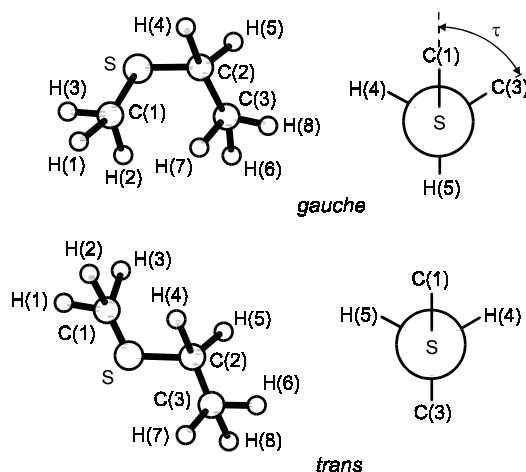


r_s	Å		θ_s	deg	
	<i>trans</i> [1]	<i>gauche</i> [2]		<i>trans</i> [1]	<i>gauche</i> [2]
C(1)–S	1.804(4)	1.802(2)	C(1)–S–C(2)	99.0(2)	100.2(1)
C(2)–S	1.804(4)	1.806(2)	C(3)–C(2)–S	109.5(3)	114.7(1)
C(2)–C(3)	1.530(4)	1.524(2)	C(3)–C(2)–H(4)	110.7(5)	112.0(2)
C(1)–H(1)	1.090(3)	1.112(4)	C(3)–C(2)–H(5)	110.7(5)	110.8(2)
C(1)–H(2)	1.089(4)	1.098(8)	S–C(2)–H(4)	108.8(4)	107.5(2)
C(1)–H(3)	1.089(4)	1.089(4)	S–C(2)–H(5)	108.8(4)	104.8(2)
C(2)–H(4,5)	1.097(3)	1.093(2)	H(4)–C(2)–H(5)	108.4(5)	106.4(3)
C(3)–H(6)	1.087(5)	1.087(2)	S–C(1)–H(1)	106.7(4)	111.6(2)
C(3)–H(7)	1.092(4)	1.113(3)	S–C(1)–H(2)	110.8(3)	109.9(4)
C(3)–H(8)	1.092(4)	1.113(1)	S–C(1)–H(3)	110.8(3)	106.9(2)
			H(1)–C(1)–H(2)	109.5(5)	108.2(5)
			H(1)–C(1)–H(3)	109.5(5)	110.3(4)
			H(2)–C(1)–H(3)	109.5(4)	110.1(8)
			C(2)–C(3)–H(6)	110.6(4)	111.2(2)
			C(2)–C(3)–H(7)	110.6(4)	109.3(2)
			C(2)–C(3)–H(8)	110.6(4)	109.8(2)
			H(6)–C(3)–H(7)	108.2(5)	108.3(3)
			H(6)–C(3)–H(8)	108.2(5)	107.9(2)
			H(7)–C(3)–H(8)	108.6(4)	110.3(3)
			tilt (SC(1)H ₃) ^b	2.7(3)	
			tilt (CC(3)H ₃) ^b	–0.1(4)	
			τ^c	180.0	69.4(8)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
<i>trans</i> [1]			
S	0.4829	–0.5733	0.0
C(1)	1.9177	0.5206	0.0
C(2)	–0.8218	0.6719	0.0
C(3)	–2.1865	–0.0189	0.0
H(1)	2.7989	–0.1187	0.0
H(2,3)	1.9248	1.1506	±0.8898
H(4,5)	–0.7074	1.3035	±0.8892
H(6)	–2.9877	0.7157	0.0
H(7,8)	–2.2990	–0.6467	±0.8869
<i>gauche</i> [2]			
S	–0.6852	0.5983	–0.1762
C(1)	–1.3665	–1.0427	0.1250
C(2)	0.9696	0.3909	0.5177
C(3)	1.8820	–0.5354	–0.2771
H(1)	–0.7845	–1.8299	–0.4029
H(2)	–1.3444	–1.2638	1.1997
H(3)	–2.3943	–1.0283	–0.2335
H(4)	0.8525	0.0617	1.5531
H(5)	1.3828	1.4016	0.5592
H(6)	2.8697	–0.5955	0.1728
H(7)	1.9938	–0.1411	–1.3126
H(8)	1.4518	–1.5623	–0.2984



^a) The tilt angle is defined by $(2/3)[(S-C(1)-H(2,3)) - (S-C(1)-H(1))]$.

^b) The tilt angle is defined by $(2/3)[(C(2)-C(3)-H(7,8)) - (C(2)-C(3)-H(6))]$.

^c) Dihedral angle C(3)–C(2)–S–C(1).

[1] Hayashi, M., Adachi, M., Nakagawa, J.: J. Mol. Spectrosc. **86** (1981) 129.

[2] Adachi, M., Nakagawa, J., Hayashi, M.: J. Mol. Spectrosc. **91** (1982) 381.

ED

r_g	\AA^a	θ_α	deg^a
C–S (average)	1.813(4)	C–S–C	97.1(11)
C(1)–S	1.806(27)	S–C–C	114.0(5)
C(2)–S	1.818(27)	H–C–H	109.6(14)
C–C	1.536(8)	τ^b	66(9)
C–H	1.111(8)		

Abundance of the *trans* conformer at room temperature was 25(10)%.
The measurements were made at room temperature.

^a) Estimated limits of error.

^b) Dihedral angle C(1)–S–C(2)–C(3) for the *gauche* conformer measured from the *syn* position.

Oyanagi, K., Kuchitsu, K.: Bull. Chem. Soc. Jpn. **51** (1978) 2243.