

Anomalous stereoselectivity in the Wittig reaction : the role of steric interactions.

Autorzy

Marcin Stępień

Rok wydania

2013

Czasopismo

Journal of Organic Chemistry

Numer woluminu

78

Strony

9512-9516

DOI

10.1021/jo401654f

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Density functional theory calculations combined with a distortion/interaction energy analysis show that the anomalous *Z* selectivity observed in Wittig reactions of *ortho*-substituted benzaldehydes is not caused by phosphorus–heteroatom interactions in the addition transition state, as assumed in earlier work, but is predominantly steric in nature. The calculations reproduced correctly the stereoselectivity preferences for a wide range of reactant pairs as well as relative reactivities for different substituent types, providing deeper structural insight into the mechanism of Wittig olefination.

Adres publiczny

<http://dx.doi.org/10.1021/jo401654f>

Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>