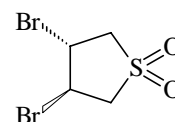


**1627**     **C<sub>4</sub>H<sub>6</sub>Br<sub>2</sub>O<sub>2</sub>S**  
ED, *ab initio* calculations  
(MP2/6-31G\*)

***trans*-3,4-Dibromotetrahydrothiophene 1,1-dioxide**

**C<sub>2</sub>**

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
S=O	1.425(1) <sup>b)</sup>	O=S=O	117.9(10) <sup>b)</sup>
S–C	1.790(3) <sup>b)</sup>	C–S–C	92.8(7) <sup>b)</sup>
C–C	1.529(4) <sup>b)</sup>	C–C–Br	109.2(3) <sup>b)</sup>
C–Br	1.948(3) <sup>b)</sup>	S–C–H	107.8 <sup>b)c)</sup>
C–H	1.120 <sup>c)</sup>	C–C–H	111.0 <sup>b)c)</sup>
		C–C–C–C (axial) <sup>d)</sup>	–51.9(10)
		C–C–C–C (equatorial) <sup>d)</sup>	59.8(9)
		Br–C–C–Br (axial) <sup>d)</sup>	–167.9(18)
		Br–C–C–Br (equatorial) <sup>d)</sup>	–70.8(11)



The molecule exists as a mixture of axial (47.2(23)%) and equatorial conformers. Differences between the bond distances and angles in the two conformers were fixed at *ab initio* values.

The nozzle was at ca. 469 K.

<sup>a)</sup> Estimated standard errors.

<sup>b)</sup> Mean value for two conformers.

<sup>c)</sup> Fixed.

<sup>d)</sup> 0° for the *syn* position.

Blake, A.J., Brain, P.T., Gosney, I., Gould, R.O., Rankin, D.W.H., Robertson, H.E., Trickey, P., Bühl, M.: J. Chem. Soc. Perkin Trans. II (1995) 2293.

