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NMR-spectroscopic study of conjugation effects. 8.13C NMR spectra of p-substituted anisoles, thioanisoles, and selenoanisoles

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Abstract

1. According to the data from13C NMR spectra, the effective conformation of anisoles, thioanisoles, and selenoanisoles is determined both by "methyl-ring" spatial interactions as well as by p, π conjugation of the O, S, and Se with the aromatic fragment which varies depending on the electronic nature of the p substituent in the ring. 2. Acceptor p substituents enhance, and donor p substituents reduce, the coplanarity of the molecules and, moreover, the greatest sensitivity to this effect is characteristic of the seleno- and thioanisoles. © 1980 Plenum Publishing Corporation.

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