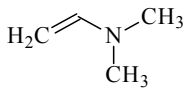
583 **C_4H_9N** ***N,N*-Dimethylethenamine** **C_1**

ED, *ab initio* and DFT calculations

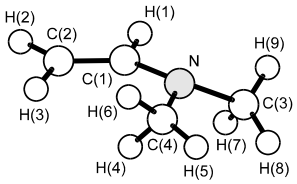


r_a	Å [a])
C(1)=C(2)	1.333(4)
N–C(1)	1.383(3)
N–C(3,4)	1.453(2)
C–H (methyl)	1.096(2) [b])
C(1)–H(1)	1.087(2) [b])
C(2)–H(2,3)	1.082(2) [b])

θ_a	deg [a])
C(2)=C(1)–N	125.3(14)
C(1)–N–C(3)	117.4(15) [b])
C(1)–N–C(4)	118.0(15) [b])
C(3)–N–C(4)	115.8(10)
H–C–H (methyl)	107.9(6)
C(2)=C(1)–H(1)	119.4 [c])
C(1)=C(2)–H(2)	119.5 [c])
C(1)=C(2)–H(3)	123.4 [c])
$\sum\alpha$(N) [d])	351.2(12)
C(3)–N–C(4)–H(6)	177(9)
C(4)–N–C(3)–H(9)	182(6)
C=C–N–lp [e])	98(6)

Local C_{3v} symmetry was assumed for the methyl groups. The vinyl group was assumed to be planar.
The nozzle was at room temperature.

[a]) Three times the estimated standard errors.
[b]) Differences between the C–H bond lengths and between the C–N–C bond angles were assumed at the values from B3LYP/6-31G* calculations.
[c]) Assumed at the value from B3LYP/6-31G* calculations.
[d]) Sum of the angles at the N atom.
[e]) lp is the lone pair axis of the nitrogen atom.



Trautner, F., Abe, T., Oberhammer, H.: J. Am. Chem. Soc. **123** (2001) 2865.