

13C-NMR spectroscopy of para-substituted benzylideneacetones. I. Long distance electronic effects

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Para-benzylideneacetones present a characteristic long distance charge transfer pattern, where the olefinic bridge (CH=CH) and the aromatic ring (Ph) carbon centers are perturbed according to the nature of the para-substituent groups. By means of 13C-NMR spectroscopy and AM1 molecular orbital calculations we have found that in this molecular series the chemical shifts (δ) and the charge densities (q_{AM1}) corresponding to the C3, C1 and C2 centers follow a functional dependence of the type: $\delta = a q_{AM1} + \delta^0$, while C4, C5 and Cco are practically constants. On the other hand, after a complete spectral assignment of the 13C-NMR signals, an analysis of the electron-donor substituent effect at the para-position of the aromatic carbonyl compounds on the C4 center, has permitted us to find a good correlation between the C4 spectral shift and the electronegativity of this vicinal center.