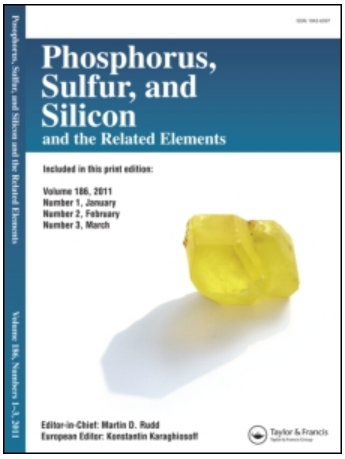

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Basicity and Reactivity of Alpha-Aminophosphonates: Theoretical Investigation

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Basicity and Reactivity of Alpha-Aminophosphonates: Theoretical Investigation

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Previously [1] we have found the possibility of the mechanism alteration for addition of substituted aminophosphonates $(RO)_2P(O)CHR^1NHR^2$ to PhNCO (where R = alkyles), which depends on the substituents at phosphorus and carbon atoms. We have performed theoretical investigation of basicity and reactivity of alpha-aminophosphonates by PM3 method using HyperChem molecular modeling package. We found that the calculated basicity parameters are in good correlation with our previous experimental data. From the results of the calculations, the whole series can be divided into three subsets: S1 with R^1=H and R^2=n-Bu; S2 with R1=Ar with electronodonating substituent, R^2=cycloHex, S3 with R^1=Ar with acceptor substituents, R^2=cycloHex. The molecules, which belong to different series, differ in MO distribution on the reaction center NH. The aminophosphinates, containing electrono-withdrawing substituents at both centers (nitrogen and alpha-carbon) are deactivated completely.

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