

Substituent Effects on the Geometrical Properties of 1-Phenylallyl Alcohol

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Optimized geometrical parameters, electron densities, heats of formation and stabilization energies have been obtained on X-substituted phenylallyl alcohols, where X is H, OCH₃, NH₂, CN, F and CH₃ at *ortho*, *meta*, and *para* positions, using MINDO-Forces SCF-molecular orbital calculations. The substituent effects on the geometrical parameters and the electron density are discussed.

Key words: Phenylallyl Alcohols; Substituent Effects; Allyl System; MINDO-Forces.