

In Situ Identification of Various Structural Features of Vanadyl Porphyrins in Crude Oil by High-Field (3.4 T) Electron-Nuclear Double Resonance Spectroscopy Combined with Density Functional Theory Calculations

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Abstract

© 2017 American Chemical Society. Structural characterization of metalloporphyrins in complex systems, such as native hydrocarbons, has been the focus of scientific and industrial interests for many years. We describe electron-nuclear double resonance (ENDOR) of crude oil from the well without any additional sample treatment (i.e., in the native environment) in the magnetic field of about 3.4 T and temperature of 50 K by applying microwave pulses at 94 GHz (W band) and radio frequency pulses at near the proton Larmor frequencies of 144 MHz to probe the paramagnetic vanadyls. By means of density functional theory calculations, ENDOR features are explained and ascribed to certain vanadyl porphyrin structural forms known to be present in crude oil.

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