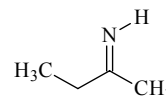


584 **C₄H₅N**ED, *ab initio* and DFT
calculations**(2*E*)-2-Butanimine****C_s (*sp*)****C₁ (*ac*)**

r_g	Å ^{a)}	θ_{α}	deg ^{a)}
N=C(2)	1.285(3)	N=C(2)–C(3)	115.8(5) ^{b)}
C(1)–C(2)	1.510(2) ^{b)}	N=C(2)–C(1)	125.0(5) ^{b)}
C(2)–C(3)	1.510(2) ^{b)}	C(2)–C(3)–C(4)	115.2(12)
C(3)–C(4)	1.521(2) ^{b)}	C(3)–C(4)–H	113.5(14)
N–H	1.046(3) ^{b)}	C(2)=N–H	109.3 ^{c)}
C–H (average)	1.113(3) ^{b)}	N=C(2)–C(3)–C(4)	0



Under the assumption that the *Z*-isomer was not present in the gas phase, it was found that the *E*-isomer exists as *sp* (60(10)%) and *ac* conformers. Local C_{3v} symmetry was assumed for the methyl groups. For the *ac* conformer, the torsional angle $\tau[\text{N}=\text{C}(2)-\text{C}(3)-\text{C}(4)]$ was assumed at the MP2/6-31G** value (117.6°) and the bond configuration around the C(2) atom was assumed to be planar. Differences between the bond lengths and angles of the conformers were constrained to the values from theoretical calculations.

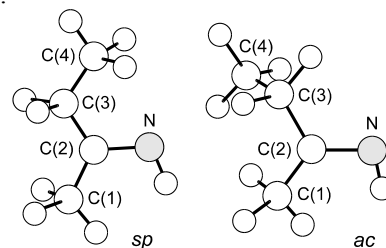
The nozzle temperature was 294 K.

The structural parameters are listed for the *sp* conformer.

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

^{b)} Differences in the C–C bond lengths and N=C–C bond angles and between the N–H and C–H bond lengths were assumed at the values from MP2/6-31G** and B3LYP/6-31G** calculations.

^{c)} Assumed at the value from MP2/6-31G** and B3LYP/6-31G** calculations.



Egawa, T., Konaka, S.: J. Phys. Chem. A **105** (2001) 2085.