

Reaction of Alkyl Halides with the Copper (100) Surface

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The interplay of alkyl halides with metal surfaces has been the focus of many experimental studies. These investigations have mainly aimed to illustrate the potential role of transitional metals and their oxides in mediating formation of toxic halogenated aromatics from the fragmentation of smaller C₁-C₃ cuts as well as from condensation of halogenated benzenes. An initial and prominent step in conversion of these precursors into heavier halogenated aromatics signifies their dissociative adsorption on metallic species present in the combustion media. This contribution represents a systematic computational study to examine thermo-kinetic parameters underlying rupture of Cl/Br-C bonds in halogenated model compounds (namely; chloromethane, 2-chloropropane, chloropropene, chlorobenzene, chloroethyne, bromomethane, 2-bromopropane, bromopropene, bromobenzene and bromoethyne) over the Cu (100) surface). These compounds adopt very weak physisorbed molecular states in several flat and vertical orientations. Calculated reaction barriers for Cl/Br-C bond fissions are scattered in the range of 40 – 120 kJ/mol. Stronger Cl – C bonds in reference to Br – C bonds translate into higher corresponding reaction barriers for the former. Results from this study should provide an insight into the heterogeneous formation of halogenated pollutants in thermal systems.

