Characterization Additive [redacted]

[redacted]

Background:

This work is to characterize the new additive [redacted] by NMR spectroscopy.

Experimental Details:

NMR Spectra were recorded on Bruker AVANCE 500 MHz NMR Spectrometer. About 10% w/w sample in $CDCl_3$ containing TMS as an internal standard was used for the analysis. The ^1H NMR spectra was recorded at 500.116 MHz with 30^o pulse length of 9.0 µs, 128 transients with 2 sec recycle delay. The 125.766 MHz ^{13}C NMR spectrum of the sample was recorded at 30-40% solution in $CDCl_3$. The quantitative spectra was obtained in the inverse gated mode and using the 0.1M $Cr(acac)_3$ as a relaxation agent. The spectral parameters used were as follows: numbers of scans 8192, relaxation delay 4 second, and spectral size 32K. The assignments of the closely packed ^{13}C NMR signals were confirmed using DEPT-135 NMR analysis.

Results and Discussion:

The ^1H NMR spectrum of the sample SP 6495 is presented in Figure 1. NMR signal at chemical shift 0.9 ppm corresponds to methyl protons ($-CH_3$) and signals between 1.0 and 2.3 ppm corresponds to methylene ($>CH_2$) and methine (>CH-) protons of the alkyl chain of the molecule. Two sharp signals appearing at 7.0 and 7.8 ppm represent the aromatic protons. In addition, there are small signals at around 7.2 ppm. Similarly, signals appearing at 2.3 and 3.2 ppm represent methylene ($-CH_2-$) protons attached to the aromatic ring.

Figure 1: ^{1}H NMR spectrum of the sample SP 6495.

The ^{13}C NMR spectrum of the [redacted] is presented in Fig 2. In general, the spectrum can be divided into two regions. The paraffinic carbons, appearing in the chemical shift region 5-55 ppm and aromatic carbons, chemical shift region 120-160 ppm. Among the paraffinic carbons, while sharp signals at 22, 29, 30 and 31 ppm represent methylene ($>CH_2$) carbons of the long paraffinic chains. The four NMR signals at 126, 128, 140 and 150 ppm suggest the presence of predominantly para-substituted aromatic compound.

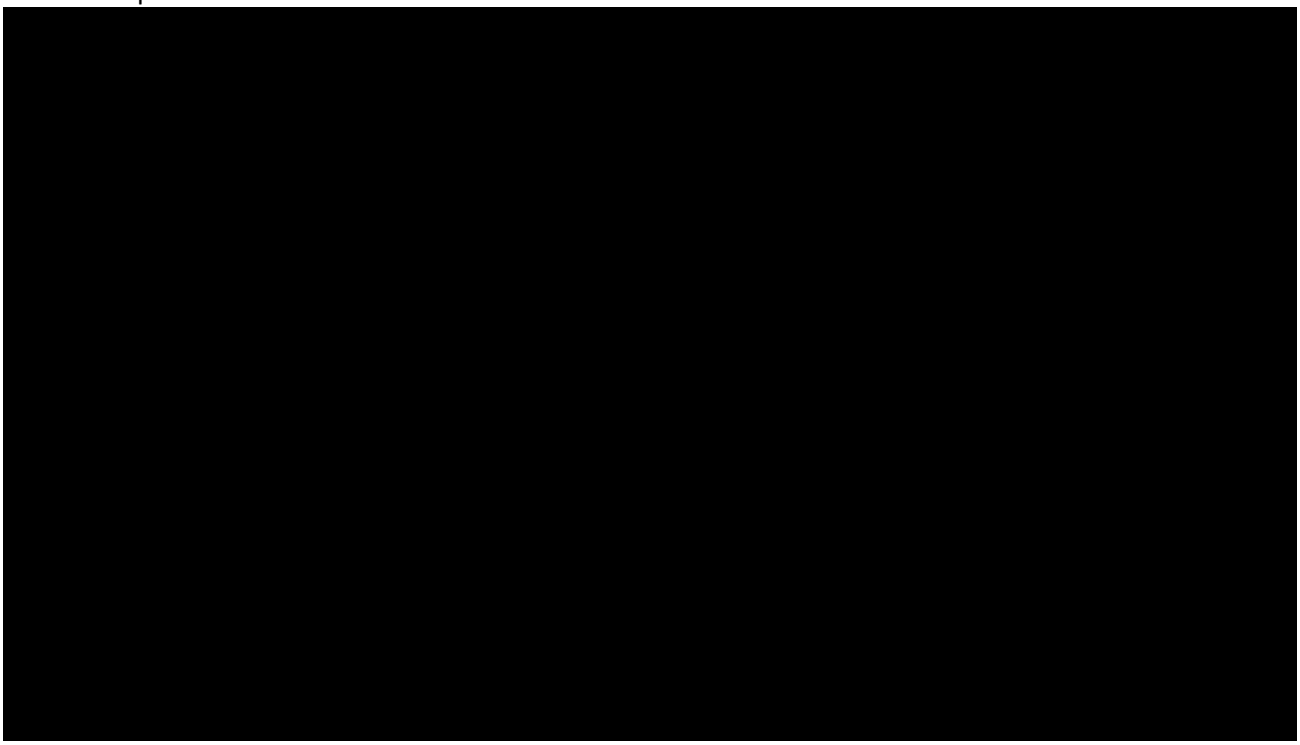

Figure 2: ^{13}C NMR spectrum of the sample [redacted]