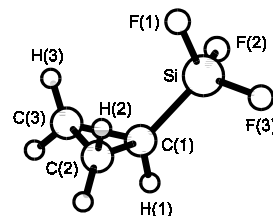
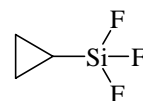


**1210**     **C<sub>3</sub>H<sub>5</sub>F<sub>3</sub>Si**  
ED, *ab initio* calculations  
(HF/4-21G\*, 6-31G\*)

**(Trifluorosilyl)cyclopropane**  
Cyclopropyltrifluorosilane

**C<sub>s</sub>**

| $r_a$     | Å <sup>a)</sup>     | $\theta_\alpha$                         | deg <sup>a)</sup> |
|-----------|---------------------|---|-------------------|
| C(1)–C(2) | 1.522(8)            | C–Si–F(1)                               | 112.3(10)         |
| C(2)–C(3) | 1.491 <sup>b)</sup> | C–Si–F(2,3)                             | 111.6(10)         |
| C–Si      | 1.807(2)            | Si–C–H                                  | 116(4)            |
| Si–F      | 1.572(3)            | H–C–H                                   | 108.8(23)         |
| C–H       | 1.104(3)            | $\theta$ <sup>c)</sup>                  | 124.5(9)          |
|           |                     | $\tau$ (CF <sub>3</sub> ) <sup>d)</sup> | 0.4(7)            |
|           |                     | $\gamma$ <sup>e)</sup>                  | 1.2 <sup>f)</sup> |
|           |                     | $\kappa$ <sup>g)</sup>                  | 3.7(64)           |
|           |                     | $\lambda$ <sup>h)</sup>                 | 2.0(71)           |



The analysis was performed applying a dynamical model, which treats the torsional vibration of the SiF<sub>3</sub> group as large-amplitude motion.  
The nozzle temperature was 22 °C.

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

<sup>b)</sup> Dependent parameter; difference between C(1)–C(2) and C(2)–C(3) was fixed at *ab initio* value.

<sup>c)</sup> Angle between the Si–C bond and the ring plane.

<sup>d)</sup> Tilt angle between the C<sub>3</sub> axis of the CF<sub>3</sub> group and the Si–C bond direction away from the ring plane.

<sup>e)</sup> Wagging angles of the CH<sub>2</sub> groups;  $\gamma$  is positive when the planes of the methylene groups move away from each other.

<sup>f)</sup> Fixed.

<sup>g)</sup> Rocking angles of the CH<sub>2</sub> groups;  $\kappa$  is positive when the atoms H(2) and H(3) move away from Si atom.

<sup>h)</sup> Twisting angles of the CH<sub>2</sub> groups;  $\lambda$  is positive when the atoms H(2) and H(3) move away from each other.

Dakkouri, M., Typke, V.: J. Mol. Struct. **320** (1994) 13.