

1104  
MW

$C_3H_3F_3O_4$

**Formic acid – trifluoroacetic acid (1/1)**  
(weakly bound complex)

$C_s$   
(effective symmetry class)  
 $CF_3COOH \cdot HCOOH$

$r_s$	$\text{\AA}$
C(1)–H(2)	1.076(1)
C(1)=O(3)	1.211(8)
C(1)–O(4)	1.320(7)
O(3)...O(5)	2.720(14)
O(4)...O(6)	2.729(3)

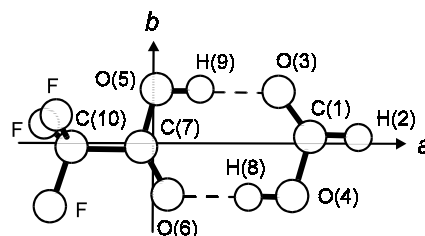
$\theta_s$	deg
H(2)–C(1)=O(3)	122.9(4)
H(2)–C(1)–O(4)	111.2(4)
C(1)=O(3)...O(5)	126.2(4)
C(1)–O(4)...O(6)	108.2(2)

$r_0$	$\text{\AA}$
C(1)–H(2)	1.077(1)
C(1)=O(3)	1.197(8)
C(1)–O(4)	1.339(7)
O(3)...O(5)	2.700(14)
O(4)...O(6)	2.729(3)
O(4)–H(8)	0.970 <sup>a)</sup>
O(5)–H(9)	0.970 <sup>a)</sup>
C(7)–O(5)	1.307 <sup>a)</sup>
C(7)=O(6)	1.190 <sup>a)</sup>
C(7)–C(10)	1.497 <sup>a)</sup>
C(10)–F	1.325 <sup>a)</sup>

$\theta_0$	deg
H(2)–C(1)=O(3)	125.0(4)
H(2)–C(1)–O(4)	109.4(4)
C(1)=O(3)...O(5)	126.7(4)
C(1)–O(4)...O(6)	107.9(2)
C(1)–O(4)–H(8)	109.6(2)
C(7)–O(5)–H(9)	117.8(11)
O(6)=C(7)–C(10)	122.5 <sup>a)</sup>
C(7)–C(10)–F	109.5 <sup>a)</sup>

<sup>a)</sup> Assumed.

Atom	$a_0$ [ $\text{\AA}$ ]	$b_0$ [ $\text{\AA}$ ]
C(1)	3.5162	0.1306
H(2)	4.5927	0.1321
O(3)	2.8278	1.1096
O(4)	3.0731	–1.1338
O(5)	0.1288	1.1854
O(6)	0.3440	–1.0681
H(8)	2.1031	–1.1392
H(9)	1.0988	1.1747
C(7)	–0.2813	–0.0556



Martinache, L., Kresa, W., Wegener, M., Vonmont, U., Bauder, A.: Chem. Phys. **148** (1990) 129.