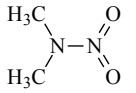
301 **$C_2H_6N_2O_2$** ***N*-Methyl-*N*-nitromethanamine** **C_s**

ED, *ab initio* and DFT calculations

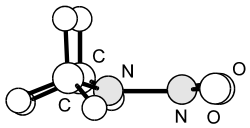
Dimethylnitramine

Nitrodimethylamine



r_g	Å [a])	θ_α	deg [a])
N=O	1.232(2)	C–N–N	116.1(6)
N–N	1.387(3)	C–N–C	122.4(27)
N–C	1.466(3)	O=N=O	127.6(12)
C–H (average) [b])	1.110(9)	N–C–H (average)	109.9(18)
		τ [c])	90.0 [d])
		$\Sigma\alpha$(N) [e])	354.6(28)

Experimental data from [1] were reanalyzed. Local C_1 symmetry was assumed for the methyl groups and C_{2v} for the nitro group.
HF/6-311++G**, MP2/6-311++G** and B3LYP/6-311++G** calculations predicted C_s symmetry for the molecule.
The nozzle temperature was 70(5) °C.



[a]) Three times the estimated standard errors.
[b]) Differences in the C–H bond lengths were assumed at the values from HF/6-311++G** calculations.
[c]) One of H–C–N–N torsional angles for each methyl group, $\tau = 0°$ for the *syn* position.
[d]) Assumed.
[e]) Sum of the bond angles around the amine N atom.

Shishkov, I.F., Khristenko, L.V., Sipachev, V.A., Vilkov, L.V., Samdal, S., Gundersen, S., Palafox, M.A.: J. Mol. Struct. **485-486** (1999) 153.
[1] Stølevik, R., Rademacher, P.: Acta Chem. Scand. **23** (1969) 672.

Replaces II/25B(**3**, 886)