COMPOUND THERMODYNAMIC PROPERTIES EVALUATION MODEL

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At present there are many databases and reference books on thermodynamic properties of individual substances, but still there remain a great number of chemical compounds, which thermodynamic properties are described poorly or not described at all.

The problem of missing data on chemical compound properties can be solved by generalizing the available data and taking it as a basis for modelling quantitative structure-property relationships. The paper presents such a model, based on fragmental descriptors approach, which summarizes data on heat capacity, enthalpy, and entropy of compounds. The model allows us to obtain thermodynamic function values for arbitrary compounds made up from fragments derived when analyzing the database of thermodynamic properties for individual substances.

The test calculations by the model are in good agreement with reference data. The relative enthalpy error is about 5%, the estimated entropy error is about 2%, and heat capacity error is 1%.

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