

1728
MW

C₄H₈N₂

3-(Methylamino)propanenitrile

C₁ (conformer I)
C_s (skeleton) (conformer II)
H₃C–NH–CH₂–CH₂–C≡N

r_0	Å	θ_0	deg
C(3)≡N	1.157 ^{a)}	C(2)–C(3)≡N	180.0 ^{a)}
N–C(4)	1.475 ^{a)}	C(2)–C(1)–N	108.0 ^{a)}
N–C(1)	1.475 ^{a)}	C(1)–N–C(4)	110.0 ^{a)}
C(2)–C(3)	1.463 ^{a)}	C(1)–C(2)–C(3)	110.5 ^{a)}
C(1)–C(2)	1.540 ^{a)}	C–C–H	109.47 ^{a)}
N–H	1.017 ^{a)}	C–N–H	109.47 ^{a)}
C–H	1.093 ^{a)}	N–C–H	109.47 ^{a)}
		C(3)–C(2)–C(1)–N ^{b)}	65(3)

Conformer I

Atom	$ a_s $ [Å]	$ b_s $ [Å]	$ c_s $ [Å]
H (NH)	0.2170	1.1491	0.3270

Two conformers, I and II, were detected, the former being more stable than the latter by 5(2) kJ mol^{–1}.

^{a)} Assumed.

^{b)} From *syn* position, for conformer I.

Marstokk, K.-M., Møllendal, H.: Acta Chem. Scand. **44** (1990) 36.

