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^{13}C NMR Spectra of *para*-Substituted Methoxybenzenes and Phenols in the Solid State Examination of Chemical Shift Nonequivalence in *ortho* and *meta* Carbons Related to Nonequivalent Electron Distribution, and Application to Assignment of Peaks in *meso*-Hexestrol and Its Derivatives*

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^{13}C-NMR spectra of *para*-substituted methoxybenzenes and phenols were recorded in the solid state to gain an insight into the manner and origin of substantial peak splittings in the *ortho* (up to 9.2 ppm) and *meta* (up to 2.5 ppm) carbon signals. It was difficult to account for these peak splittings only by the steric interaction with the methyl group of the substituent, because their magnitude varied widely from 4.6 to 9.2 ppm with a variety of substituents at the *para* position, and the *meta* carbon peaks are also split into doublets. Instead, it was found that the electron density nonequivalence between the two *ortho* and the two *meta* carbons is mainly responsible for the splittings, as manifested by the presence of an approximate linear relationship between the displacements of the ^{13}C-NMR peaks and total electron density. The observed additional splitting in the ^{13}C-NMR spectra of meso-hexestrol and its methyl or ethyl ether(s) in the solid state was similarly explained. Stereochemical features of these molecules in the solid state are discussed on the basis of the ^{13}C-NMR data.

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