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Analysis of interaction of the metallic mercury surface with ammonium bases under the density functional theory

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Abstract

The calculations have been conducted of some mercury-containing molecules in the gas phase based on the DFT using the pseudopotential basis set for mercury atom and 6-311+G (d,p) for other atoms in a software packages GAUSSIAN'03 and TZ2P+ in the Amsterdam density functional. It has been shown that the ammonium cation is more likely than ammonium radical to interact with the surface of metallic mercury. The thermodynamic parameters indicate inability to interact with the surface of metallic mercury amines such as hydroxylamine, hydrazine and tetramethylamine.