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Stacking-Conformations in Functionally Substituted Phosphines

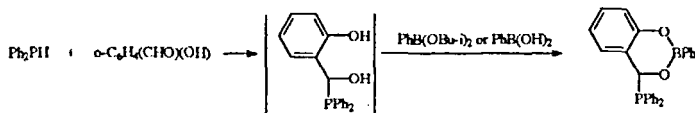
GEORGE N. NIKONOV, ANNA S. BALUEVA, ELVIRA I. MUSINA,
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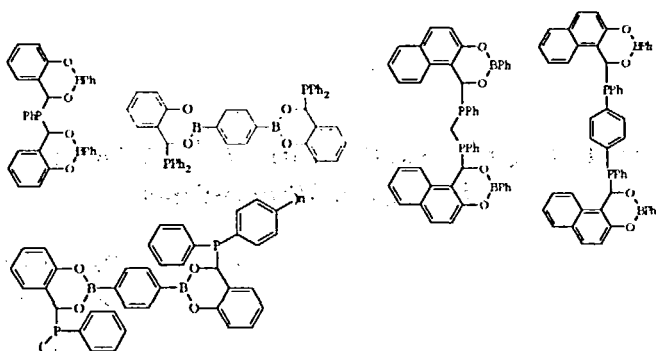
The methods of synthesis and space structure of phosphorus-containing compounds, in which stacking conformation is realized, are considered. It is shown that intramolecular stacking can be observed in monoheterocyclic compounds, bi- and polycyclic compounds, complexes of metals and acyclic compounds.

Keywords: phosphorus; boron; heterocycles; stacking-effect; complexes of metals

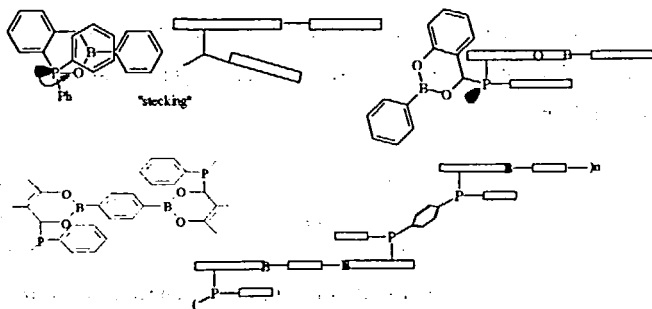
The methods of synthesis and space structure of phosphorus-containing compounds, in which stacking conformation is realized, are considered. A series of 1,3,2-dioxaborinanes with exocyclic phosphine fragment was obtained by the following scheme:



A variation of phosphines and ether of boron acids allowed to synthesize the compounds with several interacting fragments, including oligomers.

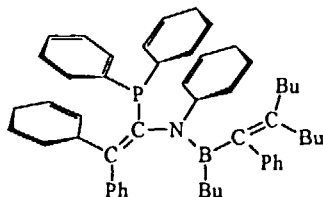


It is shown that when keeping some conditions as in crystall state (by X-ray method), also in solutions (by NMR method), the intramolecular stacking of planar heterocyclic dioxaborinane fragment and phenyl ring of substituent at the phosphorus atom is observed. Staking-conformations are probably conditioned by intramolecular dispersion interactions between a phenyl substituent and heterocyclic fragment with a delocalized unclosed system of multiple bonds.

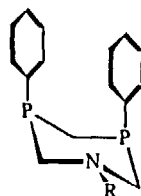
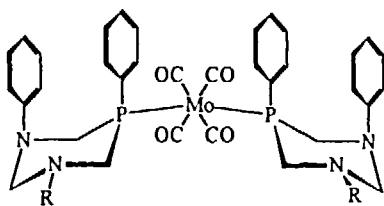
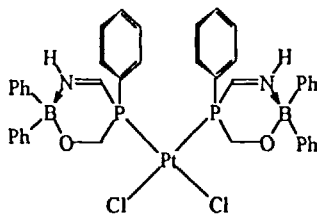
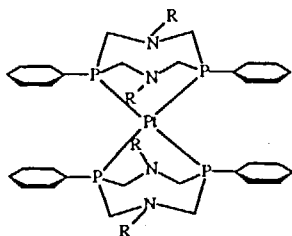


For the existence of intramolecular stacking in compounds of 4-phosphino-1,3,2-dioxaborinane series the combination of a number of conditions is necessary: the hard planar conformation of heterocycle, the delocalized π -system with the participation of the boron atom, the steric accessibility of the boron atom and the availability of two aryl groups at the phosphorus atom. The NMR ^{31}P spectroscopy can be used for the detection of stacking only in 4-diarylphosphino-1,3,2-dioxaborinanes series. The intramolecular electron interactions an a stacking-effect type are shown for some other classes of compounds. Two pairs

of interacting phenyl ring are observed in 4,6-dibutyl-2-diphenylphosphino-1,1,3,5-tetraphenyl-3-aza-4-boradeca-1,5-dien molecule.



The intramolecular stacking of phenyl rings is found in 1,5,3,7-diazadiphosphacyclooctanes, 1,3,5-azadiphospharinanes and some complexes of metals with heterocyclic phosphine ligands.



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