

^{13}C -NMR spectroscopy of β -nitrostyrenes. II 11. Mono-, bi- and tri-methoxy phenyl-substitutions and long distance electronic effects

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By means of ^{13}C -NMR spectroscopy and AM1 molecular orbital calculations of mono-, bi- and tri-methoxy- β -nitrostyrenes at the meta and para positions, we have characterized a long distance electronic charge transfer pattern on the ethylenic bridge ($\text{CH}=\text{CH}$) and on the aromatic ring (Ph) carbon centers, determined by the electron-donor nature of the methoxy-substituent groups. After a complete spectral assignment of the ^{13}C -NMR signals, we have found a functional dependence of the chemical shifts on the C1 and C β centers respect to the C4 and C3 methoxy substitution sites on the aromatic ring, while in the same molecular series C β -chemical shifts are practically constants. On the other hand, the ^{13}C -NMR chemical shifts of the C3 and C4 centers plus the analysis of the AM1 electronic charge density have permitted us determine the long distance charge transfer effect induced by the C4 methoxy substitutions as well as the attenuation of this effect due to the C3 methoxy substitutions.