

## Estimation of Physical Properties for Thermal Hazard Assessment Based on Neural Networks

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As required procedures for reactive chemical hazard evaluation, it would be useful to predict the amount of heat release of the reactions and adiabatic temperature rise by reactions. However, it is not easy to get those data, especially for the new materials or the high molecular substances. Considerable researches have been studied about determining physical property values from a compound's molecular structure. However, the existing estimation methods have problems in the accuracy and applicability. In order to improve the prediction of the physical properties in accuracy and applicability, we extended the database in large numbers, modified the existing group contribution methods and then established a new method for predicting the physical properties using neural networks. The results from the new estimation method were found to be more reliable and applicable. New method is expected to play an important part in the thermal hazard assessment by reducing the expenses and time.