

Investigation of infrared spectra-structure correlation using Kohonen and counterpropagation neural network

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Abstract

Two different artificial neural networks (ANNs) for infrared spectra analysis are presented: the self-organising Kohonen ANN for mapping of the infrared spectra into a 2-D plane and the counterpropagation ANN for determination of the structural features of organic compounds based on their infrared spectra. The preliminary learning in the Kohonen ANN with all spectra from the collection yields the information of possible grouping. The preliminary grouping has been used for the separation of spectra into the training and into the test set containing 755 and 2529 "spectrum-structure" pairs, respectively. The counterpropagation ANN trained on the "spectrum-structure" pairs from the training set has the ability to predict, with an average prediction ability of 0.77 and an average reliability of 0.82, structural fragments of an unknown compound from its infrared spectrum. Additionally, the counter-propagation ANN offers the possibility to simulate the infrared spectra from the structure representation.

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