

1290 C₃H₆S
Methyl vinyl sulfide

 ED, *ab initio* calculations

(STO-3G, 44-31G)

 C_s (*syn*)

 C₁ (*gauche*)

 H₂C=CH-S-CH₃

<i>r</i> _a	Å ^{a)}		<i>θ</i> _α	deg ^{a)}	
	<i>syn</i>	<i>gauche</i>		<i>syn</i>	<i>gauche</i>
C=C	1.343(1)		C=C-S	127.5(7)	122.5 °
C(2)-S	1.759(8)	1.767 °	C-S-C	102.1(5)	89.9 °
C(4)-S	1.795(8)		S-C(2)-H	112.3(30)	117.1 °
C(1,2)-H	1.088(9)		C(2)=C(1)-H(6)	113.5(19)	
C(4)-H	1.106(8)		C(2)=C(1)-H(7)	130.6(29)	
			S-C(4)-H	110.1(11)	
			tilt (CH ₃) ^{b)}	3.0 °	
			<i>φ</i> ^{d)}	0.0 °	135.8(65)

 Abundance of the *syn* conformer was 38(7)%.

The nozzle temperature was 200...211 °C.

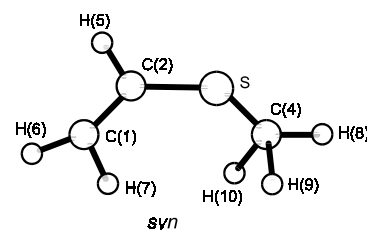
 $\Delta H^\circ = H^\circ(\textit{gauche}) - H^\circ(\textit{syn}) = 1.0...2.0 \text{ kcal mol}^{-1}$.

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

^{b)} Tilt angle, positive when the C₃-axis in the C(2)SC(4) plane is tilted towards the S atom.

^{c)} The difference from the *syn* parameter was fixed at the *ab initio* value.

^{d)} Torsional angle C=C-S-C, *φ* = 0° for *syn* position.

^{e)} Assumed.

 Samdal, S., Seip, H.M., Torggrimsen, T.: J. Mol. Struct. **57** (1979) 105.