

Quantum Chemical Study of the Effect of Zwitterionic Derived Supramolecular Complexes on the Wettability of Oil-Limestone and Water-Limestone Systems

Ernesto Lopez-Chavez^C, Alberto Garcia Quiroz^S, Rodrigo Muñoz Vega and Jorge I. Benitez Puebla
Universidad Autónoma de la Ciudad de México, Colegio de Ciencia y Tecnología, México D.F., México
elopezc_h@hotmail.com

Luis S. Zamudio Rivera, Jose M. Martinez Magadan, Eduardo Buenrostro Gonzalez
and Raul Hernandez Altamirano
Instituto Mexicano del Petróleo, México D.F., México

The newest methods for enhanced oil recovery involve surfactants, chemical products modifying the wettability of the rocks under high temperatures and pressures. In this work we present computational results pertaining to some supramolecular complexes acting as wettability modifiers of oil-limestone and water-limestone systems. The complexes studied are derived from superionic liquids of the types N'-alkyl-bis, N-alqueniil , N-cycloalkyl , N-amyl-bis-beta amino acid or salts acting as sparkling agents. In each instance, the HOMO and LUMO levels, and the energy gap between them, were calculated both for complexes as well as for the separate species, in order to obtain their dipole moment, softness and total energy.