

r_a	\AA^a	θ_α	deg^a
$C(1)\equiv C(2)$	1.216(15) ^{b)}	$C(2)-C(3)-N(1)$	114.6(2)
$C(2)-C(3)$	1.48(3) ^{b)}	$C(3)-N(1)=N(2)$	114.5(15)
$C(3)-N(1)$	1.46(3) ^{b)}	$N(1)=N(2)\equiv N(3)^c)$	169(4)
$N(1)=N(2)$	1.249(7)	$C(2)-C(3)-H$	108(3)
$N(2)\equiv N(3)$	1.137(6)	$N(1)-C(3)-H$	108(3)
$C(3)-H$	1.111(46)	$C(1)\equiv C(2)-C(3)$	180 ^{d)}
$C(1)-H^e)$	1.084	$\phi^f)$	37(8)
		$\tau^g)$	27(8)

The nozzle temperature was 293 K.

^{a)} Uncertainties were unidentified, possibly estimated standard errors.

^{b)} Uncertainty is larger than that estimated in the original paper.

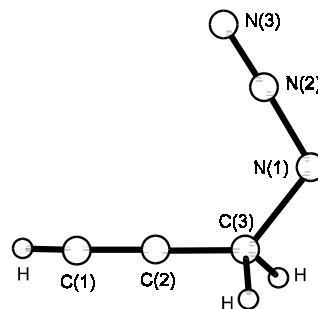
^{c)} Oriented *anti* to the C—N bond.

^{d)} Assumed.

^{e)} Difference $[C(3)-H] - [C(1)-H]$ was fixed at the *ab initio* value of 0.027 Å.

^{f)} Dihedral angle $C(2)-C(3)-N(1)=N(2)$ from *syn*.

^{g)} The root-mean-square amplitude of the torsional motion about the $C(3)-N(1)$ bond.



Almlöf, J., Braathen, G.O., Klæboe, P., Nielsen, C.J., Priebe, H., Schei, S.H.: J. Mol. Struct. **160** (1987) 1.