

过程系统工程

## 基于基团贡献神经网络集成法估算有机物常压凝固点

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**摘要** 基于基团贡献法应用神经网络对有机物的常压凝固点进行了估算, 输入参数为有机物的基团数和表征异构体的参数, 输出为常压凝固点. 分析了采用最速梯度下降法的BP算法在训练过程中产生误差饱和情况的原因, 采用在隐含层节点中加入误差饱和和预防函数用来防止误差饱和情况的出现. 仿真结果表明, 所采用的方法能有效地减小网络在误差表面陷入低谷的可能性和提高网络的收敛速率. 采用神经网络集成法建立了神经网络集成模型, 通过仿真合理选择隐含层节点数和采用交叉验证法用于防止BP网络的过度训练, 增强了网络的泛化能力. 估算结果表明, 所建立的神经网络集成模型, 其网络有良好的稳定性和预测精度, 207个样本估算的绝对平均相对误差为8.62%.

**关键词** [神经网络集成](#) [常压凝固点](#) [基团贡献](#) [误差饱和和预防函数](#) [交叉验证](#) [泛化](#)

分类号

## GROUP-CONTRIBUTION BASED ENSEMBLE NEURAL NETWORK APPROACH TO ESTIMATION OF NORMAL FREEZING POINT OF ORGANIC COMPOUND

### Abstract

A model was developed to evaluate and predict normal freezing point of organic compounds. This study was based on the group-contribution method and the neural network ensemble technology. The input parameters of neural network were group numbers of organic compounds and isomeric characterization parameters, the output was normal freezing point. The error saturation (ES) condition, which was caused by the use of gradient descent method, would greatly slow down the learning speed of BP algorithm. Having analyzed the causes of the ES condition, an ESP function was proposed to avoid the ES condition from hidden nodes. The simulation result of using ESP method in hidden layers showed that it would reduce the probability of trapping into local minimum in the error surface and accelerate the convergence speed. The ensemble method was used and the neural network ensemble model was established. The nodes in the hidden layer were chosen rationally through simulation, and the cross-validation method was adopted for preventing the BP network from overfitting, which improved the generalization ability of network. According to the ensemble neural network model established in this paper, the estimation result showed that the network had good stability and prediction accuracy and the estimation absolute mean relative error of 207 samples was 8.62%.

**Key words** [ensemble neural network](#) [normal freezing point](#) [group-contribution](#) [error saturation prevention \(ESP\) function](#) [cross-validation](#) [generalization](#)

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