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Conformational and Crystal Packing Differences in (+)-7,8-Di-*tert*-butoxy-1-phenyloctahydro-1*H*-pyrrolo(1,2-*b*)-1*H*-phospholo(2,3-*d*)isoxazole 1-Oxide Diastereoisomers

Rafal Kruszynski[1] and Wanda Wieczorek[1,2]

[1]*Institute of General and Ecological Chemistry, Lodz University of Technology, Żeromskiego 116, 90-924 Łódź, Poland*

[2]*Institute of Chemistry and Environmental Protection, Jan Dlugosz University, Al. Armii Krajowej 13/15, 42-201 Częstochowa, Poland*

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ABSTRACT: *The crystal and molecular structures of (1S,3aR,7S,8S,8aR,8bR)-(+)-7,8-Di-tert-butoxy-1-phenyloctahydro-1H-pyrrolo(1,2-b)-1H-phospholo(2,3-d)isoxazole 1-oxide (* **III**, *hereafter) and (1R,3aS,7S,8S,8aS,8bS)-(+)-7,8-Di-tert-butoxy-1-phenyloctahydro-1H-pyrrolo(1,2-b)-1H-phospholo(2,3-d)isoxazole1-oxide (* **IV**, *hereafter) have been determined.* **III** *crystallizes in space group* $P2_12_12_1$, *and* **IV** *in* $P2_1$ *one. The conformational analysis of the puckered heteroatom three-ring system shows the conformation of noticeable distorted envelope with puckering amplitude* $Q_2 = 0.397$ Å, *the intermediate conformation between twisted and envelope with* $Q_2 = 0.353$ Å, *and half-chair conformation with* $Q_2 = 0.451$ Å, *for phospholane, oxazolidine, and pyrrolidine rings of* **III**, *respectively. Rings in molecule of* **IV** *adopt conformations of envelopes with* $Q_2 = 0.381$ Å, $Q_2 = 0.367$ Å, *and* $Q_2 = 0.363$ Å, *respectively, for the rings as described above. The molecules of* **III** *are assembled by intermolecular weak hydrogen bonds to the one-dimensional chain along x-axis. The structure of* **IV** *is built-up of weak intermolecular hydrogen bonds to form a two-dimensional hydrogen bond network. The differences in conformation between compounds* **III** *and* **IV** *cause changes in hydrogen bonding pattern, because in molecule* **IV** *there is no hydrogen cavern filled with three hydrogen bond donors, and one weak hydrogen bond has not enough strength to force such an arrangement as it is in* **III**. Heteroatom Chem 16:613–620, 2005; Published online in Wiley InterScience (www.interscience.wiley.com). DOI 10.1002/hc.20160

INTRODUCTION

One of the elemental principles of racemic compounds' kinetic resolution is the phenomenon of different synthesis rates of different enantiomers [1,2]. Brandi et al. [3] described kinetic resolution in 1,3-dipolar cycloaddition of tartaric acid derived nitrones to 2,3-dihydro-1-phenyl-1*H*-phospholes, characterized by formation of diastereomeric products where both the resolved unreacted substrate and the selectively formed diastereoisomeric products are desired as synthetic targets. However, the

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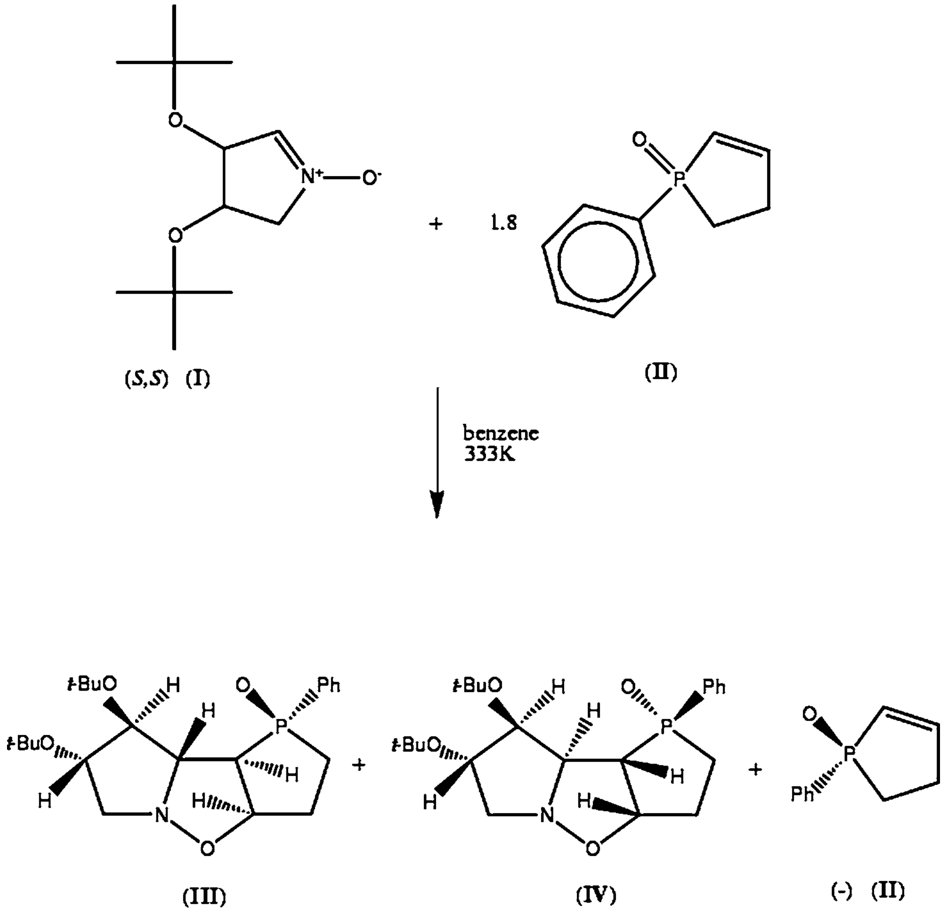
Correspondence to: Rafal Kruszynski; e-mail: kruszyna@p.lodz.pl. Contract grant sponsor: Ministry of Scientific Research and Information Technology, Poland.

absolute configuration of obtained 14 enantiomerically pure products was postulated only on the basis of ^{1}H NMR. The absolute configuration only for one of them, (+)-(1*S*,3a*R*,7*S*,8*S*,8a*R*,8b*R*)-7, 8-di-*tert*-butoxy-1-phenyloctahydro-1*H*-pyrrolo(1,2-*b*)-1*H*-phospholo(2,3-*d*)isoxazole 1-sulfide (**III-A**, hereafter), was determined [4] by X-ray crystallography (CCDC reference code: TIWZUU [5]). Thus, we decided to determine the structure and absolute configuration of the obtained diasteromeric products in the reaction of (*S*,*S*)-3,4-*tert*-butoxy-3,4-dihydro-2*H*-pyrrole 1-oxide (**I**) with an excess of racemic 2,3-dihydro-1-phenyl-1*H*-phosphole 1-oxide (**II**): (1*S*, 3a*R*,7*S*,8*S*,8a*R*,8b*R*)-(+)-7,8-di-*tert*-butoxy-1-phenyloctahydro-1*H*-pyrrolo(1,2-*b*)-1*H*-phospholo(2,3-*d*) isoxazole 1-oxide (**III**, hereafter) and (1*R*,3a*S*, 7*S*,8*S*,8a*S*,8b*S*)-(+)-7,8-di-*tert*-butoxy-1-phenyloctahydro-1*H*-pyrrolo(1,2-*b*)-1*H*-phospholo(2,3-*d*)isoxazole 1-oxide (**IV**,hereafter). In addition, we explicated hydrogen bonding pattern differences in terms of molecules conformational differences between diasteromers.

EXPERIMENTAL

Synthesis

Title compounds **III** and **IV** were prepared according to the procedure depicted in Scheme 1, based on the method of Brandi et al. [3], with total yield of 67%. The ratio of products established by integration of ^{31}P and ^{1}H NMR spectra of the crude mixtures after 8 h was 6.38:1. 38% of phosphole was recovered. $[\alpha]_D^{25}$ (**III**) = +29.2°, $[\alpha]_D^{25}$ (**IV**) = +38.7°. Elemental analysis: (calculated/ found (**III**)/found (**IV**)) C: 64.85/64.79/64.71; H: 8.41/8.49/8.44; N: 3.44/3.39/3.41. The remaining experimental data were in fully agreement with the previously reported ones.



SCHEME 1 Reaction in synthesis.

TABLE 1 Crystal Data and Structures Refinement

	Molecule **III**		*Molecule* **IV**
Empirical formula		$C_{22}H_{34}NO_4P$	
Formula weight		407.47	
Temperature (K)		293	
Crystal system	Orthorhombic		Monoclinic
Space group	$P2_12_12_1$		$P2_1$
Unit cell dimensions (Å, deg)	$a = 10.605(1)$		$a = 10.171(1)$
	$b = 11.400(1)$		$b = 11.358(2)$
	$c = 19.207(1)$		$c = 11.169(1)$
			$\beta = 113.18(3)$
Volume (Å^3)	2322.1(3)		1186.1(3)
Z	4		2
D_x (mg/m^3)	1.166		1.141
D_m (mg/m^3)	1.16		1.14
μ (mm^{-1})	1.25		1.26
Crystal description		Colorless, transparent sphere	
Crystal radius (mm)	0.42		0.39
$F(000)$	880		440
Diffractometer/scan type		CAD-4/ω-2θ	
Radiation		Cu Kα	
$\theta_{\max}$ (°)	66.98		74.94
Range of h, k, l	$0 \le h \le 12$		$-12 \le h \le 12$
	$0 \le k \le 13$		$0 \le k \le 14$
	$-22 \le l \le 22$		$-13 \le l \le 13$
Independent/collected reflections	4161/4610		2567/5127
Observed reflections	3811 [$I > 2\sigma(I)$]		2396 [$I > 2\sigma(I)$]
Completeness	1.000		1.000
Refinement method		Full-matrix least-squares	
Extinction coefficient	—		0.010(1)
Flack parameter	0.07(4)		0.03(3)
Parameters	285		294
S	1.131		1.158
R	0.0492		0.0421
R_w	0.2278		0.1137
Absorption correction		ψ-scan [6,7]	
Absorption coefficient	1.252		1.226
$T_{\min}$	0.883		0.720
$T_{\max}$	0.998		0.841
$\Delta\rho_{\max}$ (e•Å^{-3})	0.742		0.332
$\Delta\rho_{\min}$ (e•Å^{-3})	–0.941		–0.338
$\Delta\rho_{\mathrm{rms}}$ (e•Å^{-3})	0.208		0.042

X-ray Crystallography

The crystals of **III** and **IV** were mounted in turn on a CAD-4 automatic four-circle diffractometer. Three-dimensional X-ray intensity data were collected with graphite monochromated Cu $K\alpha$ radiation at room temperature using the ω-2θ scan technique. A quarter and half of Ewald sphere was collected, respectively. The unit cell parameters were determined from least-squares refinement of the setting angles of 99 reflections in the θ range from 5 to 40° [6]. Details concerning crystal data and refinement are given in Table 1.

An examination of two standard reflections, monitored after each 100 reflections measured, showed final coefficients for decay correction that are equal to 1.117 and 1.264 for **III** and **IV**, respectively. During data reduction, the decay correction coefficient was taken into account. The Lorentz polarization corrections were applied to the intensity data.

An empirical absorption correction based on ψ–scan technique [7] was used. The maximum and minimum transmission factors were 0.998 and 0.883 for **III** and 0.841 and 0.720 for **IV**. The structures were solved by direct methods. All non-hydrogen atoms

TABLE 2 Selected Bond Lengths (Å) and Angles (deg)

	III	IV
P(1)–O(1)	1.482(3)	1.482(2)
P(1)–C(9)	1.805(4)	1.794(3)
P(1)–C(1)	1.808(4)	1.816(3)
P(1)–C(8)	1.839(3)	1.840(2)
N(1)–O(2)	1.446(4)	1.441(3)
O(2)–C(3)	1.449(5)	1.442(4)
N(1)–C(4)	1.463(6)	1.483(4)
N(1)–C(7)	1.503(4)	1.486(3)
O(3)–C(15)	1.449(5)	1.451(4)
O(4)–C(6)	1.420(4)	1.406(3)
O(4)–C(19)	1.439(4)	1.446(4)
O(3)–C(5)	1.417(5)	1.413(3)
C(1)–C(2)	1.541(8)	1.514(4)
C(2)–C(3)	1.514(6)	1.517(4)
C(3)–C(8)	1.525(5)	1.532(3)
C(4)–C(5)	1.517(5)	1.528(4)
C(5)–C(6)	1.528(5)	1.523(4)
C(6)–C(7)	1.556(4)	1.537(4)
C(7)–C(8)	1.533(5)	1.537(3)
O(1)–P(1)–C(9)	111.2(2)	111.7(1)
O(1)–P(1)–C(1)	115.8(2)	114.9(1)
C(9)–P(1)–C(1)	105.1(2)	108.2(1)
O(1)–P(1)–C(8)	115.4(2)	116.8(1)
C(9)–P(1)–C(8)	110.9(2)	107.6(1)
C(1)–P(1)–C(8)	97.2(2)	96.3(1)
O(2)–N(1)–C(4)	110.0(3)	110.3(3)
O(2)–N(1)–C(7)	105.9(3)	104.2(2)
C(4)–N(1)–C(7)	107.1(3)	107.4(2)
N(1)–O(2)–C(3)	107.8(3)	107.3(2)
C(5)–O(3)–C(15)	118.0(3)	118.6(2)
C(6)–O(4)–C(19)	118.4(2)	118.2(2)
C(2)–C(1)–P(1)	104.1(3)	104.5(2)
C(3)–C(2)–C(1)	107.0(3)	108.0(2)
O(2)–C(3)–C(2)	106.5(3)	107.4(2)
O(2)–C(3)–C(8)	102.7(3)	102.7(2)
C(2)–C(3)–C(8)	110.6(4)	110.9(2)
N(1)–C(4)–C(5)	102.1(3)	108.0(2)
O(3)–C(5)–C(4)	113.6(3)	111.7(2)
O(3)–C(5)–C(6)	110.3(3)	110.4(2)
C(4)–C(5)–C(6)	101.2(3)	103.0(2)
O(4)–C(6)–C(5)	111.0(3)	110.6(2)
O(4)–C(6)–C(7)	111.9(3)	113.8(2)
C(5)–C(6)–C(7)	102.8(3)	103.3(2)
N(1)–C(7)–C(6)	104.7(3)	104.5(2)
N(1)–C(7)–C(8)	105.8(3)	106.3(2)
C(8)–C(7)–C(6)	116.2(3)	114.1(2)
C(3)–C(8)–C(7)	103.7(3)	103.7(2)
C(3)–C(8)–P(1)	103.9(2)	104.8(2)
C(7)–C(8)–P(1)	112.0(2)	112.9(2)
P(1)–C(1)–C(2)–C(3)	–38.1(4)	39.0(3)
C(1)–C(2)–C(3)–C(8)	44.9(5)	–40.8(3)
C(2)–C(3)–C(8)–P(1)	–28.7(4)	21.9(3)
C(3)–C(8)–P(1)–C(1)	4.7(3)	1.2(2)
C(8)–P(1)–C(1)–C(2)	19.2(3)	–23.2(2)
C(3)–O(2)–N(1)–C(7)	–28.6(4)	37.8(3)
O(2)–N(1)–C(7)–C(8)	6.7(4)	–19.3(3)
N(1)–C(7)–C(8)–C(3)	16.0(4)	–4.2(3)
C(7)–C(8)–C(3)–O(2)	–32.6(4)	26.0(2)
C(8)–C(3)–O(2)–N(1)	38.5(4)	–40.2(2)
N(1)–C(4)–C(5)–C(6)	47.0(4)	21.1(3)
C(4)–C(5)–C(6)–C(7)	–38.6(3)	–34.7(3)
C(5)–C(6)–C(7)–N(1)	16.8(3)	36.3(3)
C(6)–C(7)–N(1)–C(4)	12.5(4)	–23.3(3)
C(7)–N(1)–C(4)–C(5)	–37.1(4)	1.4(4)
C(6)–C(5)–O(3)–C(15)	–142.6(3)	–137.1(3)
C(5)–C(6)–O(4)–C(19)	–124.9(3)	–146.6(3)
C(4)–C(5)–O(3)–C(15)	104.5(4)	108.9(3)
C(7)–C(6)–O(4)–C(19)	120.9(3)	97.6(3)

were refined anisotropically using full-matrix, least-squares technique on F^2. The hydrogen atoms were found on difference Fourier synthesis, and next were refined as “riding” on the adjacent carbon atom with geometry idealization after each cycle. The methyl groups were allowed to rotate about their local three-fold axis. At the end of refinement, a root mean square difference of 0.208 and 0.042 $e \cdot Å^{-3}$ appeared in a difference Fourier synthesis. Because data of **III** were collected with k running from 0 to 14, the non-centrosymmetric intensities information was lost. This, together with large amount of reflections with small intensities, affects the quality of the structure and exhibits in relatively large weighted R factor. The solution and refinements were performed with SHELXS97 [8] and SHELXL97 [9]. The graphical manipulations were performed using the XP routine of the SHELXTL [10] and ORTEP [11]. Atomic scattering factors were taken according to [12]. The selected geometrical parameters of **III** and **IV** are listed in Table 2

RESULTS AND DISCUSSION

A perspective view of the structures showing absolute configuration [13], together with the atom-numbering scheme is depicted in Figs. 1 and 2 for **III** and **IV**, respectively. The methyl groups of *tert*-butyl substituents of **IV** show, signs of dynamic disorder, which exhibit in rather large displacement parameters (Fig. 2). According to Cahn–Ingold–Prelog rules [14,15], conformation of major cycloadduct (**III**) is (1*S*,3a*R*,7*S*,8*S*,8a*R*,8b*R*) and conformation of minor cycloadduct (**IV**) is (1*R*,3a*S*,7*S*,8*S*,8a*S*,8b*S*). It follows unequivocally from this finding that the preferred stereochemical cycloaddition from **I** to **II** involves an *exo* transition state in which the two five-membered ring reactants attack each other from the faces opposite to the P-Ph and C(3)-O-*t*-Bu substituents, respectively. It further follows that in the studied reaction involving nitrone (**I**) of the *S*,*S*

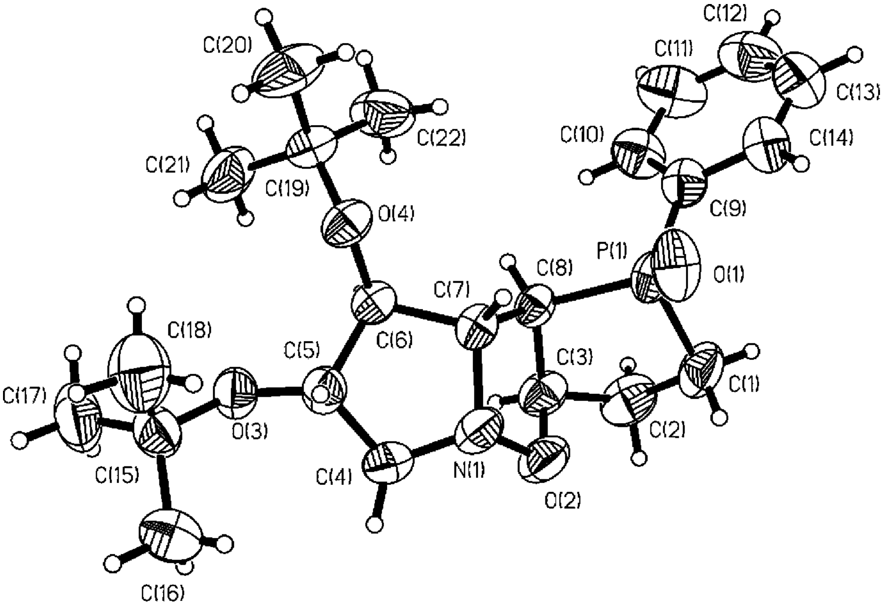


FIGURE 1 The molecular conformation of **III** plotted with 50% probability of displacement ellipsoids.

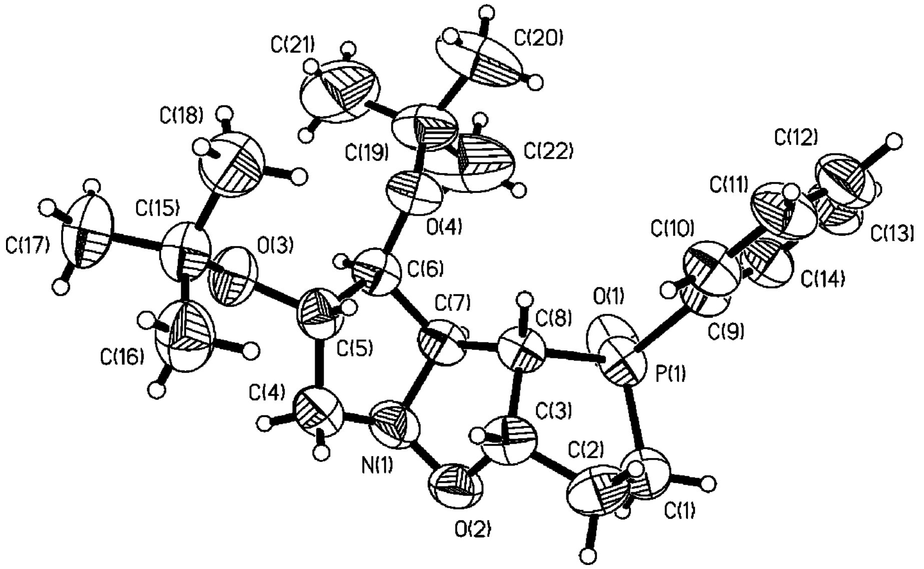


FIGURE 2 The molecular conformation of **IV** plotted with 50% probability of displacement ellipsoids.

configuration, the *S* enantiomer of dihydrophosphole sulfide was consumed preferentially and therefore the isolated unreacted laevorotatory (**II**) can be assigned unambiguously as *R*.

The general conformational preferences of molecule **III** are close to **III-A**. The main differences are in the arrangement of phenyl ring toward double bond at phosphorus (1.89° in **III-A** and 39.4(2)° in **III**) and in placement of *tert*-butyl substituents, which are more equatorial in **III-A**. The weighted root mean square deviation of superimposed molecules **III** and **III-A** is 0.138 Å for atoms of three fused rings and is 0.785 Å for all non-hydrogen atoms. In addition, **III** crystallizes in $P2_12_12_1$ space group and **III-A** crystallizes in $P3_1$ space group.

The differences between molecules of **III** and **IV** are significantly greater than between **III** and **III-A** (Fig. 3). However, the arrangement of phenyl ring toward double bond at phosphorus in **IV** is close to this founded in **III** (value of 33.0(2)°), and the angle between weighted least squares plane of phospholane ring and $P{-}C_{Ph}$ bond does not show greater differences (65.2(2) and 69.8(2)° for **III** and **IV**, respectively); the conformation of fused rings is

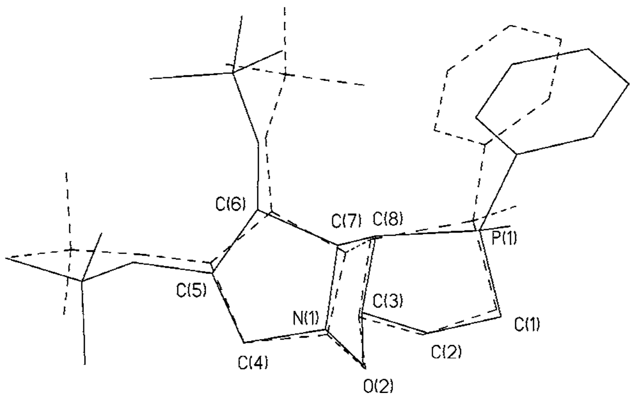


FIGURE 3 Superposition of **III** and **IV**. The molecule of **IV** is indicated by dashed lines. The hydrogen atoms have been omitted for clarity.

completely different. The conformational analysis of the puckered heteroatom three-ring system based on asymmetry parameters, introduced by Duax and Norton [16,17], shows the conformation of noticeable distorted envelope on C(2) with puckering amplitude [18] $Q_2 = 0.397$ Å, the intermediate conformation between twisted through the mid point of C(3)—O(2) bond and envelope on C(3) with $Q_2 =$ 0.353 Å, and half-chair conformation on the mid point of C(4)—O(5) bond with $Q_2 = 0.451$ Å, for phospholane, oxazolidine, and pyrrolidine rings of **III**, respectively. Rings in molecule of **IV** adopt conformations of envelopes on C(2) with $Q_2 = 0.381$ Å, on O(2) with$Q_2 = 0.367$ Å, and on C(6) with $Q_2 = 0.363$ Å, respectively, for the rings as described above. The values and placement of asymmetry parameters are shown on Fig. 4. The total puckering amplitude of the 11-membered ring created by the atoms of three fused rings is 1.755 and 1.881 Å for the compounds **III** and **IV**, respectively.

The phosphorus atom tetrahedron, in both molecules, exhibits deformation (Table 2) typical for similar compounds [4,19,20]. The most distorted is intraring angle, which is caused by steric constrains imposed by relatively stiff five-membered ring. Also O=P—$C_{phospholane}$ angles are distorted. The main reason for this behavior is comparatively great conformational freedom of small oxygen atom, and thus phosphorus environment adopts the most geometrically and energetically preferred conformation by

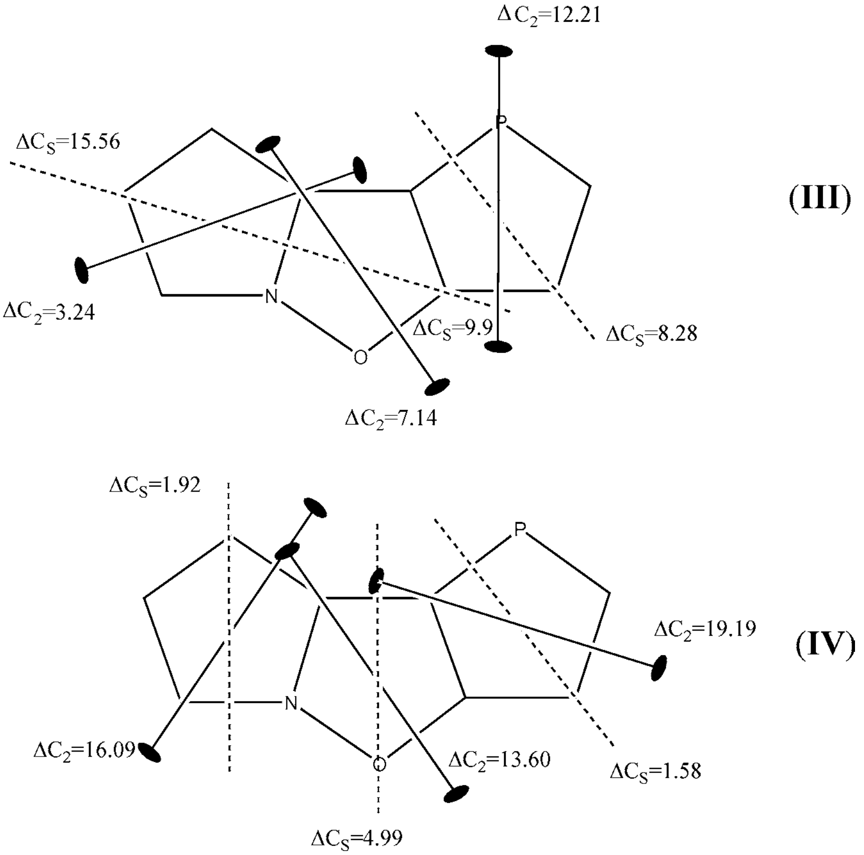


FIGURE 4 The values and placement of asymmetry parameters of **III** and **IV**.

TABLE 3 Hydrogen Bonds

III					**IV**				
D–H•••A	*d* (D–H)	*d* (H•••A)	*d* (D•••A)	(D–H•••A)	D–H•••A	*d* (D–H)	*d* (H•••A)	*d* (D•••A)	(D–H•••A)
C(3)–H(3)•••O(1)#1	0.98	2.57	3.247(5)	126.1	C(3)–H(3)•••O(1)#2	0.98	2.27	3.222(3)	163.2
C(6)–H(6)•••O(1)#1	0.98	2.35	3.275(4)	156.4	C(13)–H(13)•••O(2)#3	0.93	2.60	3.366(4)	140.0
C(7)–H(7)•••O(1)	0.98	2.50	3.055(4)	115.4	C(7)–H(7)•••O(1)	0.98	2.54	3.120(3)	117.9
C(8)–H(8)•••O(1)#1	0.98	2.51	3.163(4)	124.1	C(8)–H(8)•••O(4)	0.98	2.44	2.888(3)	107.2

Distances are in Å and angles in degrees. Symmetry transformations used to generate equivalent atoms: #1 $x + 1/2, -y + 1/2, -z + 2$; #2 $-x, y + 1/2, -z$; #3 $x-1, y, z$.

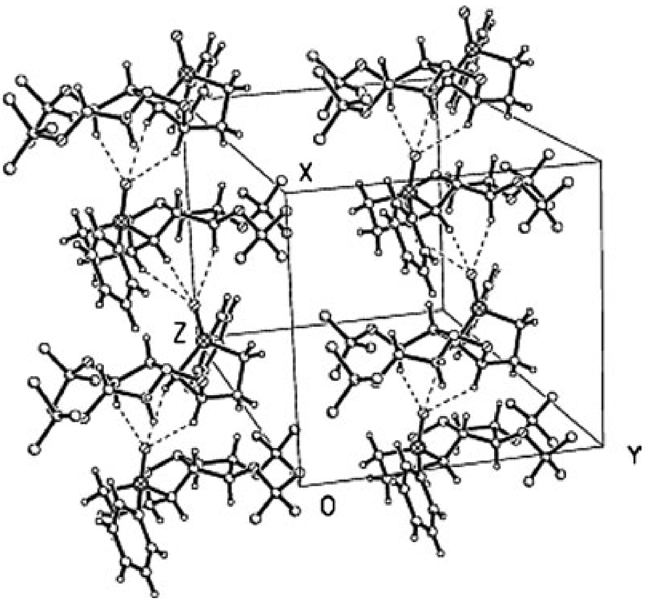


FIGURE 5 Part of the molecular packing of **III** showing intermolecular hydrogen bonds creating a chain structure along *x*-axis. Hydrogen bonds are indicated by dashed lines. Methyl groups' hydrogen atoms have been omitted for clarity.

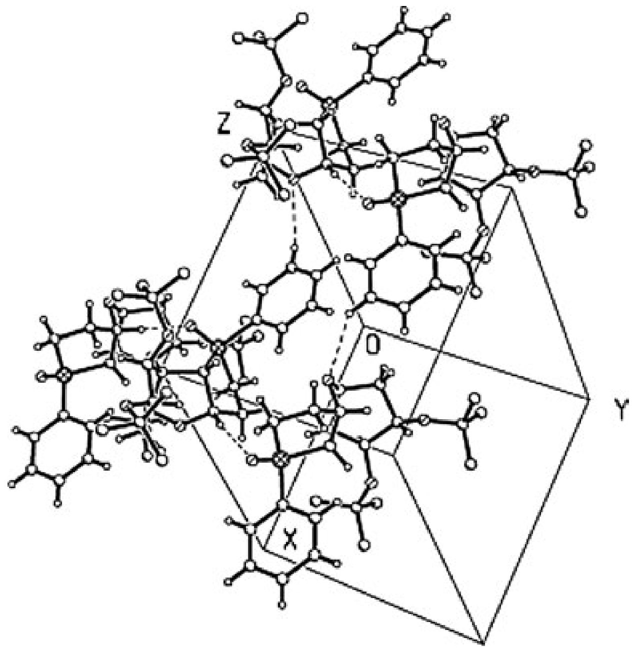


FIGURE 6 Part of the molecular packing of **IV** showing intermolecular hydrogen bonds creating a two-dimensional net structure. Hydrogen bonds are indicated by dashed lines. Methyl groups' hydrogen atoms have been omitted for clarity.

deformation of tetrahedron corner at oxygen. However, the dihedral angle between phospholane and phenyl ring planes for both compounds is the same and is equal to 86.9(2)°; the angles between weighted least squares planes of oxazolidine–pyrrolidine and phospholane–oxazolidine rings are clearly different, and their amounts are, respectively, 57.32(12), 73.83(13)° for compound **III** and 80.03(10), 67.79(9)° for compound **IV**. Analogous angles in **III-A** are 60.42 and 66.13°. The angle between phospholane weighted least squares plane and double bond at phosphorus enlarges in sequence **IV** < **III** < **III-A** and is equal to 41.3(1), 44.1(2) and 45.54°, respectively. The last difference between compounds is conformation of *tert*-butoxy substituents, which are bent in molecule **IV** in opposite direction than in molecule **III**. This is connected with differences in conformation of pyrrolidine ring.

In the structure **III**, one C(7)–H(7)•••O(1) short intramolecular interaction can be found, which, according to Desiraju and Steiner [21], can be considered as a weak hydrogen bond (Table 3). The molecules of **III** are assembled by intermolecular weak hydrogen bonds [22,23] C(3)–H(3)•••O (1# $x + 1/2, -y + 1/2$), C(6)–H(6)•••O (1# $x + 1/2, -y + 1/2$), and C(8)–H(8)•••O (1# $x + 1/2, -y + 1/2$) (Table 3) to the one-dimensional infinite chain along x-axis (Fig. 5). The structure of **IV** is built up from C(3)–H(3)•••O (1# $-x, y + 1/2, -z$) and C(13)–H(13)•••O (2# x–1, y, z) weak intermolecular hydrogen bonds (Table 3) to form the two-dimensional, infinite hydrogen bond network (Fig. 6). The two intramolecular weak hydrogen bonds C(7)—H(7)•••O(1) and C(8)—H(8)•••O(4) (Table 3) provide additional stabilization to this molecule.

The differences in conformation between compounds **III** and **IV** cause changes in hydrogen bonding pattern, because in molecule **IV** there is no hydrogen cavern filled with three hydrogen bond donors (C(3), C(6), and C(8)), and one weak hydrogen bond has not enough strength to force such an arrangement as it is in **III**.

Supporting Information. Tables of crystal data and structure refinement, anisotropic displacement coefficients, atomic coordinates and equivalent isotropic displacement parameters for non-hydrogen atoms, H-atom coordinates and isotropic displacement parameters, bond lengths and interbond angles have been deposited with the Cambridge Crystallographic Data Centre Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB1 1EW, United Kingdom, under CCDC256157 and CCDC 256158.

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