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# Prediction of the Thermodynamic Properties of Hydrocarbons Using Gaussian Process Regression

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**Abstract :** Knowing the thermodynamics properties of hydrocarbons is vital when it comes to analyzing the related chemical reaction outcomes and understanding the reaction process, especially in terms of petrochemical industrial applications, combustions, and catalytic reactions. However, measuring the thermodynamics properties experimentally is time-consuming and costly. In this paper, Gaussian process regression (GPR) has been used to directly predict the main thermodynamic properties - standard enthalpy of formation, standard entropy, and heat capacity -for more than 360 cyclic and non-cyclic alkanes, alkenes, and alkynes. A simple workflow has been proposed that can be applied to directly predict the main properties of any hydrocarbon by knowing its descriptors and chemical structure and can be generalized to predict the main properties of any material. The model was evaluated by calculating the statistical error $R^2$, which was more than 0.9794 for all the predicted properties.

**Keywords :** thermodynamic, Gaussian process regression, hydrocarbons, regression, supervised learning, entropy, enthalpy, heat capacity
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