

**1067 C<sub>3</sub>H<sub>2</sub>F<sub>6</sub>S<sub>2</sub>**ED, *ab initio* calculations  
(HF/3-21G\*)**Bis[(trifluoromethyl)thio]methane****C<sub>2</sub> (+*sc*, +*sc*)****C<sub>1</sub> (*sc*, *ap*)**F<sub>3</sub>C–S–CH<sub>2</sub>–S–CF<sub>3</sub>

<i>r</i> <sub>a</sub>	Å <sup>a)</sup>	<i>θ</i> <sub>α</sub>	deg <sup>a)</sup>
C–S (mean)	1.814(3)	F–C–F	107.3(1)
Δ(C–S) <sup>b)</sup>	0.043 <sup>c)</sup>	H–C–H	107.6 <sup>c)</sup>
C(1)–S	1.836(3)	C–S–C	98.2(10)
C–H	1.095 <sup>d)</sup>	S–C–S	112.1(6) <sup>e)</sup>
S–C(2,2')	1.793(3)	S–C–S	109.4(6) <sup>f)</sup>
C–F	1.342(2)	<i>φ</i> <sup>g)</sup>	79.1(10)
		<i>φ</i> <sub>1</sub> <sup>h)</sup>	76.7 <sup>c)</sup>
		<i>φ</i> <sub>2</sub> <sup>i)</sup>	154.2 <sup>c)</sup>
		<i>τ</i> (CF <sub>3</sub> ) <sup>j)</sup>	12.8(12) <sup>k)</sup>

The compound exists as a mixture of two conformers (+*sc*, +*sc*) and (*sc*, *ap*) in the ratio 70(15):30.

The nozzle was at room temperature.

<sup>a)</sup> Three times the estimated standard errors including a scale error.

<sup>b)</sup> [C(1)–S] – [S–C(2,2')].

<sup>c)</sup> *Ab initio* value.

<sup>d)</sup> Assumed.

<sup>e)</sup> For the (+*sc*, +*sc*) conformer.

<sup>f)</sup> For the (*sc*, *ap*) conformer. The conformational difference was fixed at the *ab initio* value.

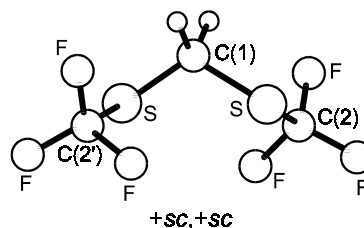
<sup>g)</sup> Dihedral angles S–C–S–C for the (+*sc*, +*sc*) conformer.

<sup>h)</sup> Dihedral angle S–C(1)–S–C(2) for the (*sc*, *ap*) conformer.

<sup>i)</sup> Dihedral angle S–C(1)–S–C(2') for the (*sc*, *ap*) conformer.

<sup>j)</sup> The torsional angle *τ* describes the deviation of the CF<sub>3</sub> groups from the exact staggered orientation.

<sup>k)</sup> Effective value due to large-amplitude torsional vibrations.



Korn, M., Haas, A., Oberhammer, H.: Chem. Ber. **128** (1995) 461.