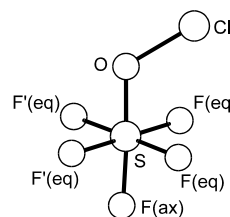


**124**      **ClF<sub>5</sub>OS**ED, *ab initio* and DFT  
calculations**Pentafluoro(hypochlorito- $\kappa$ O)sulfur**

Sulfur pentafluoride hypochlorite

**C<sub>s</sub>**  
**F<sub>5</sub>S–OCl**

$r_a$	$\text{\AA}^a$	$\theta_a$	$\text{deg}^a$
S–F (ax,eq)	1.560(2)	F(ax)–S–F(eq)	89.6(3)
S–O	1.657(14)	S–O–Cl	119.2(6)
O–Cl	1.667(16)	tilt (SF <sub>5</sub> ) <sup>b</sup>	2.9(8)



The SF<sub>5</sub> group was constrained to C<sub>4v</sub> symmetry,  
and all S–F bonds were assumed to be equal.

These assumptions were justified by HF/3-21G\* and B3PW91/6-31G\* calculations.

The O–Cl bond was assumed to be staggered with respect to the S–F(eq) bonds.

The nozzle was at room temperature.

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

<sup>b</sup>) Tilt angle between the C<sub>4</sub> axis of the SF<sub>5</sub> group and the S–O bond direction away from F(eq) and towards F'(eq).

Kornath, A., Hartfeld, N., Oberhammer, H.: Inorg. Chem. **36** (1997) 5156.