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### Molecular and Electronic Structure of 2,2,4,4-Tetrachlorodiphosphetanes

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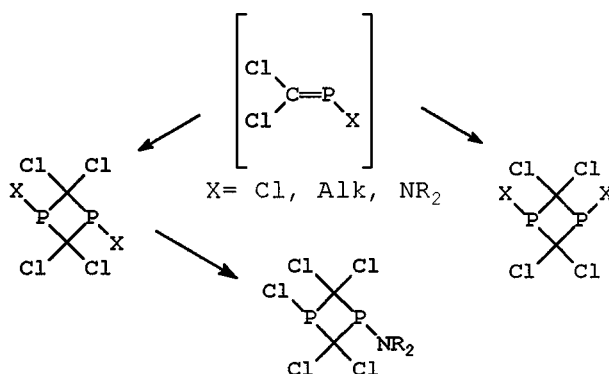
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## MOLECULAR AND ELECTRONIC STRUCTURE OF 2,2,4,4-TETRACHLORODIPHOSPHETANES

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The number of 2,2,4,4-tetrachlorodiphosphetanes (products of dimerization of kinetically unstable phosphaaalkenes) have been characterized by  $^1\text{H}$ ,  $^{13}\text{C}$ , and  $^{31}\text{P}$  NMR spectroscopy and x-ray diffraction method.



SCHEME 1

It has been discovered that the saturated diphosphetanes depending on substituents properties could exist not only as *trans*- and *cis-trans* isomers but also as *cis-cis* isomers. The main peculiarities and characteristic features of molecular and electronic structure of system investigated have been discussed on the basis of ab initio (RHF/6-31 + G\*\*) calculations.

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