

Selective mono-chlorination of CH<sub>4</sub> with Cl<sub>2</sub> Gas using ion-exchanged zeolites: Electrophilic chlorination controlled by surface properties of catalysts

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CH<sub>4</sub> chlorination is one of the energy-efficient conversion pathways of CH<sub>4</sub> using the reactive chlorine gas molecule, which produces various chlorinated methane products. Among the products, CH<sub>3</sub>Cl is highly valuable since it can be used as a building block of olefin producing process. For selective CH<sub>3</sub>Cl production, free-radical mediated pathway which generates poly-chloromethane by chain chlorination should be avoided. The Ionic chlorination process can be an alternative, as it prefers the mono-chlorination that selectively produces CH<sub>3</sub>Cl. The pathway requires superacid catalysts that can induce polarization of chlorine molecules. In this work, ion-exchanged zeolites and hence having controlled surface acidity and polarity were investigated in CH<sub>4</sub> chlorination. The CH<sub>3</sub>Cl yield was remarkably changed depending on the cations on the zeolite surface, and the chemical properties of elements (i.e., electron affinity, standard reduction potential) could be correlated. Furthermore, the physical adsorption enthalpy of CH<sub>3</sub>Cl and natural-bond-orbital charges of cations on the catalysts were derived by DFT calculations, suggesting catalytic property for the selective production of CH<sub>3</sub>Cl.