慶應義塾大学学術情報リポジトリ

Keio Associated Repository of Academic resouces

Title	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
Sub Title	
Author	斉藤, 肇(Saito, Hajime)
	横井, もと子(Yokoi, Motoko)
	相田, 美砂子(Aida, Misako)
	児玉, 昌彦(Kodama, Masahiko)
	小田, 泰子(Oda, Taiko)
	佐藤, 良博(Sato, Yoshihiro)
Publisher	共立薬科大学
Publication year	1988
Jtitle	共立薬科大学研究年報 (The annual report of the Kyoritsu College of
	Pharmacy). No.33 (1988.),p.162-162
JaLC DOI	
Abstract	
Notes	沙 録
Genre	Technical Report
URL	https://koara.lib.keio.ac.jp/xoonips/modules/xoonips/detail.php?koara_id=AN00062898-00000033-0162

慶應義塾大学学術情報リポジトリ(KOARA)に掲載されているコンテンツの著作権は、それぞれの著作者、学会または出版社/発行者に帰属し、その権利は著作権法によって 保護されています。引用にあたっては、著作権法を遵守してご利用ください。

The copyrights of content available on the KeiO Associated Repository of Academic resources (KOARA) belong to the respective authors, academic societies, or publishers/issuers, and these rights are protected by the Japanese Copyright Act. When quoting the content, please follow the Japanese copyright act.

¹³C 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*

Hajime Saito,** Motoko Yokoi,** Misako Aida,** Masahiko Kodama**, Taiko Oda, and Yoshihiro Sato

> 斉藤 肇**, 横井とも子**, 相田美砂子**, 児玉昌彦**, 小田泰子, 佐藤良博

¹³C-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 non-equivalence 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 ¹³C-NMR peaks and total electron density. The observed additional splitting in the ¹³C-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 ¹³C-NMR data.

^{*} 本報告は Mage. Reson. Chem., 26, 155-161 (1988) に発表.

^{**} 国立がんセンター研究所, 生物物理