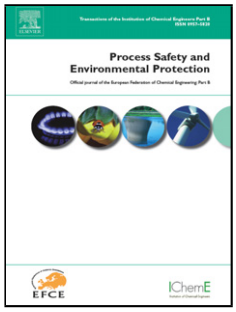

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Reliable method for safety assessment of melting points of energetic compounds

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Abstract

This work presents a widely applicable model for the prediction of melting points of energetic compounds including organic peroxides, organic azides, organic nitrates, polynitro arenes, polynitro heteroarenes, acyclic and cyclic nitramines, nitrate esters and nitroaliphatic compounds. This method is based on the elemental composition of an energetic compound and the contribution of some specific polar groups/structural moieties as additive and non-additive functions, respectively. The new model was applied for 288 different energetic compounds including complex molecular structures. The average and maximum deviations of the suggested method are 6.8 and 21.1, respectively, which are much lower than the predicted values of two well-known different methods.

Keywords: Melting point, Energetic compound, Correlation, Safety