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**C<sub>3</sub>H<sub>3</sub>Cl<sub>2</sub>OP**

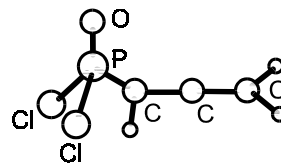
**1,2-Propadienylphosphonic dichloride**

**C<sub>s</sub> (*sp*)**

**C<sub>1</sub> (*ac*)**



$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
P–C	1.795(6)	C=C–P	121.1(15)
P–Cl	2.011(1)	C–P–Cl	105.9(5)
P=O	1.461(3)	Cl–P–Cl	101.9(6)
C=C	1.318(4)	O=P–Cl	113.3(4)
C–H	1.084(15)	O=P–C	115.4(10)
		C=C–H	124.4(42)
		$\tau_1$ <sup>b)</sup>	0
		$\tau_2$ <sup>c)</sup>	123.1(244)



The molecule exists as a mixture of *sp* (72(25)%) and *ac* (28(25)%) conformers.

The conformers were assumed to have the same parameters except for the torsion angle  $\tau$ .

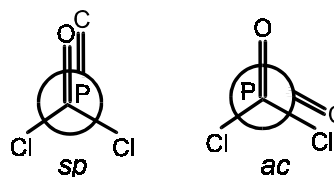
The carbon skeleton C=C=C was assumed to be linear.

The nozzle temperature was about 80 °C.

<sup>a)</sup> Three times the estimated standard errors.

<sup>b)</sup> Torsion angle O=P–C=C for the *sp*-conformer.

<sup>c)</sup> Torsion angle O=P–C=C for the *ac*-conformer.



Nesterov, V.Yu., Naumov, V.A.: Zh. Obshch. Khim. **63** (1993) 2585; Russ. J. Gen. Chem. (Engl. Transl.) **63** (1993) 1794.