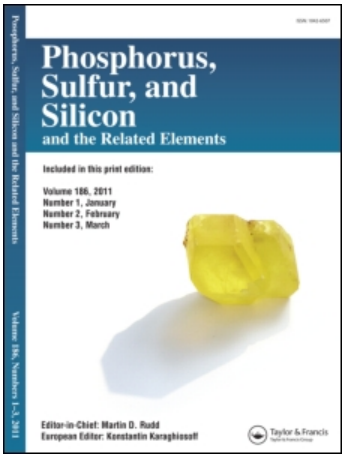

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Molecular Mechanics Study of Organophosphorus Compounds

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Molecular Mechanics Study of Organophosphorus Compounds

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Molecular Mechanics calculation (Allinger's force field and MM2 1985 program) was successfully applied for the structure-reactivity studies of organophosphorus compounds in our laboratory.

1. Structural effect of organophosphorus compounds on ^{31}P NMR chemical shifts. Our results reveal that the substituent effect on ^{31}P NMR chemical shifts of various organophosphorus compounds are governed chiefly by the local van der Waals(VDW) steric energy of phosphorus nucleus. A series of linear relationship between the E_{VDW} and ^{31}P NMR chemical shift in different kinds of organophosphorus compounds was established.

2. Substituent effect in alkaline hydrolysis of esters of phosphorus acids. A significant difference in hydrolytic behaviours between carboxylate and phosphonate was found. Based on regression analysis, a new set of parameters $\Delta\Delta E$ as measure of steric effect of substituents of organophosphorus compounds was suggested.

3. Induced asymmetric addition of dialkylphosphite to C=N bond. MM is good for understanding the reaction mechanism and the important factors that determine the de value of the reaction.

4. Extraction reaction of metals by phosphorus-based ligands. MM was successfully applied to study metal extraction reactions. A series of typical examples was reported for uranium, thorium, cobalt, nickel and lanthanides based on solvation and ion-exchange mechanism.

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