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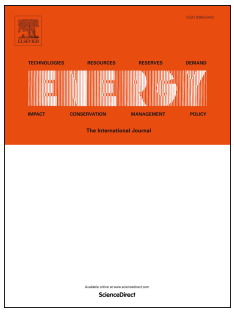

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Standard Molar Chemical Exergy: A New Accurate Model

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Abstract — One of the key challenges in exergy analysis is computation of the standard molar chemical exergies of the compounds involved in the process or system. Here, we present a new, data-driven model for computation of the standard molar chemical exergies of pure organic compounds composed of C, H, N, O, S, F, Cl, Br, I and Si. The model is obtained by considering the formation of a pure organic compound from its constituent elements. The compound's standard molar chemical exergy is related to its standard state enthalpy and entropy of formation, and to the standard molar chemical exergies of its constituent elements. A database of 3,148 pure organic compounds is used to develop correlations for the enthalpy and entropy of formation of an arbitrary organic compound based on a group contribution approach. Using these correlations, the standard molar chemical exergy of a given organic compound can be computed from our model. Comparison of model predictions with experimental data for 3,148 compounds produces an average absolute relative deviation of only 0.3%. The new model provides a reasonable basis to estimate the standard molar chemical exergies of various organic compounds when experimental data are not available.

Keywords: Chemical exergy; enthalpy of formation; entropy of formation; organic compounds; thermodynamic modeling.

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