eraspec: Advanced FTIR spectrometry for determining cetane improvers in diesel fuel

The **cetane number** of diesel fuel is a critical parameter that defines its ignition quality. High cetane numbers provide a multitude of benefits, including shortened ignition delays, improved cold-start performance, reduced engine noise, decreased fuel consumption, and lower emissions of hydrocarbons, carbon monoxide, nitrogen oxides (NO_x), and particulate matter.

To achieve these benefits without making major changes to fuel formulations, refineries use cetane number improvers. These additives offer a simple, cost-effective way to upgrade diesel performance, providing processing flexibility when crude oil sources have a lower natural cetane number. Furthermore, they allow refineries to produce premium diesel from lower-cost base stocks, such as light cycle oil. The market primarily relies on two chemical compounds for this purpose: 2-ethylhexyl nitrate (2-EHN) and di-tert-butyl peroxide (DTBP).

eralytics' eraspec is a Fourier Transform Infrared (FTIR) spectrometer explicitly designed to measure liquid samples in the mid-infrared (MIR) region using transmission geometry. Because fuels like diesel are complex mixtures of hydrocarbons, they display fundamental vibrational modes that absorb light in the MIR region, giving every chemical compound a unique spectral fingerprint. For quantitative analysis, eraspec relies on the Classical Least Squares (CLS) method, which functions as a multivariate linear regression where each component's distinct spectrum contributes linearly to the fuel's overall absorbance.

2-EHN is a nitrate ester and is the most popular cetane improver. It is generally applied to diesel fuel at treat rates between 0.025 and 0.40 vol%. The nitrate functional group leaves highly characteristic absorption bands in the MIR region. The eraspec evaluates 2-EHN concentration by targeting the absorption peak at approximately 1720 cm^{-1}. The system applies a local baseline correction and calculates the area under the peak (from 1630 to 1855 cm^{-1}), which is directly proportional to the amount of 2-EHN present in the sample.

Through this technique, eraspec provides a highly precise measurement range of 50 to 20,000 mg/L. The instrument is capable of detecting 2-EHN with an estimated limit of detection of 50 mg/L.

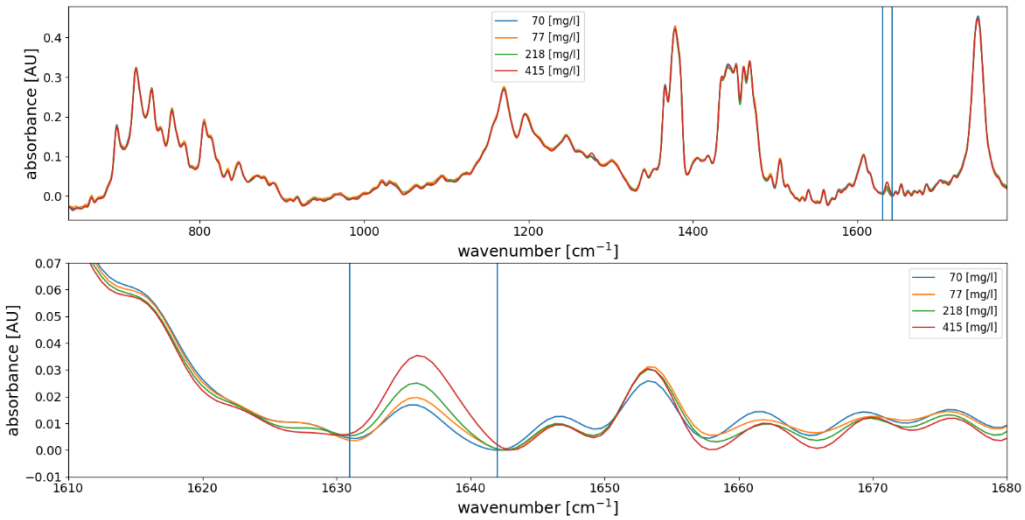

Figure 1: 2-EHN in Diesel at various concentrations

DTBP is an organic peroxide typically utilized at concentrations of 0.05 to 0.50 vol%. Compared to 2-EHN, DTBP offers a distinct advantage: it is nitrogen-free, meaning it improves the cetane number without raising the nitrogen content of the fuel.
Because of its C-O stretch, DTBP exhibits a dominant absorption peak around 1190 cm^{-1} and a smaller secondary peak at 1240 cm^{-1}. The eraspec analyzer successfully distinguishes DTBP from other common diesel components, such as fatty acid methyl esters (FAME) found in diesel blends, which instead display peaks at 1170, 1200, and 1245 cm^{-1}. Via its classical least squares evaluation of the spectrum, eraspec is able to measure DTBP without any interference from FAME (and vice versa) and the analysis can be applied to all diesel blends. For DTBP, eraspec achieves a reliable limit of detection of 0.05 vol%.

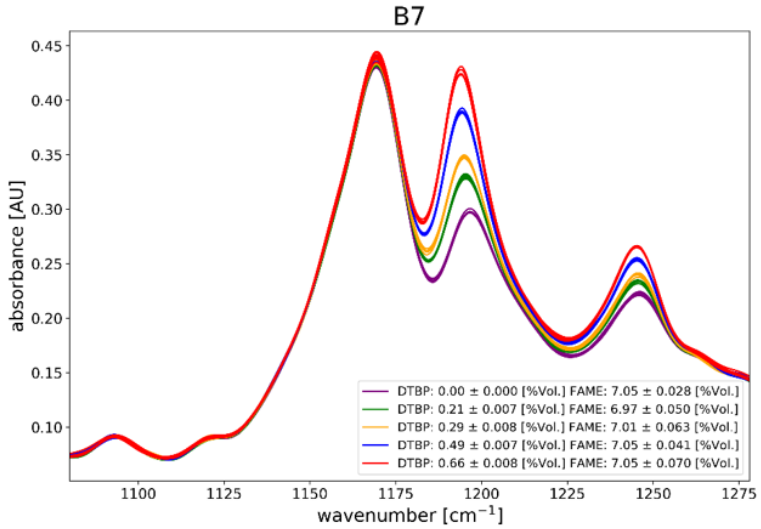

Figure 2: Measured absorbance of B7 diesel with various levels of DTBP. The corresponding concentration of FAME and DTBP as determined by eraspec is shown in the legend.

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Summary: By leveraging advanced FTIR technology and CLS multivariate regression, the analyzer successfully targets the unique spectral fingerprints of fuel additives. It provides refineries and testing laboratories with a highly reliable and precise method for quantifying both 2-EHN and DTBP, ensuring diesel fuels meet strict ignition quality and environmental standards.