Long distance electronic effects on the rotational potential barriers around the Caromatic-Cethylenic bond

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A systematic study of the rotational activation free energy around the Caromatic-Cethylenic bond of para-substituted styrene systems is carried out in the present work from a quantum chemistry point of view. Calculations of the rotational potential barriers in the AM1 approach are developed as function of the electron-donor groups localized on the aromatic ring. Based on these calculations and thermodynamical data, we predict changes in the activation free energy barriers due to the long distance electronic effects of the substituents in acetophenones, cinnamaldehydes and benzalketones according to the following equation ?G?exp = (2.41±0.16) VAM1 + 5.43 ± 1.79, in kJmol-1. Our results agree the experimental measurements registered up to date and the standard deviations are similar to experimental determinations.