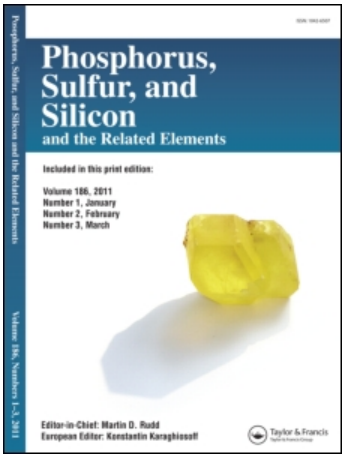

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Conformational Behaviour of Substituted 2-Methoxy-2-Oxo-1,2-Oxaphospholan-3-Ols

Andrzej E. Wroblewski[a]
[a] Institute of Organic Chemistry, Technical University, Łódź, Poland

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CONFORMATIONAL BEHAVIOUR OF SUBSTITUTED 2-METHOXY--2-OXO-1,2-OXAPHOSPHOLAN-3-OLS

ANDRZEJ E. WRÓBLEWSKI
Institute of Organic Chemistry, Technical University, Politechnika, Żwirki 36, 90-924 Łódź, Poland

Conformational behaviour of about 30 2-methoxy-2-oxo-1,2--oxaphospholan-3-ols containing various substituents was examined by ^{1}H and ^{13}C NMR. Vicinal coupling constants J(HCCH), J(HCCP), J(HCOP), J(CCOP) and J(CCCP) were employed in this study. Conformation of the 1,2-oxaphospholane ring is governed almost exclusively by substituents at C-3, C-4 and C-5, as well as by their orientation. The configuration of the P atom has little or no influence on conformation of the ring in diastereomeric pairs. Strong preference of phenyl, methyl and substituted methyl groups to occupy the equatorial or pseudoequatorial positions was observed for all but one compounds studied. In the cis--fused bicyclic systems conformationally rigid 6-membered rings forced the 1,2-oxaphospholane rings to adopt an envelope-like (E_4) conformation. No influence of the P=O····HO-C-3 hydrogen bond on conformation of the 1,2-oxaphospholane ring was found. Preferred conformations for (2R, 3R, 4R)-3-(hydroxymethyl)-2-methoxy-2-oxo-1,2-oxaphospholane-3,4-diol and its triacetate are shown below.