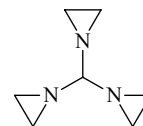


813 **C₇H₁₃N₃**
ED, *ab initio* and DFT
calculations

1,1',1''-Methyldynetrizaziridine
Tris(1-aziridinyl)methane

C₃

r_a	Å ^{a)}	θ_a	deg ^{a)}
C(1)–N ^{b)}	1.471(2)	H–C–N	104.4(14)
C(ring)–N ^{b)}	1.464(2)	C(1)–N–C(ring)	115.9(14)
C–C ^{b)}	1.497(2)	N–C–N ^{c)}	114.0(11)
		τ_1 ^{d)}	59.3(17)
		τ_2 ^{e)}	172.6(51)



The molecule was found to have the *gauche-gauche-gauche* conformation. According to the results of HF/6-31G**, B3PW91/6-31G* and MP2/6-31G** calculations, it was assumed in the ED analysis that the aziridine rings have identical parameters and C_{2v} local symmetry and the HCN₃ fragment has C_{3v} symmetry.

The nozzle temperature was 20 °C.

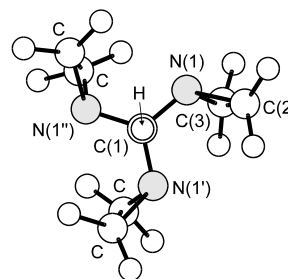
^{a)} Three times the estimated standard errors.

^{b)} Differences between the C(ring)–N and C(1)–N and between the C(1)–N and C–C bond lengths were assumed at the values from HF/6-31G** calculations.

^{c)} Dependent parameter.

^{d)} Torsional angles around C(1)–N(1,1',1'') bonds, lp–N(1,1',1'')–C(1)–H, where lp is the lone pair.

^{e)} Torsional angle lp–N–C–N.



Novikov, V.P., Dakkouri, M., Golubinskii, A.V., Popik, M.V., Vilkov, L.V., Dormov, P.E., Lyssenko, K.A., Kostyanovsky, R.G.: *Mendeleev Commun.* (2000) 103.