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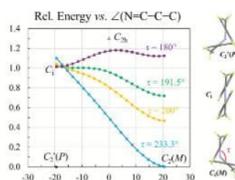
RESEARCH ARTICLE

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

Kaidi Yang, Harmeet Bhoday, Rainer Glaser

First Published: 27 January 2026

#### Graphical Abstract



Steric strain between the azine-Me groups in (*E,E*)-acetophenone azines and N lone pairs causes small rotations about the Az-CH<sub>3</sub> bonds, and geared phenyl twisting may lead to C<sub>2</sub>- or C<sub>1</sub>-structures. Exploration of the ( $\tau$ ,  $\phi_1$ ,  $\phi_2$ ) conformational space clarifies the role of C<sub>1</sub>-like structures in a  $\tau$ -plateau region for enantiomerization.

10:36 AM · Feb 2, 2026 · 7 Views

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