

**1661 C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>**

 ED, MW, *ab initio*  
 calculations (HF/4-21G)

**Cyclopropanecarboxylic acid**

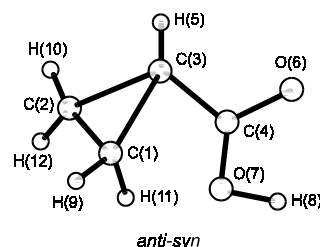
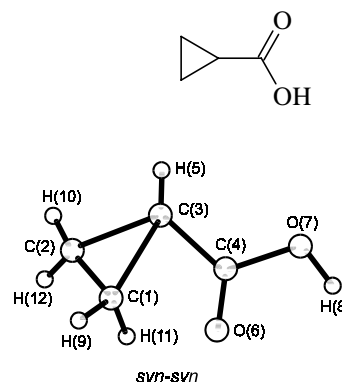
 C<sub>s</sub> (*syn-syn*)

 C<sub>s</sub> (*anti-syn*)

$r_g$	Å <sup>c)</sup>	Å <sup>c)</sup>
	Static model <sup>a)</sup>	Dynamic model <sup>b)</sup>
C(1)–C(2)	1.497(6)	1.493(7)
C(1)–C(3)	1.522(3)	1.524(3)
C(3)–C(4)	1.475(4)	1.478(5)
C(4)=O(6)	1.214(2)	1.214(2)
C(4)–O(7)	1.349(3)	1.349(3)
C(1)–H(9)	1.103(4) <sup>d)</sup>	1.104(4) <sup>d)</sup>
C(1)–H(11)	1.103(4) <sup>d)</sup>	1.104(4) <sup>d)</sup>
C(3)–H(5)	1.099(4) <sup>d)</sup>	1.100(4) <sup>d)</sup>
O(7)–H(8)	0.985(11)	0.982(12)

$\theta_\alpha$	deg <sup>c)</sup>	deg <sup>c)</sup>
	Static model <sup>a)</sup>	Dynamic model <sup>b)</sup>
C(1)–C(3)–C(4)	116.8(3)	116.6(3)
C(3)–C(4)=O(6)	124.7(4)	124.1(6)
C(3)–C(4)–O(7)	112.5(3)	112.6(3)
C(3)–C(1)–H(9)	116.4(9) <sup>d)</sup>	117.0(10) <sup>d)</sup>
C(3)–C(1)–H(11)	115.4(9) <sup>d)</sup>	116.0(10) <sup>d)</sup>
C(2)–C(1)–H(9)	118.1(9) <sup>d)</sup>	118.7(10) <sup>d)</sup>
C(2)–C(1)–H(11)	116.9(9) <sup>d)</sup>	117.5(10) <sup>d)</sup>
C(4)–C(3)–H(5)	115.6(9) <sup>d)</sup>	115.6(10) <sup>d)</sup>
C(4)–O(7)–H(8)	105.4(8)	105.4(12)



The molecule is found to prefer a conformation that has the carbonyl group *syn* to the cyclopropyl ring. A second conformer is also present with an energy 3...5 kJ mol<sup>−1</sup> less stable. This conformer is found to have the carbonyl group *anti* to the ring. The nozzle temperature of the ED experiment was 48...52 °C.

<sup>a)</sup> 65(5)% *syn-syn* and 35(5)% *anti-syn*.

<sup>b)</sup>  $V_1 = 2.1(9)$  kJ mol<sup>−1</sup> and  $V_2 = 13(2)$  kJ mol<sup>−1</sup>, where the potential energy related to the C(3)–C(4) torsion ( $\phi = 0^\circ$  for the *syn* position of the C(4)=O(6) bond with respect to the ring) is represented by  $V(\phi) = (1/2)[V_1(1 - \cos \phi) + V_2(1 - \cos 2\phi)]$ .

<sup>c)</sup> Twice the estimated standard errors.

<sup>d)</sup> The differences were fixed at the *ab initio* values.

Marstokk, K.-M., Møllendal, H., Samdal, S.: Acta Chem. Scand. **45** (1991) 37.