Environmental Engineering and Management Journal *February 2014, Vol.13, No. 2, 315-322*
http://omicron.ch.tuiasi.ro/EEMJ/

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PREDICTION OF RATE CONSTANTS FOR NITRATE RADICAL REACTIONS USING A SVM MODEL BASED ON DENSITY FUNCTIONAL THEORY

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Abstract

In the present paper, support vector machines (SVMs) are used to develop a quantitative structure-activity relationships (QSAR) model for the reaction rate constants ($-\log k_{NO3}$) of 115 heterogeneous organic compounds, through reaction with nitrate radicals ($NO_3^{\bullet}$) in the troposphere. Two quantum chemical descriptors used as the inputs for the SVM model were calculated with density functional theory (DFT), at the B3LYP level of theory with 6-31G(d) basis set. The best predictions were obtained with the Gaussian radical basis kernel (C = 4, ε =0.15 and γ =3). The average root-mean square (RMS) error for the prediction of k_{NO3} is 0.502 log units, indicating good robustness and predictive ability. The SVM model, reported here, shows better statistical characteristics compared to existing QSAR models.

Key words: density functional theory, quantum chemical, quantitative structure-activity relationships, rate constant, support vector machine

Received: August 2011; Revised final: May, 2012; Accepted: June, 2012

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