458f A Theoretical Cluster Approach to Understanding Mercury Adsorption on Bromine-Embedded Activated Carbon

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Emissions from coal combustion processes constitute a significant amount of the elemental mercury released into the atmosphere today. Current technologies only allow for the capture of oxidized forms of mercury, while gaseous elemental mercury passes on to the environment freely. This investigation looked into the ways that activated carbon, with adsorbed bromine, can attract and adsorb mercury. Understanding the way in which bromine adsorbs to the surface of activated carbon, and subsequently mercury, can lead to the development of new technologies for the capture of mercury from the flue gases of coal combustion.

For the theoretical model it was assumed that the activated carbon molecular framework is similar to that of graphite. Both four-fused and seven-fused six-membered carbon atom rings were examined to serve as representative cluster species to model the activated carbon surface. *Ab initio* energetics calculations were performed using QCISD and CCSD methods with the Stuttgart and SBJK relativistic pseudopotentials for mercury using Gaussian03 software. Energetics associated with the adsorption of bromine at different sites on the graphite were calculated to determine a stable bromine-embedded activated carbon cluster. Using this cluster model, further *ab initio* calculations were performed to find the lowest energy interactions between mercury and the bromine-embedded graphite surface. The quantum mechanical level of theory chosen was based upon a previous detailed analysis comparing theoretical and experimental geometries and heats of reaction for mercury-containing compounds. Overall, this work will allow for a better understanding of interactions between mercury and bromine on activated carbon for mercury capture applications, and will eventually be extended to include the interactions with other halogens as well.