

Dipole moments and conformational analysis of tris(2-pyridyl)phosphine and tris(2-pyridyl)phosphine chalcogenides. Experimental and theoretical study



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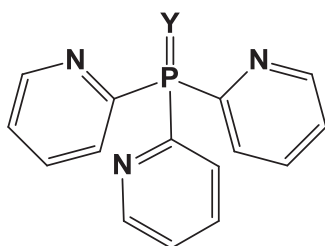
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HIGHLIGHTS

- Dipole moments of tris(2-pyridyl) phosphine and its chalcogenides were determined.
- Possible conformers of phosphines were optimized using density functional theory.
- Conformational analysis of tris(2-pyridyl)phosphine and its chalcogenides was performed.
- Tris(2-pyridyl)phosphine and its chalcogenides have preferred *gauche*- and *trans*-forms.

GRAPHICAL ABSTRACT



Y = lone pair 1, O 2, S 3, Se 4

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ABSTRACT

Conformational analysis of tris(2-pyridyl)phosphine and tris(2-pyridyl)phosphine chalcogenides was carried out by the method of dipole moments and density functional theory calculations. The conformations of the examined compounds fit into the overall conformational picture for the P^{III} and P^{IV} compounds: namely, these phosphines have non-eclipsed *gauche*- and *trans*-forms with propeller arrangement of the pyridyl radicals about the P = Y bond (Y = lone pair, O, S, Se).

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Introduction

Extensive utilization of organophosphorus compounds for practical purposes prompted the progress in the field of their conformational analysis and necessitated synthesis of compounds with predefined useful properties, and identification of their structure and fine conformational features. Structural and polarity data are

necessary for studying of reaction mechanisms and reactivity of organophosphorus compounds. For complex polyfunctional organoelement compounds in general and for organophosphorus compounds with several axes of internal rotation in particular, the majority of articles usually describes the mutual arrangement of separate fragments of molecules established without conformational analysis of an entire molecule as a whole. In this study, we used a comprehensive approach to investigate the structure of molecules in solution using various complementary physical methods taking into account all their advantages and/or

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