

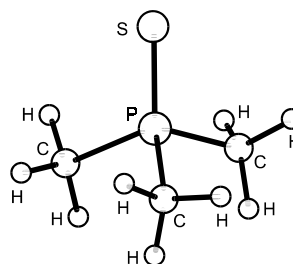
1415
ED

C₃H₉PS

Trimethylphosphine sulfide

C₃
S=P(CH₃)₃

r_a	\AA^a	θ_a	deg ^{a)}
P=S	1.940(2)	S=P-C	114.1(2)
P-C	1.818(2)	C-P-C	104.5(3)
C-H	1.106(5)	P-C-H	108.6(8)
		τ^b	42.7(73)



With models simulating free rotation of the methyl groups, approximately the same parameter values were obtained. The nozzle temperature was 160 °C.

^{a)} Twice the estimated standard errors including a systematic error.

^{b)} The torsional angle S=P-C-H, $\tau = 0^\circ$ for the *syn* position. The tilt (CH₃) angle was assumed to be zero.

Wilkins, C.J., Hagen, K., Hedberg, L., Shen, Q., Hedberg, K.: J. Am. Chem. Soc. **97** (1975) 6352.

MW

C_{3v} assumed

r_0	\AA	θ_0	deg
P=S	1.936(3)	S=P-C	114.36(9)
P-C	1.814(1)	P-C-H(s)	113.17(125) ^{a)}
C-H	1.094(3)	P-C-H(a)	107.52(69) ^{a)}
		H(s)-C-H(a)	109.52(4)
		H(a)-C-H(a)	109.52(4)
		tilt (CH ₃) ^{b)}	3.74(128)

^{a)} Dependent parameters.

^{b)} Towards the P=S bond.

Durig, J.R., Chatterjee, K.K.: Inorg. Chem. **28** (1989) 298.