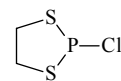


262 **C₂H₄CIPS₂**
ED, *ab initio* and DFT
calculations

2-Chloro-1,3,2-dithiaphospholane**C₁**

r_a	Å ^{a)}	θ_a	deg ^{a)}
P–Cl	2.103(14) ^{b)}	S–P–Cl	102.9(4)
P–S(3)	2.117(14) ^{b)}	S–P–S	96.7(5)
P–S(1)	2.081(28)	P–S(3)–C(4)	102.0(7)
C(4)–S(3)	1.836(5) ^{c)}	S(3)–C(4)–C(5)	112.1(8) ^{d)}
C(5)–S(1)	1.816(5) ^{c)}	H–C–S	107.6(45)
C(4)–C(5)	1.514(11)	P–S(3)–C(4)–C(5)	–17.9(32)
C–H	1.121(16)	S(3)–C(4)–C(5)–S(1)	42.7(31)
		C(4)–C(5)–S(1)–P	–45.2(32)
		C(5)–S(1)–P–S(3)	27.5(31)
		S(1)–P–S(3)–C(4)	–8.9(32)
		Cl–P–S(3)–C(4)	96.0(34)
		Cl–P–S(1)–C(5)	–77.4(33)

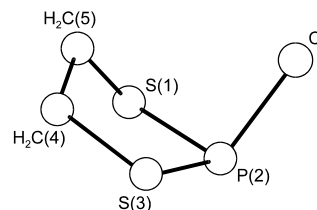
The ED intensities from [1] were reanalyzed. Contrary to the results of [1], the molecule has no C_s symmetry. The molecular ring was found to have the P-envelope form twisted about the C–C bond with an axial P–Cl bond. According to the results of *ab initio* calculations, the less stable conformers have C_s ($\Delta E = 2.53$ kcal mol^{–1}) and C₂ ($\Delta E = 2.74$ kcal mol^{–1}) symmetry. The nozzle was *ca.* 130 °C.

^{a)} Uncertainties were unidentified, probably estimated total errors.

^{b)} Difference between the P–Cl and P–S(3) bond lengths was assumed at the value from HF/6-31G** calculations.

^{c)} Difference in the C–S bond lengths was assumed at the value from HF/6-31G** calculations.

^{d)} The C–C–S bond angles were assumed to be equal.



Naumov, V.A., Dakkouri, M., Naumov, A.V.: Zh. Obshch. Khim. **71** No.7 (2001) 1089;
Russ. J. Gen. Chem. (Engl. Transl.) **71** (2001) 1024.

[1] Schultz, G., Hargittai, I., Martin, J., Robert, J.B.: Tetrahedron **30** (1974) 2365.

Replaces [II/25B\(3, 734\)](#)