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Formation of the acrylonitrile self-associates

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Abstract

The structures of the acrylonitrile self-associates (the dimer A3 structure is optimal) were calculated by quantum-chemical methods and proved by NMR ^{1}H and ^{13}C spectroscopy. The self-association constants from ~0.070 till 0.103 l/mol were determined by chemical shifts of the *trans*- and *cis*-hydrogen in the $=CH_2$ and carbon in the =CH of the acrylonitrile isomers. It is recommended to use the chemical shift of the carbon in the =CH for the self-association constants calculations. The obtained data are important not only for the further acrylonitrile polymerization, but also for its copolymerization with other vinyl monomers.