

A Vibrational and Theoretical Interpretation of the Conformation of Mono- and Disubstituted N-Benzylideneanilines

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Infrared data for N-benzylideneanilines mono- and disubstituted predict, in agreement with CNDO molecular orbital calculations, that the internal energy transfer is induced mainly by a donor group in para position of the benzylidene ring; this effect confers to this molecular portion a prevalent planar structure. However, the charge transfer is restricted by a steric interaction between one of the ortho hydrogen atoms of the aniline ring and the azomethine hydrogen; this situation constraints this molecular portion to adopt a major non planar conformation. © 1991, Taylor & Francis Group, LLC.

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