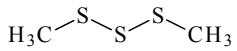
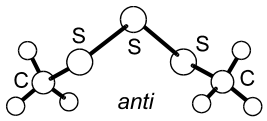
307 **$C_2H_6S_3$** **Dimethyl trisulfide** **C_2** (*anti*) **C_s** (*syn*)

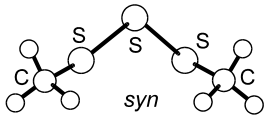
ED, *ab initio* and DFT calculations



r_g	Å [a])	θ_α	deg [a])
C–H [b])	1.084(7)	C–S–S	103.1(5)
S–C	1.817(2)	S–S–S	107.3(5)
S–S	2.046(2)	H–C–S [b])	112(2)
		C–S–S–S [c])	79(5)

According to the results of MP2/6-311+G(d) calculations, the molecule exists as a mixture of *anti* (71.5%) and *syn* (28.5%) conformers, where the CH_3 groups are on the opposite and the same sides, respectively (see figure), at the temperature of the ED experiment; the energy difference between these conformers was calculated to be 7.65 kJ mol^{-1}. The differences in the geometrical parameters between the two conformers were constrained in the ED analysis at the *ab initio* values. The parameters are listed here for the *anti* conformer. The nozzle was at 383 K.





[a]) Twice the estimated standard errors including a systematic error.
[b]) Average value.
[c]) Zero degree for the eclipsed position.

Shen, Q., Wells, C., Hagen, K.: Inorg. Chem. **37** (1998) 3895.