

310
MW N_2O_5 **Dinitrogen pentaoxide**

Nitryl nitrate

 C_2 (effective symmetry class)
(large-amplitude motion) N_2O_5

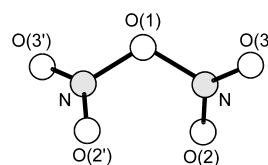
The measurements support a picture of N_2O_5 as a C_2 symmetry molecule with facile geared internal rotation of the two equivalent NO_2 groups.

Domenech, J.L., Fraser, G.T., Walker, A.R.H., Lafferty, W.J., Suenram, R.D.: J. Mol. Spectrosc. **184** (1997) 172.

Grabow, J.-U., Andrews, A.M., Fraser, G.T., Irikura, K.K., Suenram, R.D., Lovas, F.J., Lafferty, W.J., Domenech, J.L.: J. Chem. Phys. **105** (1996) 7249.

ED, DFT
calculations C_2

r_g	\AA^a	θ_α	deg a
N–O(1)	1.505(4)	N–O–N	112.3(17)
N=O(2,3) b	1.188(2)	O(2)=N=O(3)	134.2(4)
N=O(2)	1.189 c	O(1)–N=O(2,3) b	112.8(2)
N=O(3)	1.187 c	O(1)–N=O(2)	115.8 c
		O(1)–N=O(3)	109.8 c
		τ^d	33.7(40)



The molecular structure from [1] was reinvestigated in terms of a more realistic model in which the C_{2v} symmetry restriction for the O–NO_2 group was relaxed. The nozzle temperature was $-11\text{ }^\circ\text{C}$.

a) Twice the estimated standard errors.

b) Average value.

c) Differences between the N=O(2) and N=O(3) bond lengths and between the O(1)–N=O(2) and O(1)–N=O(3) bond angles were assumed at the values from B3LYP/6-311+G(d) calculations.

d) N–O(1)–N=O(2) torsional angle.

McClelland, B.M., Richardson, A.D., Hedberg, K.: Helv. Chim. Acta **84** (2001) 1612.

[1] McClelland, B.W., Hedberg, L., Hedberg, K., Hagen, K.: J. Am. Chem. Soc. **105** (1983) 3789.

Replaces [II/25A\(2, 838\)](#)