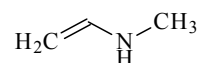


423 **C₃H₇N**ED, *ab initio*
calculations***N*-Methylethenamine***N*-MethylvinylamineC₁ assumed (*syn*)C₁ assumed (*anti*)

r_g	\AA^a		θ_α	deg^a	
	<i>syn</i>	<i>anti</i>		<i>syn</i>	<i>anti</i>
N–C(1)	1.391(3)	1.395(3)	C–N–C	119.5(9)	118.4(9)
N–C(m)	1.465(3)	1.472(3)	N–C=C	126.5(7)	126.1(7)
C(1)=C(2)	1.343(4)	1.341(4)	τ^b	13.1 ^{c)}	–145.1 ^{c)}
C(1)–H	1.105(2)	1.106(2)			
N–H	1.029(2)	1.033(2)			

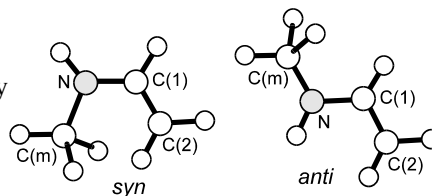
The pyrolysis product of propyleneimine at 470 °C was found to consist of the following short-lived species: *syn* and *anti* conformers of *N*-methylethenamine and (*E*)-*N*-ethylidenemethanamine (CH₃–N=CH–CH₃) with the mole fractions of 0.63(7), 0.28(8) and 0.09(4), respectively. The differences between the structural parameters of different species and the differences in some structural parameters of the same species, as well as all the dihedral angles and all the bond angles including H atoms, were assumed at the MP2/6-31G** values.

The nozzle temperature was about 24 °C.

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

^{b)} C–N–C=C torsional angle from the exactly *syn* position.

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



Fujiwara, H., Egawa, T., Konaka, S.: J. Am. Chem. Soc. **119** (1997) 1346.