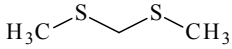
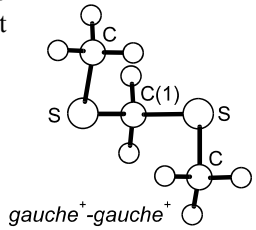
443 **$C_3H_8S_2$** **Bis(methylthio)methane** **C_2** (*gauche*$^+$-*gauche*$^+$)
ED, *ab initio* and DFT calculations Methylenedithiobismethane **C_1** (*gauche-anti*)

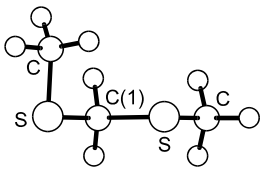


r_g	Å [a])	θ_α	deg [a])
S–C(methyl)	1.805(2) [b])	C–S–C	102.8(24)
C(1)–S	1.806(2) [b])	S–C–S	115.9(3)
C(methyl)–H	1.108(5)	H–C(1)–H	107.5 [c])
C(1)–H	1.098(5)	S–C(methyl)–H	108.9 [c])
		τ [d])	54(6)

The molecule was found to exist as a mixture of *gauche*$^+$-*gauche*$^+$ and *gauche-anti* conformers in the ratio of 70(18):30(18). The differences in bond distances and bond angles between these conformers as well as the differences between the different types of C–H distances in the same conformer were assumed at the values from HF/6-311+G(d) calculations. Torsional angles C–S–C–S in the *gauche-anti* conformer were assumed at the values of 74° and 186° from HF/6-311+G(d) calculations. Local C_{3v} symmetry was assumed for methyl groups. The structural parameters are listed for the *gauche*$^+$-*gauche*$^+$ conformer.
The nozzle temperature was 90...105 °C.



gauche$^+$-*gauche*$^+$



gauche-anti

[a]) Twice the estimated standard errors including a systematic error.
[b]) Difference between the r_α[S–C(methyl)] and r_α[C(1)–S] bond lengths was assumed at the value from HF/6-311+G(d) calculations.
[c]) Assumed at the value from HF/6-311+G(d) calculations.
[d]) Torsional angle C–S–C–S from the *syn* position.

Page, E.M., Rice, D.A., Aarset, K., Hagen, K., Genge, A.R.J.: J. Phys. Chem. A **104** (2000) 6672.