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Prediction of Thermal Decomposition Temperatures Using Statistical Methods ARIANA BESTE, BRIAN BARNES, US Army Research Laboratory — We present development of a computational tool for the prediction of thermal decomposition onset temperatures using machine learning techniques. Our focus is on energetic materials, for which such a tool currently does not exist. Our models are trained and tested on published differential scanning calorimetry data consisting of decomposition temperatures and molecular formulas. Therefore, the models do not require any quantum mechanical calculations and may easily be transitioned to an experimentalist. We explore a variety of molecular fingerprints for encoding chemical information, and contrast their performance. We expect a complex, nonlinear relationship between molecular fingerprint and decomposition temperature and, therefore, test nonlinear methods such as Gaussian process regression, kernel ridge regression, and random forest regression, adaptive boosting of decision trees, and neural networks. We discuss the effect of outliers with particularly high or low decomposition temperatures on model performance. Due to the high dimensionality of the employed fingerprints, we analyze the utility of input reduction methods such as principal component analysis prior to model optimization. Further, we investigate the influence of specific functional groups on prediction quality.

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