

MINDO – Forces Calculation of Some Substituted Phenylallyl Cations

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Z. Naturforsch. **59a**, 971 – 976 (2004); received February 17, 2004

MINDO-Forces SCF-molecular orbital calculations with complete geometry optimization have been performed on x-substituted phenylallyl cations, where x is H, OCH₃, NH₂, NO₂, CN, F and CH₃, in ortho, meta, or para positions. Optimized geometrical parameters, electron densities, heats of formation and stabilization energies were obtained. The substituent effect on the geometrical parameters and the electron density are discussed by correlation analysis.

Key words: Phenylallyl Cations; Substituted Allyl System; MINDO-Forces.