

1736 **C<sub>4</sub>H<sub>8</sub>O**  
ED, MW, *ab initio*  
calculations (HF/6-31G\*)

**Isobutyraldehyde**  
2-Methylpropanal

**C<sub>1</sub> (*gauche*)**  
**C<sub>s</sub> (*syn*)**  
**H(O)C–CH(CH<sub>3</sub>)<sub>2</sub>**

$r_g$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C–H (methyl)	1.109(3)	C(2)–C(1)–C(3)	113.5(7)
C(1)–H <sup>b)</sup>	1.104(3)	C(2)–C(1)–C(4)	109.2(7)
C(2)–H <sup>b)</sup>	1.108(3)	C(3)–C(1)–C(4)	111.6(4)
C(1)–C(2)	1.513(2)	C(1)–C(3,4)–H	112.3(8)
C(1)–C(3) <sup>c)</sup>	1.526(2)	C(1)–C(2)=O	123.8(9)
C(1)–C(4) <sup>c)</sup>	1.537(2)	C(1)–C(2)–H	114.7 <sup>d)</sup>
C=O	1.226(3)	C(2)–C(1)–H	105.6 <sup>d)</sup>
		$\phi_1$ <sup>e)</sup>	115.4(14)
		$\phi_2$ <sup>f)</sup>	60 <sup>d)</sup>

The molecule exists as a mixture of the *gauche* (88(14)%) and *syn* conformers. The differences in the corresponding bond distances and valence angles between the two conformers were fixed at *ab initio* values. Local C<sub>3v</sub> symmetry was assumed for the methyl groups. The parameters were given for the *gauche* conformer.

The nozzle temperature was 299 K.

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

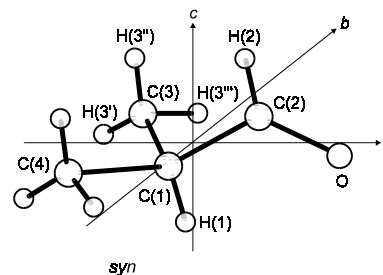
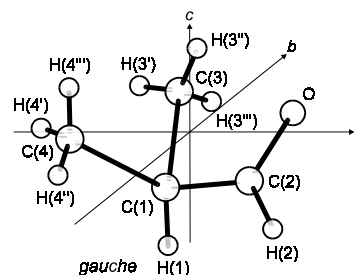
<sup>b)</sup> Dependent parameter. Difference between this parameter and C–H (methyl) was fixed at the *ab initio* value.

<sup>c)</sup> Dependent parameter. Difference between this parameter and C(1)–C(2) was fixed at the *ab initio* value.

<sup>d)</sup> Fixed at the *ab initio* value.

<sup>e)</sup> Dihedral angle O=C–C–H;  $\phi_1 = 0^\circ$  for the *syn* position.

<sup>f)</sup> Dihedral angle H(1)–C(1)–C(3)–H(3'').



Aarset, K., Faksnes, L.G., Nygård, I., Hagen, K.: J. Phys. Chem. **98** (1994) 2848.

MW

<i>gauche</i>			
$r_0$	Å	$\theta_0$	deg
C(2)=O	1.209(2)	H–C(2)=O	121.4(1)
C(2)–H	1.118(2)	C(1)–C(2)=O	125.5(3)
C(1)–C(2)	1.509(3)	C(1)–C(2)–H	113.1(3)
C(1)–C(3,4)	1.525(2)	C(2)–C(1)–C(3)	111.9(3)
C(1)–H	1.119(2)	C(2)–C(1)–C(4)	109.3(3)
		C(2)–C(1)–H(1)	100.9(6)
		$\alpha$ <sup>a)</sup>	113.0(14)
		$\beta$ <sup>b)</sup>	126.2(3)
		$\gamma$ <sup>c)</sup>	120.8(14)

Atom	$a_s$ [Å]	$b_s$ [Å]	$c_s$ [Å]
C(1)	-0.5236	0.0101	-0.4088
H(1)	-0.5963	0.0321	-1.5260
C(2)	0.8410	-0.6003	-0.2213
H(2)	0.8964	-1.6643	-0.5584
O	1.8053	-0.0352	0.2410
C(3)	-0.5693	1.4607	0.0599
H(3')	-1.5651	1.8783	-0.0871
H(3'')	-0.3183	1.5216	1.1168
H(3''')	0.1437	2.0588	-0.5036
C(4)	-1.5702	-0.8705	0.2698
H(4')	-2.5625	-0.4425	0.1429
H(4'')	-1.5613	-1.8674	-0.1660
H(4''')	-1.3584	-0.9523	1.3338

*syn*

$r_0$	Å	$\theta_0$	deg
C(2)=O	1.209(2)	H-C(2)=O	120.4(1)
C(2)-H	1.116(2)	C(1)-C(2)=O	125.7(3)
C(1)-C(2)	1.507(5)	C(1)-C(2)-H	113.9(3)
C(1)-C(3,4)	1.526(3)	C(2)-C(1)-C(3)	109.3(3)
C(1)-H	1.114(4)	C(2)-C(1)-C(4)	109.3(3)
		C(2)-C(1)-H(1)	105.1(5)
		$\alpha^a$	118.7(3)
		$\beta^b$	122.6(4)
		$\gamma^c$	118.7(3)

Atom	$a_s$ [Å]	$b_s$ [Å]	$c_s$ [Å]
C(1)	-0.4423		-0.3294
H(1)	-0.1952		-1.4152
C(2)	0.8896		0.3757
H(2)	0.8122		1.4894
O	1.9727		-0.1620
C(3,4)	-1.2114	$\pm 1.2633$	0.0466
H(3')	-2.1768	$\pm 1.2786$	-0.4549
H(3'')	-1.3755	$\pm 1.2972$	1.1216
H(3''')	-0.6499	$\pm 2.1470$	-0.2492

<sup>a)</sup> Dihedral angle between the C(2)C(1)H(1) and C(2)C(1)C(3) planes.

<sup>b)</sup> Dihedral angle between the C(2)C(1)C(3) and C(2)C(1)C(4) planes.

<sup>c)</sup> Dihedral angle between the C(2)C(1)H(1) and C(2)C(1)C(4) planes.

Stiefvater, O.L.: Z. Naturforsch. **41a** (1986) 641.