

1414 C₃H₉PS

 ED, *ab initio* calculations
 (HF/3-21G*, HF/6-31G*)

Dimethyl(methylthio)phosphine

 C_s (*trans*)
 C_s (*cis*) or C₁ (*near-cis*)
 H₃C–S–P(CH₃)₂

	<i>r</i> ^{a)} Å ^{b)}		<i>θ</i> ^{a)}	deg ^{b)}	
	<i>near-cis</i>	<i>trans</i>		<i>near-cis</i>	<i>trans</i>
P–S	2.111(2)	2.103(2)	P–S–C	102.3(26)	108.5(25)
P–C	1.862(2)	1.862(2)	C–P–C	96.7(8)	96.7(8)
S–C	1.769(6)	1.769(6)	C–P–S	96.8(15)	99.9(15)
C–H	1.081(2)	1.081(2)	H–C–P	113.1(20)	113.1(20)
			H–C–S	110.8(40)	110.8(40)
			H–C–H	108.9 ^{d)}	108.9 ^{d)}
			H–C–H	105.7 ^{e)}	105.7 ^{e)}
			C–S–P–D ^{c)}	15.7(16)	180

Two distinct conformers, *trans* and *cis* or *near-cis* (the *cis* conformer has the thiomethyl group eclipsing the non-bonded electron pair on the P atom and the *trans* conformer has this methyl group staggered with respect to the two methyl groups attached to the P atom) were identified with the conformational composition of 78(5)% of the *cis* form.

The potential energy surface near the *cis* conformation is likely to be very close to flat.

Local C_{3v} and C_{2v} symmetry for the CH₃ and PC₂ groups, respectively, were assumed. One of the C–H bonds in the SCH₃ group was assumed to eclipse the S–P bond.

The nozzle was at room temperature.

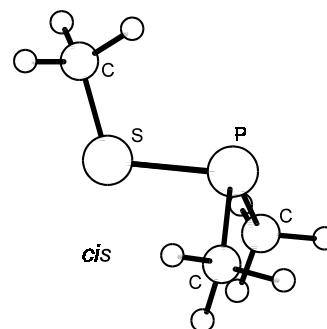
^{a)} Undefined, possibly *r*_a and *θ*_a.

^{b)} Estimated standard errors including a systematic error.

^{c)} Effective torsional angle where D is a dummy atom defined as the bisector of the angle C–P–C.

^{d)} Assumed for the S–CH₃ group.

^{e)} Assumed for the P–CH₃ groups.



Durig, J.R., Barron, D.A., Sullivan, J.F., Anderson, D.G., Craddock, S., Rankin, D.W.H.: J. Mol. Struct. **268** (1992) 143.