

**1063**      **C<sub>3</sub>H<sub>2</sub>F<sub>2</sub>O<sub>2</sub>**  
ED, *ab initio* calculations  
(HF/3-21G, HF/6-31G\*\*)

**Propanedioyl difluoride**  
Malonyl difluoride

**C<sub>1</sub> (S-*gauche*)**  
**C<sub>2</sub> (W-*gauche*)**  
F(O)C-CH<sub>2</sub>-C(O)F

$r_a$	$\text{\AA}^a$	$\theta_\alpha$	deg <sup>a)</sup>
C-H	1.10 <sup>b)</sup>	C-C-C	110.2(10)
C-C	1.502(5)	H-C-H	108.0 <sup>b)</sup>
C=O	1.177(3)	C-C=O	129.1(8)
C-F	1.349(4)	C-C-F	109.7(7)
		F-C=O	121.2(11) <sup>c)</sup>
		$\delta_1(\text{C}(1)-\text{C}(2)-\text{C}(3)=\text{O})$	112.0(20)
		$\delta_2(\text{C}(3)-\text{C}(2)-\text{C}(1)=\text{O})$	0.0 <sup>b)</sup>

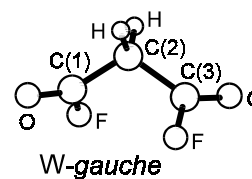
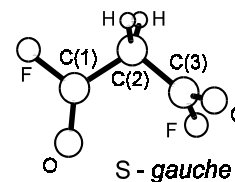
The presence of a small amount (10(10)%) of a second conformer (W-*gauche*) with C<sub>2</sub> symmetry and with both C=O bonds eclipsing the C-H bonds is likely. Parameters for the S-*gauche* conformer are listed.

The nozzle was at room temperature.

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

<sup>b)</sup> Assumed.

<sup>c)</sup> Dependent parameter.



Jin, A., Mack, H.-G., Waterfeld, A., Oberhammer, H.: J. Am. Chem. Soc. **113** (1991) 7847.