

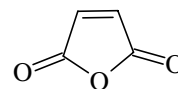
1512  
MW

$C_4H_2O_3$

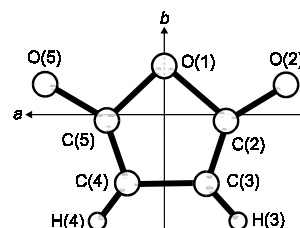
**2,5-Furandione**  
Maleic anhydride

$C_{2v}$

$r_s$	$\text{\AA}^a$	$\theta_s$	$\text{deg}^a$
O(1)–C(2,5)	1.3876(10)	C(2)–O(1)–C(5)	108.06(10)
C(2,5)–C	1.4849(25)	O(1)–C–C	108.07(5)
C(3)=C(4)	1.3331(40)	C(2,5)–C=C	107.90(10)
O(2,5)=C	1.1962(6)	O(1)–C=O(2,5)	122.32(10)
C(3,4)–H	1.0791(30)	O(2,5)=C–C	129.61(10)
		C(2,5)–C–H	122.10(10)
		C(3,4)=C–H	129.99(5)



Atom	$a_s$ [ $\text{\AA}$ ]	$b_s$ [ $\text{\AA}$ ]
O(1)	–	0.92971
O(2,5)	2.23442	0.55732
C(2,5)	1.12314	0.11464
C(3,4)	0.66675	–1.29863
H(3,4)	1.36007	–2.10508



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

Stiefvater, O.L.: Z. Naturforsch. **32a** (1977) 1480.

ED

$r_g$	$\text{\AA}^a$	$\theta_a$	$\text{deg}^a$
O(1)–C(2,5)	1.394(11)	C(2)–O(1)–C(5)	107.0(11)
C(2,5)–C	1.500(5)	O(1)–C–C	108.8(12)
C(3)=C(4) <sup>b</sup>	1.330(30)	C(2,5)–C=C <sup>b</sup>	107.7(10)
O(2,5)=C	1.195(3)	O(1)–C=O(2,5) <sup>b</sup>	121.9(12)
C(3,4)–H	1.091(21)	O(2,5)=C–C	129.3(20)
		C(3,4)=C–H	128.9(33)

A planar model agrees with the experimental results.

The nozzle temperature was 90 °C.

<sup>a</sup>) Estimated limits of error.

<sup>b</sup>) Values for these parameters are obtained from the eight independent parameters.

Uncertainties in these dependent parameters are obtained by transforming the error matrix.

Hilderbrandt, R.L., Peixoto, E.M.A.: J. Mol. Struct. **12** (1972) 31.