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ENDOR study of nitrogen hyperfine and quadrupole tensors in vanadyl porphyrins of heavy crude oil

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Abstract

© Kazan Federal University (KFU). We report the observation of pulsed electron-nuclear double resonance (ENDOR) spectrum caused by interactions of the nitrogen nuclei ^{14}N with the unpaired electron of the paramagnetic vanadyl complexes VO_2^+ of vanadyl porphyrins in natural crude oil. We provide detailed experimental and theoretical characterization of the nitrogen hyperfine and quadrupole tensors.

Keywords

Crude oil, DFT, ENDOR, EPR, Vanadyl porphyrins