

1416
ED

C₃H₉PS₃

Trimethyl trithiophosphite
Trimethyl phosphorotrithioite

C₃ (*gauche-gauche-gauche*)
C_s (*gauche⁻-gauche-anti*)
C₁ (*gauche-gauche-anti*)
P(SCH₃)₃

r_a	\AA^a	θ_a	deg ^{a)}
C–H	1.150(21)	H–C–H	109.0(40) ^{b)}
C–S	1.834(5)	C–S–P	96.9(11)
S–P	2.115(3)	S–P–S	97.7(6)

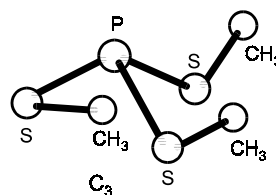
	<i>gauche-gauche-gauche</i>	<i>gauche⁻-gauche-anti</i>	<i>gauche-gauche-anti</i>
ϕ_1 [deg] ^{a) c)}	64.5(15)	–64.5(15)	64.5(15)
ϕ_2 [deg] ^{a) c)}	64.5(15)	64.5(15)	64.5(15)
ϕ_3 [deg] ^{a) c)}	64.5(15)	180.0	180.0

The ED intensity measured in [1] was reanalyzed to study possible conformational equilibrium. The molecule exists as a mixture of *gauche-gauche-gauche* (80%), *gauche⁻-gauche-anti* (10%) and *gauche-gauche-anti* (10%) conformers. The nozzle temperature was 80 °C.

^{a)} Three times the estimated standard errors.

^{b)} Not estimated in the original paper.

^{c)} Dihedral angle M–P–S–C measured from the *syn* position, where M denotes the lone pair of the P atom.



Kataeva, O.N., Naumov, V.A.: Zh. Strukt. Khim. **28** No.5 (1987) 153; Russ. J. Struct. Chem. (Engl. Transl.) **28** (1987) 770.

[1] Tuzova, L.L., Naumov, V.A., Galiakberov, R.M., Ofitserov, E.N., Pudovik, A.N.: Dokl. Akad. Nauk SSSR **256** (1981) 891; Proc. Acad. Sci. USSR (Engl. Transl.) **256** (1981) 51.