

Multinuclear (^1H , ^{13}C and ^{15}N) Magnetic Resonance Spectroscopy and Substituent Effects on *N*-Phenoxyethylanilines

Jorge L. Jios^a, Gustavo P. Romanelli^a, Juan C. Autino^a, Damian Magiera^b, and Helmut Duddeck^b

^a LADECOR, Departamento de Química, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, Calles 47 y 115, 1900 La Plata, Argentina

^b Universität Hannover, Institut für Organische Chemie. Schneiderberg 1B, D-30167 Hannover Germany

Reprint requests to Dr. Jorge L. Jios. E-mail: jlj@sinectis.com.ar

Z. Naturforsch. **57b**, 226–232 (2002); received September 6, 2001

NMR Data, Phenoxyethylanilines, Substituent Effects

^1H , ^{13}C and ^{15}N NMR spectra of twenty substituted *N*-phenoxyethylanilines **1–20** were completely and unambiguously assigned using a combination of both homo- and heteronuclear (gs-COSY), ^1H detected heteronuclear one-bond (gs-HMQC) and long-range (gs-HMBC) gradient-selected correlation experiments. Correlations between chemical shifts and substituent constants are analyzed separately for both phenyl rings using variable substituents *para* to the fixed substituent $-\text{OCH}_2\text{CH}_2\text{NHC}_6\text{H}_5$ (series I) and $-\text{NHCH}_2\text{CH}_2\text{OC}_6\text{H}_5$ (series II), respectively. The correlation coefficient for chemical shifts *vs.* a linear combination of inductive and resonance substituent constants is high and improves when only the six values, corresponding to each *para*-monosubstituted series, were used. For nitrogen chemical shifts excellent linear dependences were obtained. The results show that the ethylene chain is not able to transmit the substituent effect from one aromatic ring to the other.