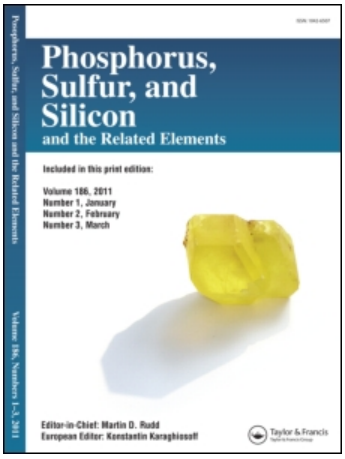


Phosphorus, Sulfur, and Silicon and the Related Elements
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713618290

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

Vladimir F. Mironov[a]; Aidar T. Gubaidullin[a]; Gulnara A. Ivkova[b]; Igor A. Litvinov[a]; Boris I. Buzykin[a]; Liliya M. Burnaeva[b]; Irina V. Konovalova[b]
[a] Organic and Physical Chemistry A.E. Arbuzov Institute, Kazan, Russia [b] Kazan State University, Kazan, Russia

To cite this Article Mironov, Vladimir F. , Gubaidullin, Aidar T. , Ivkova, Gulnara A. , Litvinov, Igor A. , Buzykin, Boris I. , Burnaeva, Liliya M. and Konovalova, Irina V.(1999) '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', Phosphorus, Sulfur, and Silicon and the Related Elements, 147: 1, 267
To link to this Article: DOI: 10.1080/10426509908053614
URL: http://dx.doi.org/10.1080/10426509908053614

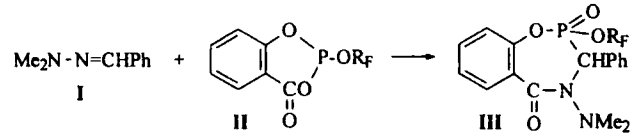
Phosphorus, Sulfur and Silicon, 1999, Vol. 147, pp. 267-267
Reprints available directly from the publisher
Photocopying permitted by license only

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

VLADIMIR F. MIRONOV[a], AIDAR T. GUBAIDULLIN[a], GULNARA A. IVKOVA[b], IGOR A. LITVINOV[a], BORIS I. BUZYKIN[a], LILIYA M. BURNAEVA[b] and IRINA V. KONOVALOVA[b]

[a]*Organic and Physical Chemistry A.E. Arbuzov Institute, Kazan, 420088, Russia and* [b]*Kazan State University, Kazan, 420008, Russia*

[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-Me_2N-2,5-dioxo-3-phenyl-6,7-benzo-1,4,2-dioxaphosphepine (**III**) [R_F = C_6F_5, $CH(CF_3)_2$] 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 = C_6F_5) has been investigated by single crystal X-ray diffraction (fig.). Heterocycle of the molecule has a distorted boat conformation. Fragment $O^1C^7C^6C^5$ is planar within 0.001(2) Å. The deviation of other atoms belonging to the cycle from this plane are P^2 -1.1537(3), C^3 -1.925(3), N^4 -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 $O^5C^5N^4N$ is practically planar (torsion angle is -9.1°). Nitrogen atom $N^4C(O)$ is planar too.