Inclusion complex formations of ferrocene and its derivatives with cyclodextrins
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Abstract: Ferrocene or bis(cyclopentadienyl)iron(II) and its derivatives are the high burning rate catalysts in composite propellants. The migration of ferrocenes from the cured propellant into the liner and onto the surface of the propellant grain which changes the main designed performance characteristics of the rocket considerably. The application of host-guest systems may use as one method of immobilizing a ferrocene. Quantum chemistry and molecular docking techniques are used to investigate the inclusion complex formations of ferrocenes with cyclodextrins. The chemical structure of ferrocene, n-butyl ferrocene, di-ter-butyl ferrocene, 1,3-diferrocenyl-1-butene, and three types of cyclodextrins (α-CD, β-CD and γ-CD) are constructed and optimized at B3LYP/m6-31G* level by GaussView5 and Gaussian 09 programs, respectively. The binding energy and the binding mode of inclusion complexes are also evaluated and analyzed.

Keywords: Ferrocene; Cyclodextrin; Inclusion complex; Host-guest interaction