

**344**      **C<sub>3</sub>H<sub>2</sub>ClF<sub>5</sub>O**ED, *ab initio* and DFT  
calculations**2-Chloro-1-(difluoromethoxy)-1,1,2-trifluoroethane**2-Chloro-1,1,2-trifluoroethyl difluoromethyl ether  
EnfluraneC<sub>1</sub> (aAg<sup>+</sup>)C<sub>1</sub> (g<sup>+</sup>Ag<sup>+</sup>)C<sub>1</sub> (g<sup>+</sup>Ag<sup>+</sup>)C<sub>1</sub> (g<sup>-</sup>Ag<sup>-</sup>)

<i>r<sub>a</sub></i>	Å <sup>a)</sup>	<i>θ<sub>a</sub></i>	deg <sup>a)</sup>
O–C(1)	1.383(5)	C(2)–C(1)–O	110.7(11)
O–C(3)	1.409 <sup>b)</sup>	C(1)–O–C(3)	117.3(21)
C(1)–C(2)	1.520(9)	C(2)–C(1)–F	110.0(11)
C(1)–F	1.343(2)	O–C(1)–F	110.0 <sup>c)</sup>
C(2)–F	1.343 <sup>b)</sup>	C(1)–C(2)–F	108.0 <sup>d)</sup>
C(3)–F	1.333 <sup>b)</sup>	O–C(3)–F	107.3 <sup>e)</sup>
C–Cl	1.752(6)	C(1)–C(2)–Cl	111.0(10)
C–H	1.100 <sup>f)</sup>	F–C(2)–Cl	111.6(11)
		F–C(1)–F	106.1(28)
		F–C(3)–F	108.0 <sup>g)</sup>
		C(1)–C(2)–H	107.8 <sup>g)</sup>
		O–C(3)–H	112.7 <sup>g)</sup>
		Cl–C(2)–H	107.8 <sup>g)</sup>
		<i>τ</i> <sub>1</sub> <sup>h)</sup>	195(4)
		<i>τ</i> <sub>2</sub> <sup>i)</sup>	180(5)
		<i>τ</i> <sub>3</sub> <sup>j)</sup>	22(4)



The experimental intensities were reproduced best with a mixture of conformers, which possess an *anti* (A) configuration of the C–C–O–C skeleton and *gauche* (g) orientation of the H atom in CHF<sub>2</sub> group with respect to the O–C(1) bond. These conformers differ by the rotational orientation of the CHFCl group, with either C–Cl (aAg<sup>+</sup> conformer, 58(8)%), C–H (g<sup>+</sup>Ag<sup>+</sup> and g<sup>-</sup>Ag<sup>-</sup> conformers, 32(10)%), or C–F (g<sup>-</sup>Ag<sup>-</sup> conformer, 10(10)%) in *anti* position to the C(1)–O bond. The structural differences between the aAg<sup>+</sup> conformer and others were assumed at the values from B3PW91/6-311G(2d) calculations.

The structural parameters are given for the aAg<sup>+</sup> conformer.

The nozzle was at room temperature.

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

<sup>b)</sup> Difference between similar parameters was assumed at the value from B3PW91/6-311G(2d) calculations.

<sup>c)</sup> O–C(1)–F and C(2)–C(1)–F were assumed to be equal.

<sup>d)</sup> Difference between C(1)–C(2)–F and C(2)–C(1)–F was assumed at the value from quantum chemical calculations.

<sup>e)</sup> Difference between O–C(3)–F and C(2)–C(1)–F was assumed at the value from quantum chemical calculations.

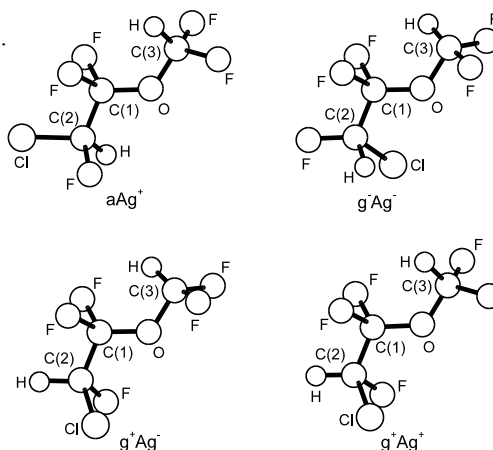
<sup>f)</sup> Assumed.

<sup>g)</sup> Assumed at the value from B3PW91/6-311G(2d) calculations.

<sup>h)</sup> Cl–C(2)–C(1)–O torsional angle.

<sup>i)</sup> C(2)–C(1)–O–C(3) torsional angle.

<sup>j)</sup> C(1)–O–C(3)–H torsional angle.



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