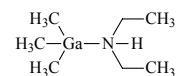


816 **C₇H₂₀GaN**
ED, *ab initio* and DFT
calculations

***N*-Ethylethanamine – trimethylgallium (1/1)**
Diethylamine – trimethylgallium (1/1)

C₁



r_g	\AA^a	θ_a	deg^a
C–H ^{b)}	1.116(3)	N–Ga–C(m) ^{c)}	98.9(13)
Ga–C(m) ^{c)}	1.993(3)	N–Ga–C(m') ^{c)}	102.8(13)
Ga–C(m'') ^{c)}	1.995(3)	N–Ga–C(m'') ^{c)}	96.8(13)
Ga–C(m''') ^{c)}	1.999(3)	Ga–N–C(1) ^{c)}	109.6(9)
Ga–N	2.204(12)	Ga–N–C(1') ^{c)}	115.5(9)
N–C(1) ^{c)}	1.473(4)	C–N–C	113.3(11)
N–C(1') ^{c)}	1.476(4)	N–C(1)–C(2) ^{c)}	115.8(8)
C(1)–C(2) ^{c)}	1.539(4)	N–C(1')–C(2') ^{c)}	113.9(8)
C(1')–C(2') ^{c)}	1.549(4)	Ga–C–H ^{b)}	110.6(10)
N–H	1.025 ^{d)}	N–C–H ^{b)}	109.0 ^{d)}
		C–C–H ^{b)}	111.1 ^{d)}
		Ga–N–H	102.9 ^{d)}
		C(m)–Ga–N–H	176(8)
		Ga–N–C(1)–C(2)	151(4)
		Ga–N–C(1')–C(2')	–100(4)
		N–C(1)–C(2)–H	180.2 ^{d)}
		N–C(1')–C(2')–H	177.6 ^{d)}
		N–Ga–C–H	173.5 ^{d)}

The molecule was found to exist as a *gauche-anti* conformer.

Local C_{3v} symmetry was assumed for the methyl groups.

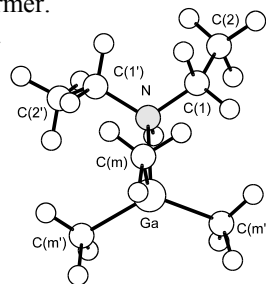
The nozzle was at room temperature.

^{a)} Twice the estimated standard errors including a systematic error.

^{b)} Average value.

^{c)} Differences in the chemically similar, but symmetry-inequivalent parameters were assumed at the values from HF/6-311G(d) calculations.

^{d)} Assumed at the value from HF/6-311G(d) calculations.



Aarset, K., Beer, C.E., Hagen, K., Page, E.M., Rice, D.A.: J. Phys. Chem. A **106** (2002) 8762.