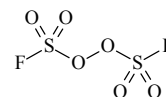


**186**      **F<sub>2</sub>O<sub>6</sub>S<sub>2</sub>**ED, *ab initio* and DFT  
calculations **$\mu$ -Peroxo-bis(fluorodioxosulfur)**

Bis(sulfuryl fluoride) peroxide

**C<sub>2</sub> (G<sup>-</sup>G<sup>-</sup>)****C<sub>2</sub> (G<sup>+</sup>G<sup>+</sup>)****C<sub>1</sub> (G<sup>+</sup>G<sup>-</sup>)**

$r_g$	$\text{\AA}^a$		$\theta_\alpha$	deg <sup>a)</sup>
	G <sup>-</sup> G <sup>-</sup>	G <sup>+</sup> G <sup>+</sup>		
S=O	1.406(2)	1.407(2)	O(1)–S–F	98.2(18)
S–O	1.620(4)	1.616(3)	O–O–S	108.6(10)
S–F	1.539(3)	1.547(3)	O(1)–S=O(2)	111.2(12) <sup>b)</sup>
O–O	1.453(14)	1.466(14)	O(1)–S=O(3)	103.1(12) <sup>b)</sup>
			O(2)=S=O(3)	126.7(15)
			F–S=O(2)	106.3(5)
			F–S=O(3)	107.6(3)
			G <sup>-</sup> G <sup>-</sup>	G <sup>+</sup> G <sup>+</sup>
			S–O–O–S	122.7(56)    135.5 <sup>c)</sup>
			O–O–S–F	-71.7(50)    70.5 <sup>c)</sup>



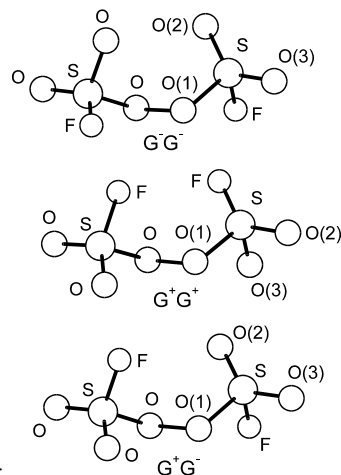
In the ED analysis, about equally good fits were found for two models, model A consisting of G<sup>-</sup>G<sup>-</sup> (57(27)%) and G<sup>+</sup>G<sup>+</sup> (43(27)%) conformers and model B, consisting of G<sup>-</sup>G<sup>-</sup> (38(14)%) and G<sup>+</sup>G<sup>+</sup> (62(14)%) conformers, where G<sup>+</sup> and G<sup>-</sup> designate positive and negative rotations around the O–S bonds. The structural parameters are listed for the conformers from model A.

The nozzle temperature was 298 K.

<sup>a)</sup> Twice the estimated standard errors.

<sup>b)</sup> Difference between the O(1)–S=O(2) and O(1)–S=O(3) bond angles was assumed at the value from MP2/6-311+G\* calculations.

<sup>c)</sup> Assumed at the value from MP2/6-311+G\* calculations.



Hagen, K., Hedberg, K., Gard, G., Aubke, F.: J. Mol. Struct. **567-568** (2001) 1.