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Sereoselective Addition of Benzaldehyde N,N-Dimethyl-Hydrazone to 2-R_fO-4-Oxo-5,6-Benzo-1,3,2-Dioxaphosphorinanes. The Spatial Structure of 2-Pentafluorophenoxy-4-Dimethylamino-2,5-Dioxo-3-Phenyl-6,7-Benzo-1,4,2-Oxazaphosphepine

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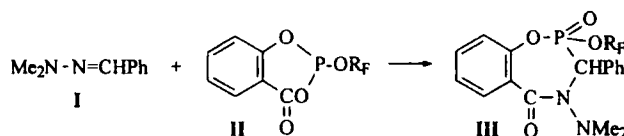
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Stereoselective Addition of Benzaldehyde N,N-Dimethyl-Hydrazone to 2-R_FO-4-Oxo- 5,6-Benzo-1,3,2-Dioxaphosphorinanes. The Spatial Structure of 2-Pentafluorophenoxy-4- Dimethylamino-2,5-Dioxo-3-Phenyl-6,7-Benzo- 1,4,2-Oxazaphosphepine

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[3+2]-Cycloaddition of N,N-dimethylhydrazone benzaldehyde (I) to 2-R_FO-4-oxo-5,6-benzo-1,3,2-dioxaphosphorinanes (II) yields the new heterocycle - 2-R_FO-4-Me₂N-2,5-dioxo-3-phenyl-6,7-benzo-1,4,2-dioxaphosphepine (III) [R_F = C₆F₅, CH(CF₃)₂] with high stereoselectivity (above 94 %). The reaction is likely to involve the initial interaction of nitrogen as a nucleophile with carbonyl carbon as an electrophile. The hydrolysis of (III) leads to phosphonic acid (IV) (OR_F = OH).



The structure of phosphepine (III, R_F = C₆F₅) has been investigated by single crystal X-ray diffraction (fig.). Heterocycle of the molecule has a distorted boat conformation. Fragment O¹C⁷C⁶C⁵ is planar within 0.001(2) Å. The deviation of other atoms belonging to the cycle from this plane are P² -1.1537(3), C³ -1.925(3), N⁴ -0.851(2) Å. The pentafluorophenoxy and dimethylamino groups occupy the pseudo axial position. Phosphoryl group and phenyl are pseudo equatorial. The angle between the carbonyl group and benzene ring is -38.98 (0.47)°. The fragment O⁵C⁵N⁴N is practically planar (torsion angle is -9.1°). Nitrogen atom N⁴C(O) is planar too.

