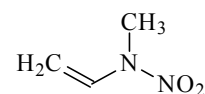


**401**      **C<sub>3</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>**ED, *ab initio*  
calculations***N*-Methyl-*N*-nitroethenamine***N*-Methyl(vinyl)-*N*-nitroamine**C<sub>1</sub> (near-*anti*)**

$r_a$	$\text{\AA}^a$	$\theta_a$	deg <sup>a)</sup>
N=O	1.214(3)	O=N=O	122.0(9)
C(1)–N	1.428(6)	C(1)–N–N	118.2(6)
C(3)–N	1.475(6)	C(3)–N–N	117.7(6)
N–N	1.368(6)	C–N–C	123.8(24)
C=C	1.340(6)	N–C=C	121.7(21)
C–H (methyl)	1.082(18)	N–C–H (mean)	119 <sup>b)</sup>
C–H (vinyl)	1.074(18)	C=C–H (mean)	104.0(27)
		C(1)–N(1)–C(3)–H(1)	36.4 <sup>c)</sup>
		$\tau[\text{C(1)–N}]^d$	161(8)
		$\tau(\text{N–N})^e$	150(5)
		$\Sigma\alpha[\text{N(amine)}]^f$	359.7

According to *ab initio* (RHF/6-31G\*) predictions, the *syn* conformer lies about 3.3 kcal mol<sup>−1</sup> above the *anti* form. Experimental data from [1] were reinvestigated. The vapor was assumed to consist only of the *anti* form. The methyl and nitro groups were assumed to have C<sub>3v</sub> and C<sub>2v</sub> local symmetry, respectively. The differences between the C(3)–N, C(1)–N, C=C and N–N bond lengths, between the C–H bond lengths in the methyl and vinyl groups and between the C(3)–N–N and C(1)–N–N angles were assumed at the *ab initio* values.

The temperature of the experiments was 75 °C.

<sup>a)</sup> Three times the estimated standard errors.

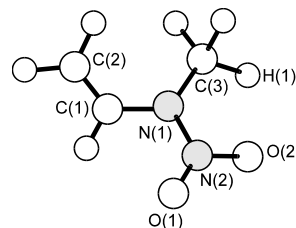
<sup>b)</sup> Fixed in the final refinement.

<sup>c)</sup> Assumed at the *ab initio* value, 0° for the *anti* position.

<sup>d)</sup> C(2)=C(1)–N–N torsional angle, 0° for the *syn* position.

<sup>e)</sup> C(1)–N–N=O(2) torsional angle, 0° for the *syn* position.

<sup>f)</sup> Sum of the bond angles around the amine nitrogen atom.



Shishkov, I.F., Vilkov, L.V., Khristenko, L.V., Skancke, P.N.: J. Mol. Struct. **413-414** (1997) 521.

[1] Batyukhnova, O.G., Sadova, N.I., Vilkov, L.V., Ivshin, V.P., Pankrushev, Yu.A.: Zh. Strukt. Khim. **25** No.6 (1984) 47; J. Struct. Chem. (Engl. Transl.) **25** (1984) 878.

Replaces [II/25C \(3, 1261\)](#)