

1170  
MW

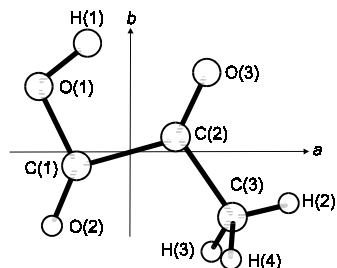
**C<sub>3</sub>H<sub>4</sub>O<sub>3</sub>**

**2-Oxopropanoic acid**  
Pyruvic acid

**C<sub>s</sub>**  
H<sub>3</sub>C–C(O)–COOH

$r_s$	Å	$\theta_s$	deg
O(1)–H(1)	0.9835(51)	C(1)–O(1)–H(1)	105.2(20)
C(1)–O(1)	1.3285(49)	O(1)–C(1)–C(2)	114.5(13)
C(1)=O(2)	1.2146(48)	C(1)–C(2)–C(3)	118.6(12)
C(2)=O(3)	1.2310(54)	C(1)–C(2)=O(3)	117.0(16)
C(1)–C(2)	1.5227(31)	C(2)–C(1)=O(2)	122.0(18)
C(2)–C(3)	1.4863(44)	C(2)–C(3)–H(2)	110.7(11)
C(3)–H(2)	1.0744(17)	C(2)–C(3)–H(3,4)	109.0(26)
C(3)–H(3,4)	1.1056(65)		
H(1)...O(3)	2.0176(43)		
O(1)...O(3)	2.6352(25)		

Atom	$a_s$ [Å]	$b_s$ [Å]	$c_s$ [Å]
C(1)	–0.7356	–0.1808	± 0.0185
C(2)	0.7517	0.1453	± 0.0178
C(3)	1.7255	–0.9774	± 0.0374
O(1)	–1.5333	0.8816	± 0.0238
O(2)	–1.1437	–1.3249	± 0.0206
O(3)	1.0624	1.3365	± 0.0250
H(1)	–0.9294	1.6579	± 0.0383
H(2)	2.7338	–0.6063	± 0.1417
H(3,4)	1.5281	–1.6254	± 0.8524



Dyllick-Brenzinger, C.E., Bauder, A., Günthard, H.H.: Chem. Phys. **23** (1977) 195.