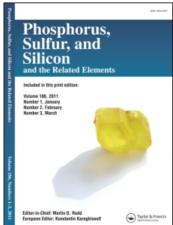
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Structure Features of 1,3,5-Tris(Diphenylphosphinoxidemethylene)Ben zene in Crystal and Solution on the Base of X-Ray, Dipole Moments and Quantum Chemical Analysis

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Structure Features of 1,3,5-Tris(Diphenylphosphinoxidemethylene)Ben zene in Crystal and Solution on the Base of X-Ray, Dipole Moments and Quantum Chemical Analysis

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The molecular structure, polarity and conformations in solution of 1,3,5-tris(diphenylphosphinoxidemethylene)benzene 1,3,5-[Ph₂P(O)CH₂]₃C₆H₃ have been studied by X-ray, dipole moments and quantum chemistry methods. It have been shown, that in crystal molecule has the conformation in which two diphenylphosphinoxide fragments dispose on one and the same side, but the third - on the other side of central benzene ring plane with torsion angles C_{SP2} - C_{SP2} - C_{SP3} -P 60-80° and C_{SP2} - C_{SP3} -P=O about 50-70°. In solution conformational picture is more rich: side by side with the structures realized in crystal, conformations with all three diphenylphosphinoxide fragments disposed on one and the same side of central benzene ring plane with torsion angles C_{SP2} - C_{SP2} - C_{SP3} -P 70-90° and C_{SP2} - C_{SP3} -P=O about 70-75° become preferable.

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