

$r_0$	Å	$\theta_0$	deg			
C(3)=C(4)	1.331 <sup>a)</sup>	C-S-H	96.0 <sup>a)</sup>			
C(2)-C(3)	1.496 <sup>a)</sup>	C-C-S	113.6 <sup>a)</sup>			
C(1)-C(2)	1.528 <sup>a)</sup>	C(1)-C(2)-C(3)	111.6 <sup>a)</sup>			
C-S	1.814 <sup>a)</sup>	C(2)-C(3)=C(4)	127.8 <sup>a)</sup>			
S-H	1.336 <sup>a)</sup>	C(2)-C(3)-H	115.5 <sup>a)</sup>			
C(1,2)-H	1.093 <sup>a)</sup>	H-C(4)=C(3)	121.5 <sup>a)</sup>			
C(3,4)-H	1.090 <sup>a)</sup>	C(2)-C(1)-H	109.47 <sup>a)</sup>			
		C(1)-C(2)-H	109.47 <sup>a)</sup>			
		H-C(2)-H	109.47 <sup>a)</sup>			
		H-C(1)-H	109.47 <sup>a)</sup>			
		H-bonded <i>gauche</i>		ext. I	ext. II	
		$\tau_1$ <sup>b)</sup>	57(3)	62(3)	62(3)	
		$\tau_2$ <sup>c)</sup>	115(3)	2(3)	5(3)	
			65(3) <sup>d)</sup>			
		$\tau_3$ <sup>e)</sup>	130(5)	60(5)	60(5)	

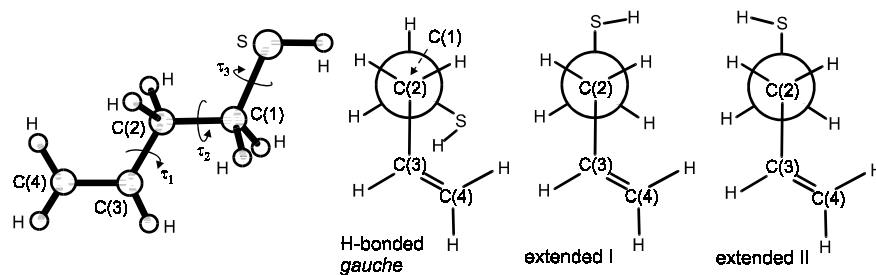
## H-bonded conformation

Atom	$ a_s $ [Å]	$ b_s $ [Å]	$ c_s $ [Å]
H (in SH)	0.47425	1.33914	0.55400

<sup>a)</sup> Assumed.<sup>b)</sup> Torsional angle C(1)-C(2)-C(3)=C(4).<sup>c)</sup> Torsional angle S-C(1)-C(2)-C(3).<sup>d)</sup> From *syn*.<sup>e)</sup> Torsional angle H-S-C(1)-C(2).

Three rotational conformers were detected.

Energy difference between

Extended I – H-bonded *gauche* = 2.9(5) kJ mol<sup>-1</sup>Extended II – H-bonded *gauche* = 3.6(6) kJ mol<sup>-1</sup>.Marstokk, K.-M., Møllendal, H.: Acta Chem. Scand., Ser. A **40** (1986) 402.

Marstokk, K.-M., Møllendal, H.: Structure and Dynamics of Weakly Bound Molecular Complexes, A. Weber (ed.), Reidel 1987, p.57.