A Theoretical Study of the Interaction of Methane Hydrate with a Vinyl Caprolaptam Polymer

Isidoro García Cruz [C, S], Ana Cristina Ramírez Gallardo and Ascención Romero Martínez
Gerncia de Refinacion de Hidrocarburos, Instituto Mexicano del Petróleo, Mexico City, México
igarcia@imp.mx

Humberto Saint-Martín
Termofísica, Instituto de Ciencias Físicas UNAM, Cuernavaca Morelos, México

In this work, we optimized the $n = 15$ clathrate with the monomer and polymer of vinyl caprolaptama and its interaction with the clathrate, using density functional theory with dispersive (vdW) forces. The clathrate was previously obtained by Bravo and Saint-Martín [1] including dispersive effects and proved to be highly stable. In fact, this methane clathrate is the precursor of an $n = 20$ cage that lies 1.2 kcal/mol lower than the 512 dodecahedral unit that takes part in crystal I. It is already known the crucial importance of the dispersive (vdW) forces in these kinds of intermolecular interaction effects. [2,3] We have considered three different orientations from the hydrate to monomer and polymer of vinyl caprolaptama, through different approaches, reaching one of its 6-ring faces, one of its 5-ring faces, and another with a 4-ring face. The results show that methane hydrate with the monomer and polymer of vinyl caprolaptama destabilizes mainly the water cage.