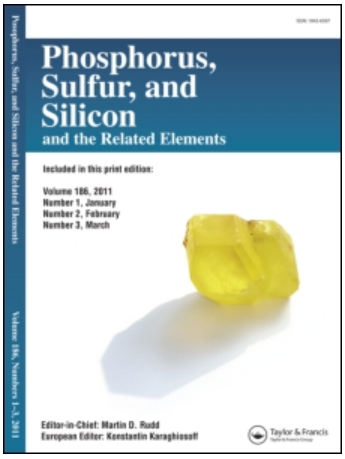

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Conformational Analysis of Novel Organophosphorus Cyclopendent Ligands

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CONFORMATIONAL ANALYSIS OF NOVEL ORGANOPHOSPHORUS CYCLOPENDENT LIGANDS

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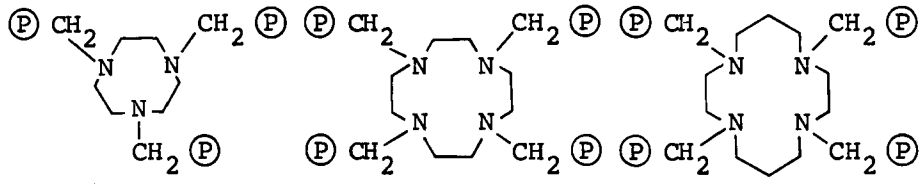
In the present work the "structure-properties" relalationship has been demonstrated on novel organophosphorus cyclopendenes, macrocyclic ligands with exocyclic groups including additional donor centres.



where Ⓟ = PO_3H_2, $P(O)Ph_2$ or $CH_2PO_3H_2$.

The ligand conformational energy has been calculated by molecular mechanics as the sum of nonvalent interaction energy (E_{nb}), the energy of rotation around ordinary bonds (E_{tors}) and of angle deformation energy (E_{angle}). The construction of a complex has been performed using the "floating point" calculation method, having XYZ coordinated and imitating the complexation ion. The necessary condition for all distances from this point to the ligand donor atoms (l_i) is to be equal to a given coordination bond distance (l_o). The distance is controlled by penalty function (E_{pen}) in the form of quasielastic law $K(l_i-l_o)^2$, where K is a force constant. The minimized function if $F = E_{nb} + E_{tors} + E_{angle} + E_{pen}$. The strain energy of ligand profiles of various denticity has been estimated by computer calculations. Found topological types of complexes have been by X-ray analysis. Conclusions have been drawn out with regard to the complexation ability.