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## Phosphorus, Sulfur, and Silicon and the Related Elements

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### Structure Features of 1,3,5-Tris(Diphenylphosphinoxidemethylene)Benzene 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-[Ph<sub>2</sub>P(O)CH<sub>2</sub>]<sub>3</sub>C<sub>6</sub>H<sub>3</sub> have been studied by X-ray, dipole moments and quantum chemistry methods. It has been shown, that in crystal molecule has the conformation in which two diphenylphosphinoyl fragments dispose on one and the same side, but the third - on the other side of central benzene ring plane with torsion angles C<sub>SP2</sub>-C<sub>SP2</sub>-C<sub>SP3</sub>-P 60-80° and C<sub>SP2</sub>-C<sub>SP3</sub>-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 diphenylphosphinoyl fragments disposed on one and the same side of central benzene ring plane with torsion angles C<sub>SP2</sub>-C<sub>SP2</sub>-C<sub>SP3</sub>-P 70-90° and C<sub>SP2</sub>-C<sub>SP3</sub>-P=O about 70-75° become preferable.

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