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NMR techniques to study gasoline-ethanol blends

Anatoly K. Khitrin

Department of Chemistry, Kent State University, OH 44242, USA

Abstract

Gasoline-ethanol blends are popular motor fuels today. Presence of ethanol greatly increases solubility of water and all such fuels contain some water. Although a miscibility of gasoline-ethanol-water systems, as well as their performance in motors, has been extensively studied, little is known about these complex systems at a microscopic molecular level. Nuclear magnetic resonance (NMR) is a microscopic probe, sensitive to molecular organization. In addition to commonly used "fingerprinting" of fuel blends, NMR may offer an arsenal of spectroscopic and pulsed-field-gradient (PFG) diffusion techniques for obtaining detail information on ethanol-water clusters in gasoline, their composition, structure and mobility. We will show that high-resolution proton NMR spectra of undiluted samples, after suppression of radiation damping, can be conveniently used to quantify both ethanol and water in the blends, that the spectra are very sensitive to proton exchange between ethanol and water, and that dynamic NMR and PFG NMR can be used to obtain a unique information about structure and dynamics of the ethanol-water clusters. Besides providing a fundamental knowledge of the mechanism of ethanol hydration in hydrocarbon blends, NMR can become a primary technique for characterization and express-tests for gasoline quality and stability.

Biography

A. K. Khitrin graduated from the Moscow Institute of Physics and Technology in 1978 and received PhD in 1985 from the Institute of Chemical Physics, Russian Academy of Sciences, where he worked until 1999. Since 2002 he is a Professor of Physical Chemistry at Kent State University, USA. Khitrin's research interests are spin dynamics and NMR spectroscopy and imaging. He has published more than 100 papers in peer-reviewed journals.