MOLECULAR FRAGMENT MACHINE LEARNING TRAINING TECHNIQUES TO PREDICT CLUSTER ENERGETICS AND FREQUENCIES IN BROWN CARBON AEROSOL CLUSTERS

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Density functional theory (DFT) has become a popular method for computational work involving larger molecular systems as it provides accuracy that rivals ab initio methods while lowering computational cost. Nevertheless, computational cost is still high for systems greater than ten atoms in size, preventing their application in modeling realistic atmospheric systems at the molecular level. Newer machine learning techniques, however, show promise as cost-effective tools in predicting chemical properties when properly trained. In the interest of furthering chemical machine learning in the field of atmospheric science, we are developing a new training method to be used in the prediction of molecular characteristics for cyclic, nitrogen-based molecules that can undergo tautomerization within brown carbon aerosols. By creating a training dataset made of small molecule DFT calculations that supplement DFT cluster models of brown carbon molecules with hydration shells ranging from one to three waters, we hope to find a significant improvement in accuracy when predicting characteristics of brown carbon compounds while being computationally efficient.

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