

1669  
ED

**C<sub>4</sub>H<sub>6</sub>O<sub>3</sub>**

**Acetic anhydride**

**C<sub>2</sub> assumed**  
H<sub>3</sub>C–C(O)–O–C(O)–CH<sub>3</sub>

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C(1)–O(1)	1.405(20)	C(1)–O(1)–C(1')	115.8(40)
C(1)=O(2)	1.183(25)	O(1)–C(1)=O(2)	121.7(20)
C(1)–C(2)	1.495(20)	O(1)–C(1)–C(2)	108.3(20)
		$\tau_1$ <sup>b)</sup>	48.5(100)
		$\tau_2$ <sup>c)</sup>	180 <sup>d)</sup>

A second model also agrees with the experimental results and cannot be ruled out. The only significant difference between the two models is the different value of the angle (for the second model O(1)–C(1)–C(2) = 114.5(20)°).

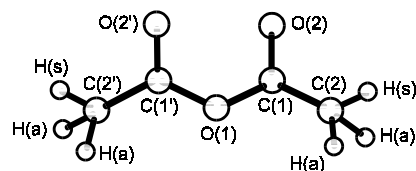
The nozzle temperature was 80 °C.

<sup>a)</sup> Uncertainty estimates are larger than those of the original data.

<sup>b)</sup> The torsional angle C(1')–O(1)–C(1)=O(2).

<sup>c)</sup> The torsional angle O(1)–C(1)–C(2)–H(s).

<sup>d)</sup> Assumed.



Vledder, H.J., Mijlhoff, F.C., Leyte, J.C., Romers, C.: J. Mol. Struct. **7** (1971) 421.