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Synthesis and Crystal Structure of 2-R-2,5-Dioxo-5,6-benzo-1,4,2- and -1,3,2-Dioxaphosphepines

Liliya M. Burnaeva^a; Vladimir F. Mironov^b; Irina V. Konovalova^a; Evgenij I. Goruynov^c; Tat'yana A. Mastruykova^a; Aidar T. Gubaidullin^b; Igor A. Litvinov^b; Olga V. Yashagina^a

^a Kazan State University, Russia ^b A. E. Arbuzov Institute of Organic and Physical Chemistry, Russian Academy of Sciences, Russia ^c A. N. Nesmeyanov Institute of Organo-Element Compounds, Russian Academy of Sciences, Russia

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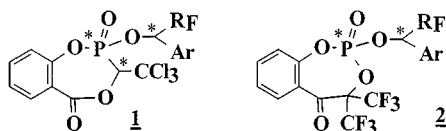
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SYNTHESIS AND CRYSTAL STRUCTURE OF 2-R-2,5-DIOXO-5,6-BENZO-1,4,2- AND –1,3,2-DIOXAPHOSPHEPINES

Liliya M. Burnaeva, Vladimir F. Mironov,^a Irina V. Konovalova,
 Evgenij I. Goruynov,^b Tat'yana A. Mastruykova,^b
 Aidar T. Gubaidullin,^a Igor A. Litvinov,^a and Olga V. Yashagina
 Kazan State University, Russia; A. E. Arbuzov Institute
 of Organic and Physical Chemistry, Russian Academy
 of Sciences, Russia;^a and A. N. Nesmeyanov Institute
 of Organo-Element Compounds, Russian Academy
 of Sciences, Russia^b

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2-R-4-oxo-5,6-benzo-1,3,2-dioxaphosphorinanes [R = OCH(R_F)Ar], containing two chiral centers (phosphorus and carbon in the substituent R) easily react with chloral and hexafluoroacetone and form diastereoisomeric 2-R-2,5-dioxo-5,6-benzo-1,4,2- and –1,3,2-dioxaphosphepines **1**, **2** respectively. The reaction with chloral has a high regio- and stereoselectivity (two diastereoisomers are obtained from starting two diastereoisomers). The individual isomers were isolated and examined by NMR and single crystal x-ray diffraction in all cases. The heterocycle of the phosphepine molecules has a distorted boat conformation. The exocyclic alkoxy substituent is axial, phosphoryl and CCl₃ groups are equatorial.



R_F = CF₃, C₃F₇, C₆F₁₁, Ar = Ph, 3-ClC₆H₄,
 3-CF₃C₆H₄, 3-MeOC₆H₄

SCHEME 1

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Address correspondence to V. F. Mironov, Kazan State University, Kremlevskaya Str., 18, Kazan, 420008 Russia. E-mail: mironov@iopc.ken.ru