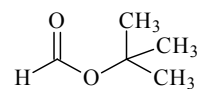
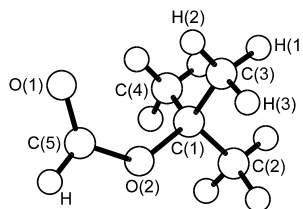


665 **C₅H₁₀O₂**ED, MW, *ab initio* and
DFT calculations**Formic acid 1,1-dimethylethyl ester**1,1-Dimethylethyl formate
t-Butyl formate**C_s**, assumed

r_g	Å ^{a)}	θ_α	deg ^{a)}
O(1)=C(5)	1.202(3)	O=C=O	128.0(9)
C(5)-O(2)	1.332(5)	C(1)-O-C(5)	122.0(9)
C(5)-H	1.08 ^{b)}	O(2)-C(5)-H	108.0 ^{b)}
O(2)-C(1)	1.456(9)	O-C(1)-C(2)	102.5(5)
C-C ^{c)}	1.529(3)	O-C(1)-C(3,4)	111.0(10)
C-H(methyl) ^{d)}	1.109(4)	C(2)-C(1)-C(3,4)	111.7(17)
		C(3)-C(1)-C(4)	109.0 ^{c)}
		C-C-H ^{d)}	108.4(9)
		\angle [O=C-O-C]	0 ^{f)}
		\angle [O-C(1)-C(3)-H(1)]	172 ^{f)}
		\angle [O-C(1)-C(3)-H(2)]	52 ^{f)}
		\angle [O-C(1)-C(3)-H(3)]	-68 ^{f)}

r_z	Å ^{a)}
O(1)=C(5)	1.197(3)
C(5)-O(2)	1.329(5)
C(5)-H	1.06 ^{b)}
O(2)-C(1)	1.454(9)
C-C ^{c)}	1.526(3)
C-H(methyl) ^{d)}	1.097(4)



Staggered conformations were assumed for the *t*-butyl group with respect to the O(2)-C(5) bond and for the C(2)H₃ group with respect to the C(1)-O bond. Local C_{3v} symmetry was assumed for the methyl groups.

The nozzle was at room temperature.

^{a)} Three times the estimated standard errors including a systematic error.

^{b)} Assumed to be equal to the value of methyl formate.

^{c)} All the C-C distances were assumed equal.

^{d)} Mean value.

^{e)} Dependent parameter.

^{f)} Assumed according to the results of MP2 and CISD calculations.

Takeuchi, H., Matsuoka, T., Tsuji, T., Takashima, H., Ito, M., Konaka, S.: J. Mol. Struct. **471** (1998) 275.