

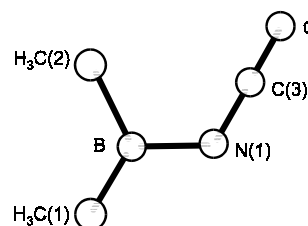
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C₃H₆BNO

Isocyanatodimethylborane
Dimethylboron isocyanate

C₁ (planar heavy
atom skeleton)
O=C=N-B(CH₃)₂

r_a	Å ^{a)}	θ_α	deg ^{a)}
B-C	1.563(4)	C-B-C	123.6(7)
B-N	1.425(5)	N-B-C(1)	115.3(11)
N=C	1.206(6)	N-B-C(2)	121.1(11)
C=O	1.167(5)	B-N=C(3)	153.8(26)
		N=C(3)=O	180 ^{b)}



Local C_{3v} symmetry was assumed for the methyl groups with no tilt. Structure analyses with a large-amplitude model and a double minimum potential for the BNCO in-plane bending motion suggest that the barrier at the linear configuration is ≥ 0.2 kcal mol⁻¹, but the *ab initio* (HF/6-31G*) method predicts a linear BNCO structure.

The nozzle was at room temperature.

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

^{b)} Assumed.

Hausser-Wallis, R., Oberhammer, H., Einholz, W.,
Paetzold, P.O.: Inorg. Chem. **29** (1990) 3286.