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Spectroscopy and structure of styrene (water)_n and styrene (methanol)_n clusters, n = 1, 2

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Abstract

Resonant two-photon ionization (R2PI) spectra of styrene-water (SW_n) and styrene-methanol (SM_n) binary clusters with n = 1, 2 are reported. The results indicate that the SW_n clusters exhibit different structures as compared to the benzene (water)_n clusters. Ab initio calculations of the lowest energy structure of the SW complex confirm that water interacts mostly with the ethylene group. Two distinct isomers are identified for the SM₂ cluster. The favorable interactions of water and methanol with the olefin group of styrene may explain the strong inhibition effects observed by trace concentrations of water or methanol on the cationic polymerization of styrene. © 2002 Published by Elsevier Science B.V.