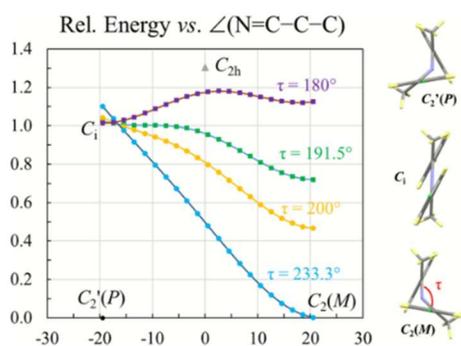


Intramolecular Nonbonding Interactions and Geared Phenyl Twisting in Para-Disubstituted 1,4-Diphenylazines: Electron Correlation Effects on Molecular Conformations and Enantiomerization

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Graphical Abstract



Steric strain between the azine-Me groups in (*E,E*)-acetophenone azines and N lone pairs causes small rotations about the Az-CH₃ bonds, and geared phenyl twisting may lead to C₂- or C_i-structures. Exploration of the (τ , ϕ_1 , ϕ_2) conformational space clarifies the role of C_i-like structures in a τ -plateau region for enantiomerization.

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