

Theoretical Studies on the Ethylene Purification Using Substituted Nickel Dithiolenes

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Abstract

World is running out of energy. It is very important to find different ways of saving energy. Ethylene is purified using the very energy intensive cryogenic distillation method. The chemical method of olefin purification that is based on the reaction of ethylene with copper salts is poisoned and deactivated by some impurities such as CO, H₂S and acetylene. The mechanism of the combined chemical and electrochemical procedure based on the redox properties of nickel bis-dithiolene complexes has been theoretically studied in order to design a more convenient complex for such a reaction. Several possible addition routes of ethylene to neutral and anionic Ni(S₂C₂(CN)₂)₂ complexes have been modeled using ω-B97XD/6-31++G(p,d). The intraligand addition and subsequent decomposition is preferred for the neutral complex, while the interligand adduct is formed in the presence of the anion, in line with previous experimental results. The effect of the anion, whose role is as a mediator in the initial step of the reaction, is discussed, and the ability of this compound to avoid poisoning by acetylene is investigated. The results from the CN substituted complex are then compared with that of ethylene addition to CF₃, H, and OH substituted nickel dithiolene complexes. It has been confirmed that the hydroxyl substitution deactivates the nickel bis-dithiolene complex towards ethylene.