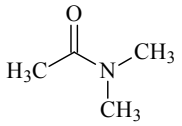
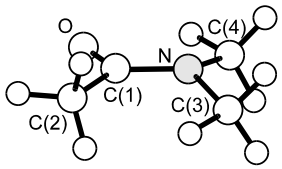
587 **C_4H_9NO** ***N*,*N*-Dimethylacetamide** **C_s** (skeleton)
ED, *ab initio* and DFT calculations or quasi-**C_s** (skeleton)



r_a	Å [a])
C–H	1.101(3)
C=O	1.226(3)
N–C(1)	1.368(5)
N–C(3,4)	1.453(3)
C(1)–C(2)	1.527(6)

θ_a	deg [a])
N–C(1)=O	121.0(7)
N–C(1)–C(2)	115.9(9)
C(1)–N–C(3)	123.8(13)
C(1)–N–C(4)	117.8(11)
$\sum\alpha$(N) [b])	354.1(17)
H–C–H	108.9(7)
tilt(C–CH_3) [c])	3.4 [d])
tilt(N–CH_3) [e])	0.5 [d])
τ_1(N–C(3)) [f])	19(12)
τ_2(N–C(4)) [f])	–19(12)
τ_3 [g])	18(3)
τ_4 [h])	–11(2)

The molecule possesses either a planar equilibrium structure of the skeleton with a large-amplitude out-of-plane vibration (a combination of inversion at nitrogen and torsion around the N–C(1) bond) or a pseudoplanar structure of the skeleton with a potential hump of 15 cal mol^{-1} lying below the vibrational ground state. Local C_{3v} symmetry was assumed for the methyl groups and one C–H bond of the acetyl CH_3 group was assumed to eclipse the C=O bond.
The nozzle temperature was 50 °C.



[a]) Three times the estimated standard errors.
[b]) Sum of the angles at the N atom.
[c]) Tilt angle of the acetyl CH_3 group towards the C=O bond.
[d]) Assumed at the value from B3PW91/6-311G(2d) calculations.
[e]) Tilt angle of the amino methyl groups away from each other.
[f]) Torsional angles of the methyl groups around the N–C bond, C(1)–N–C–H; zero degree for the *syn* position. $\tau_1 = -\tau_2$ was assumed.
[g]) C(2)–C(1)–N–C(3) torsional angle from the *syn* position.
[h]) O–C(1)–N–C(4) torsional angle from the *syn* position. The correlation $\tau_4 = -\alpha\tau_3$ was assumed with α taken from *ab initio* calculations.

Mack, H.-G., Oberhammer, H.: J. Am. Chem. Soc. **119** (1997) 3567.