

**1473**      **C<sub>4</sub>F<sub>6</sub>OS<sub>2</sub>**  
ED, *ab initio* calculations

**Bis[(trifluoromethyl)thio]ethenone**  
Bis(trifluoromethylthio)ketene

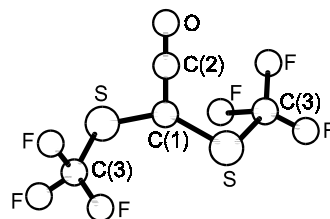
**C<sub>2</sub> assumed**  
O=C=C(SCF<sub>3</sub>)<sub>2</sub>

(HF/3-21G\*, HF/6-31G\*)

$r_a$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
S–C (mean)	1.778(3)	S–C(1)–S	127.3(8)
$\Delta(\text{C–S})$ <sup>b)</sup>	0.066(11)	C(1)–S–C(3)	102.1(9)
C(1)–S	1.745(12)	F–C(3)–F	107.6(3)
S–C(3)	1.811(12)	tilt (CF <sub>3</sub> ) <sup>c)</sup>	3.0 <sup>d)</sup>
C(1)=C(2)	1.335(21)	C(2)=C(1)–S–C	95.8(13)
C(2)=O	1.180(8)		
C–F	1.337(3)		

Local C<sub>3v</sub> symmetry and staggered orientation with respect to the C(1)–S bonds were assumed for the CF<sub>3</sub> groups.

The nozzle temperature was 20 °C.



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

<sup>b)</sup>  $\Delta(\text{C–S}) = [\text{C(1)–S}] - [\text{S–C(3)}]$ .

<sup>c)</sup> Tilt angle of the CF<sub>3</sub> group towards the C(1) atom.

<sup>d)</sup> Assumed.

Korn, M., Mack, H.-G., Praas, H.-W., Della Védova, C.O., Oberhammer, H.: J. Mol. Struct. **352/353** (1995) 145.