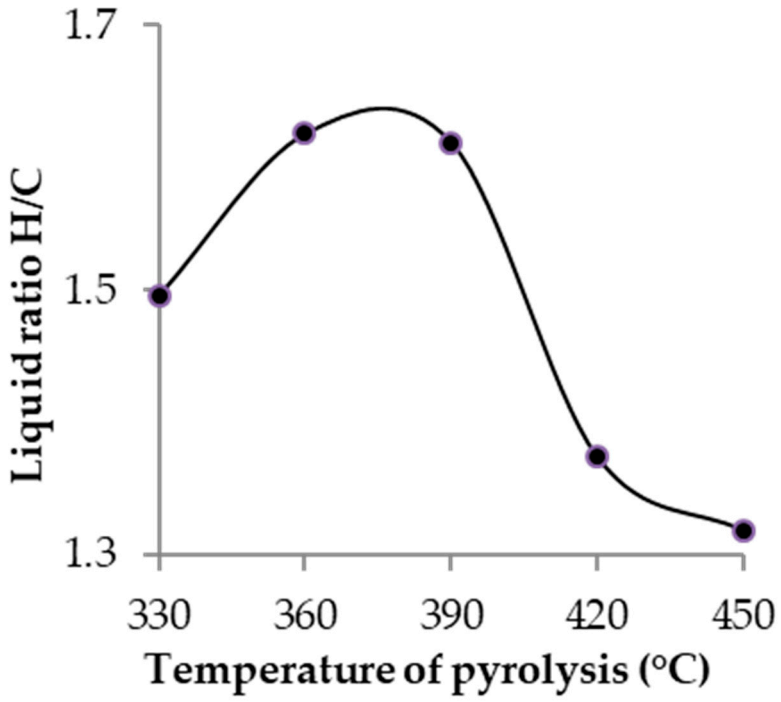

Figure S3. H/C ratio of the liquid product against the pyrolysis temperature.

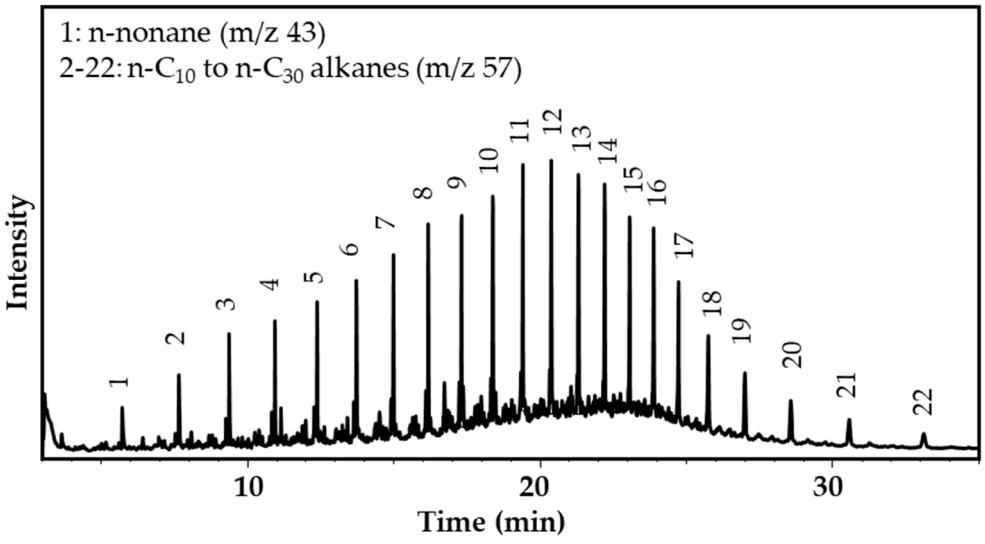

Figure S4. GC-MS analysis of the saturates fraction from the liquid product obtained through asphaltenes pyrolysis at 390 °C.

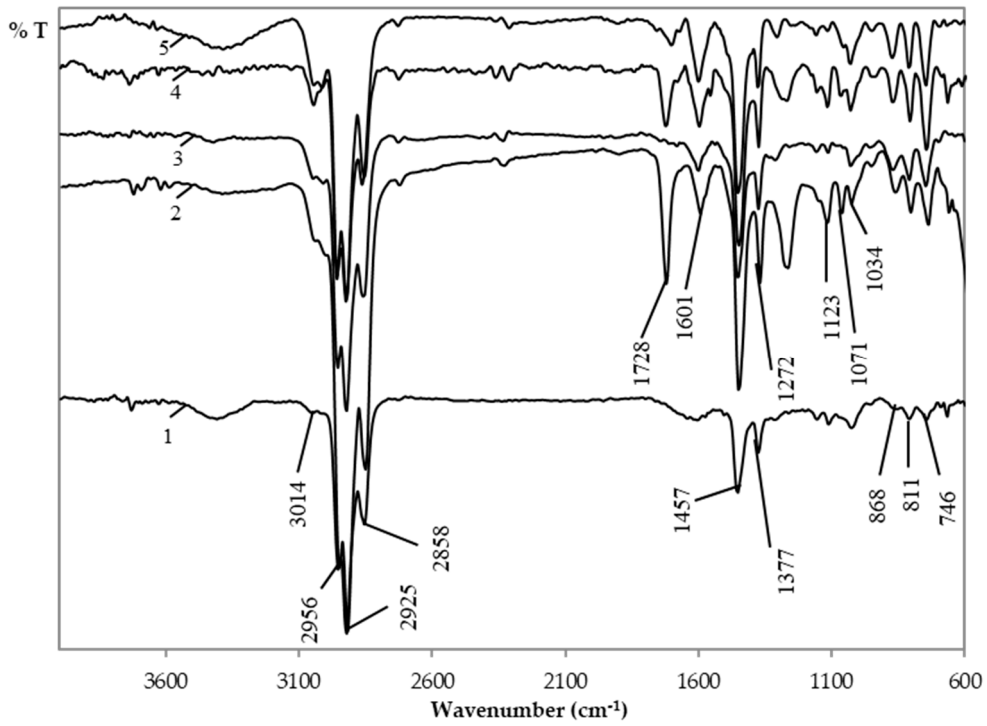

Figure S5. FTIR spectra of the naphthene aromatics from the liquid product obtained to the temperature (°C): (1) 330, (2) 360, (3) 390, (4) 420, (5) 450.

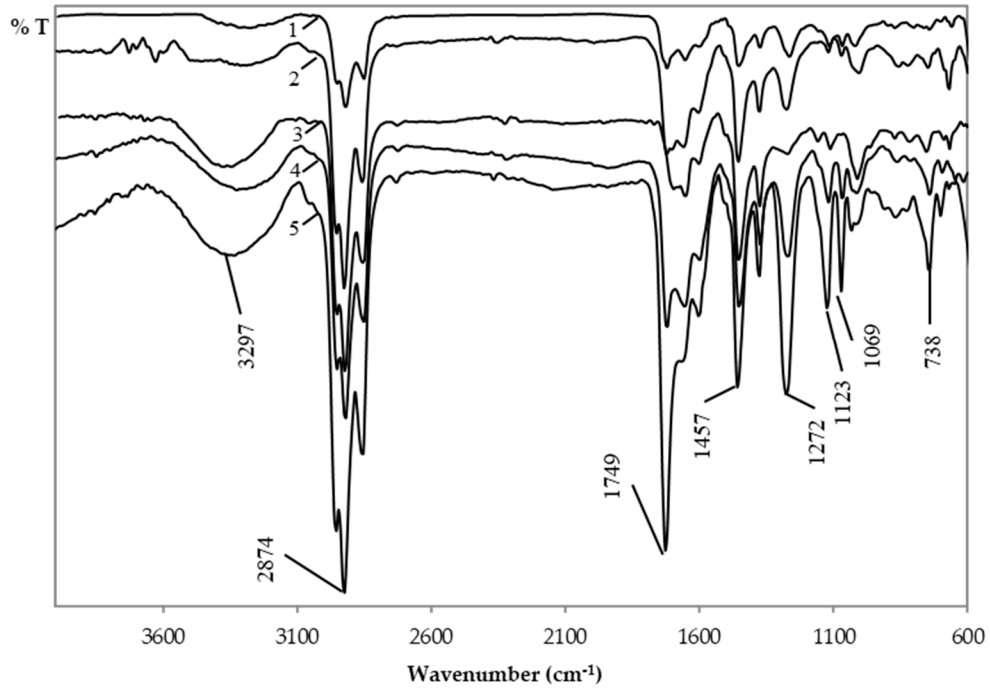

Figure S6. FTIR spectra of the polar aromatics from the liquid product obtained to the temperature (°C): (1) 330, (2) 360, (3) 390, (4) 420, (5) 450.

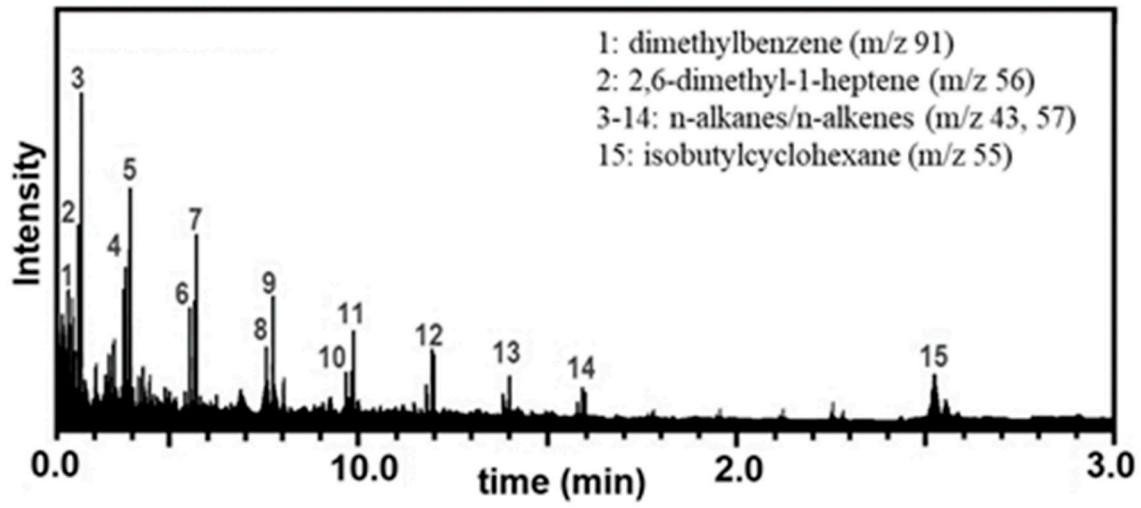

Figure S7. GC-MS analysis of the liquid product obtained through asphaltenes pyrolysis at 390 °C.

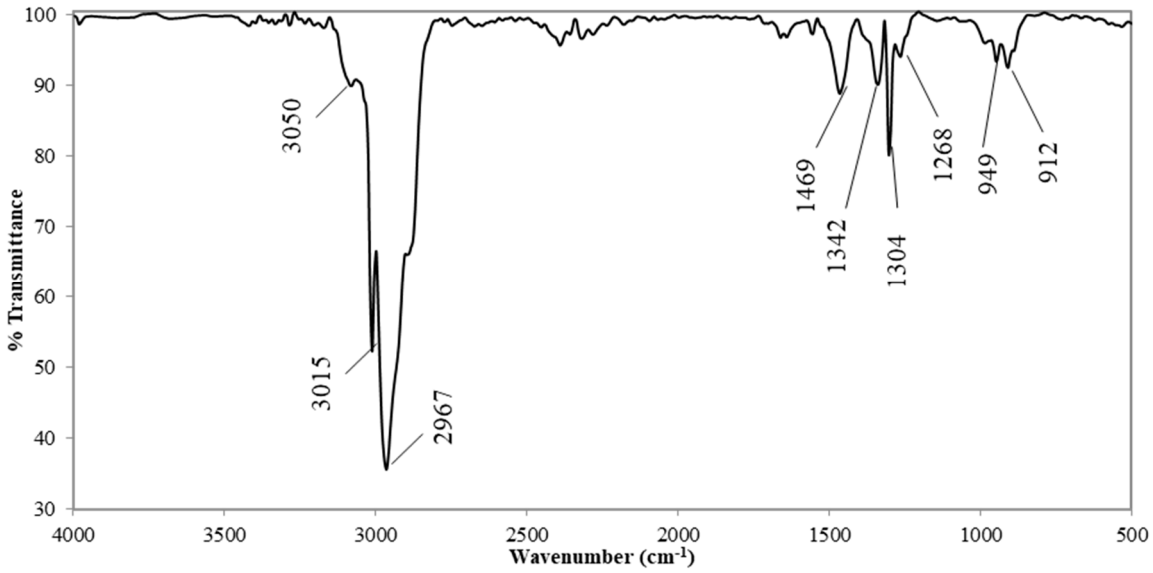

Figure S8. Infrared spectrum of the gases from the pyrolysis of the asphaltenes.

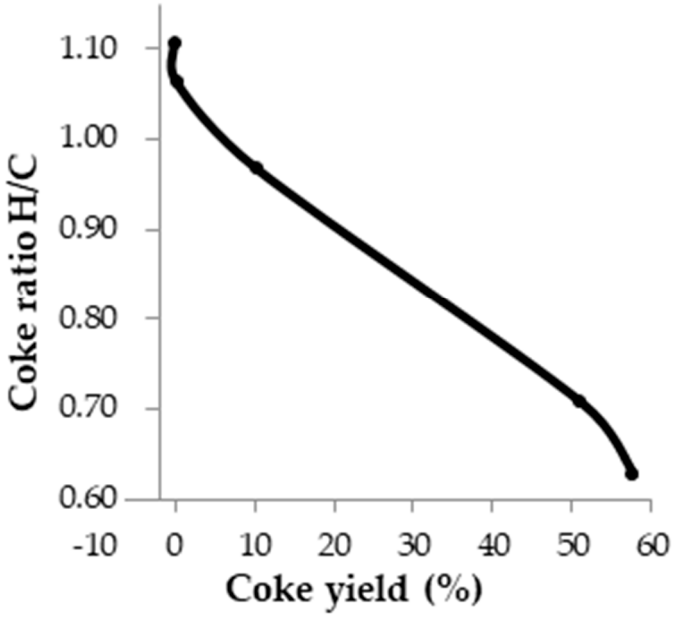

Figure S9. H/C ratio of the reacted asphaltenes against the pyrolysis temperature.

Supplementary Tables:

Table 1. Areas of the absorption bands of infrared spectra of the pyrolyzed asphaltenes.

Band	**ν(CH_3+CH_2)**	**ν(C=C)**	**δ(CH_3+CH_2)**	**δ(CH_3)**	**γ(CH_{AR1})**	**γ($CH_{AR2,3}$)**	**γ(CH_{AR4})**
Wavenumber (cm^{-1})	2922-2852	1605	1465	1365	870	814	750
Temperature of pyrolysis (°C)	Area	Area	Area	Area	Area	Area	Area
25 [1]	6.3145	1.9432	1.4920	1.0382	0.6651	0.6191	0.7180
330	4.3947	1.2362	1.1534	0.3751	0.4577	0.3655	0.4049
360	3.0709	0.8649	0.7985	0.3884	0.3476	0.3241	0.3901
390	0.5925	0.7230	0.2997	0.4019	0.2705	0.1074	0.2321
420	0.1731	0.3696	0.1897	0.2832	0.3531	0.3240	0.2297
450	0.1164	0.2287	0.1104	0.1315	0.1013	0.1473	0.1712

[1] Non-pyrolyzed asphaltenes corresponds at 25 °C.

*Equations used to calculate asphaltenes structural relationships from the bands of the IR spectra are:

Relative aromaticity (*RA*) is calculated from:

$$RA = \frac{\nu(C=C)}{\nu(CH_3 + CH_2)} \quad (1)$$

Where $\nu_{C=C}$ is the vibration band of aromatic carbons, and $\nu_{CH3+CH2}$ is the asymmetric vibration band of CH_3 and CH_2 links.

Degree of aromatic condensation (*ACD*), are aromatic rings penta-substituted related to hydrogen in aromatic carbons:

$$ACD = \frac{\gamma_{\text{CH-AR 2,3}}}{\gamma_{\text{CH-AR 1}}} \quad (2)$$

Where $\gamma_{CH\text{-}AR\ 2,3}$ is the in-plane bending vibration band from two or three C-H groups, and $\gamma_{CH\text{-}AR1}$ is the in-plane bending band from a C-H aromatic link.

Degree of disubstitution (DD), and degree of aromatic substitution (ASD):

$$DD = \frac{\gamma_{\text{CH-AR 4}}}{\gamma_{\text{CH-AR 1}}} \quad (3)$$

$$ASD = \frac{ACD}{DD} \quad (4)$$

Ramification degree (RD) is calculated:

$$RD = \frac{\delta_{CH_3}}{\delta_{\text{CH}_3\text{+CH}_2}} \quad (5)$$

Where δ_{CH3} is the out-of-plane bending or deformation symmetric vibration band of methyl groups, and $\delta_{CH3+CH2}$ is the bending band asymmetric of methyl-methylene groups.