

Diastereoselective synthesis of tetraalkyl (*R,R*)-1,2-cyclohexylene-diamino-di-phosphonates bearing thiophene, furan and pyrrole moieties. Computational and experimental study on their formation.

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Streszczenie

Diastereoselective additions of dialkyl phosphites to three diimines bearing DACH moiety and thiophene, furan or pyrrole rings were studied in the aspect of their stereochemistry, structure of predominant products and mechanism. For these reasons, analysis of reaction mixture, X-ray studies of products, UV-photoelectron spectroscopy and ionization energies of the starting imines were performed experimentally while reaction profiles were calculated at the CAM-B3LYP/6-311G(d,p) level of theory. The calculated energy barriers corresponding to the gas phase are significantly low and seem to explain why the products are formed relatively easily.

Słowa kluczowe

diamino-phosphonate with DACH moiety, diastereoselective addition of phosphite, X-ray structural study, UV-photoelectron spectroscopy, ionization energies, quantum calculation

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