PREDICTION OF MONOMER REACTIVITY PARAMETERS USING QUANTUM CHEMICAL DESCRIPTORS

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To construct artificial neural network (ANN) models for the prediction of reactivity parameters (*u*, *v*), density functional theory (DFT) calculations are carried out for 55 vinyl monomers, at the B3LYP level of theory with a 6-31G(*d*) basis set. After the generation of quantum chemical descriptors, the stepwise multiple linear regression (MLR) analysis and the ANN method are used to develop quantitative structure-property relationship (QSPR) models of parameters *u* and *v*. The ANN models produced test set root-mean-square (rms) errors of 0.35 for the parameter *u* and 0.34 for the parameter *v*. Research results indicate that the QSPR models based on DFT calculations and ANN techniques are accurate and possess the ability to generalize.

Keywords: artificial neural network, density functional theory, monomer, radical copolymerization, QSPR, quantum chemical descriptors.