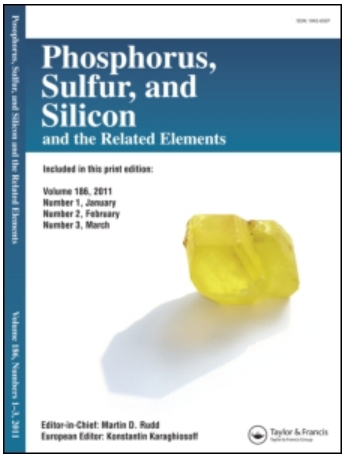

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Structure of 4-Oxo-5,6-benzo-1,3,2-dioxaphosphorinanes in Solution

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STRUCTURE OF 4-OXO-5,6-BENZO-1,3,2-DIOXAPHOSPHORINANES IN SOLUTION

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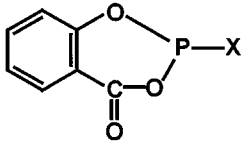
Structure of 4-oxo-5,6-benzo-1,3,2-dioxaphosphorinanes (salicylphosphites), compounds of P^{III} that have a six-membered heterocycle ring joined to the planar fragments (a Ph ring and a carbonyl group), was studied by methods of dipole moments (DM) and IR spectroscopy (solutions of compounds in CH_2Cl_2 and CH_3CN).



	X	dipole moment (expt.), D	
1	N=C=O	–	4.23 (C_6H_6)
2	Cl	3.80 (CCl_4)	4.02 (C_6H_6)
3	NEt_2	3.88 (CCl_4)	4.17 (C_6H_6)

SCHEME 1

In the IR spectra of compound **1** there were small changes in the region of all characteristic frequencies except isocyanate group (2256 cm^{-1}). The latter indicated existence of only one conformation. Low conformational mobility of phosphoric heterocycle was even more conclusive for dioxaphosphorinane **2**: ν(P—Cl) 480 cm^{-1}. Identification of realizable conformations was carried out by the DM method. Experimental DM of salicylphosphites **1–3** are described by values calculated for the "sofa" form with an axial (N=C=O, NEt_2) or an equatorial (Cl) exocyclic substituent.

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