

1037  
MW

**C<sub>3</sub>HF<sub>3</sub>O**

**3,3-Difluoro-2-propenoyl fluoride**  
3,3-Difluoroacryloyl fluoride

C<sub>s</sub> (*syn*)  
C<sub>s</sub> (*anti*)  
F<sub>2</sub>C=CH-C(O)F

<i>r</i> <sub>0</sub>	Å	Å	<i>θ</i> <sub>0</sub>	deg <sup>a)</sup>	deg <sup>a)</sup>
	<i>syn</i>	<i>anti</i>		<i>syn</i>	<i>anti</i>
C(1)–F(1)	1.355 <sup>b)</sup>	1.352 <sup>b)</sup>	F(2)–C(3)=C(2)	126.3 <sup>b)</sup>	127.5 <sup>b)</sup>
C(1)–C(2)	1.450 <sup>b)</sup>	1.449 <sup>b)</sup>	F(3)–C(3)=C(2)	123.4 <sup>b)</sup>	122.6 <sup>b)</sup>
C(2)=C(3)	1.307 <sup>b)</sup>	1.307 <sup>b)</sup>	H–C(2)=C(3)	119.3 <sup>b)</sup>	118.5 <sup>b)</sup>
C(1)=O	1.185 <sup>b)</sup>	1.185 <sup>b)</sup>	C(1)–C(2)=C(3)	123.8(20)	126.6(20)
C(3)–F(2)	1.317 <sup>b)</sup>	1.317 <sup>b)</sup>	O=C(1)–C(2) <sup>c)</sup>	130.9(20)	124.3(20)
C(3)–F(3)	1.323 <sup>b)</sup>	1.325 <sup>b)</sup>	F(1)–C(1)–C(2)	108.7(20)	115.2(20)
C(2)–H	1.064 <sup>b)</sup>	1.065 <sup>b)</sup>			

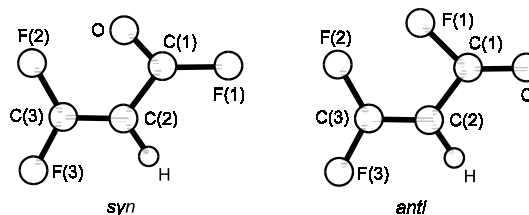
Two conformers, *syn* and *anti*, were detected, the *syn* form being more stable by 170(100) cal mol<sup>–1</sup>.

<sup>a)</sup> Uncertainties were not estimated in the original paper.

<sup>b)</sup> Assumed *ab initio* values.

<sup>c)</sup> Dependent parameter

determined by planarity constraint and fixed value of angle F(1)–C(1)=O.



Tam, H.S., Harmony, M.D., Brahms, J.C., Dailey, W.P.: J. Mol. Struct. **244** (1991) 59.