Theoretical Study of Clusters of HNO_3, H_2O_2, SO_2 and H_2O.

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Abstract

Clusters of HNO_3, H_2O_2 and SO_2, important atmospheric trace species, have been examined in DFT optimizations with the BPW91 functional and numerical basis sets. In addition several structures of the three subject molecules clustered with as many as 16 water molecules have been optimized to examine general aspects of stability. HNO_3, H_2O_2 and SO_2 form a number of stable clusters. The most stable water clusters were those in which the water molecules cohere as they would essentially in the absence of solutes and the solute molecules reside on the surface. The results indicate that reactions among the solute molecules in atmospheric clusters are most likely surface reactions even at elevated temperatures.