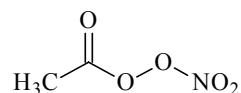


**247 C<sub>2</sub>H<sub>3</sub>NO<sub>5</sub>****Acetyl nitro peroxide****C<sub>1</sub>**ED, MW, *ab initio* and DFT calculations

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C(1)=O(2)	1.184 <sup>b)</sup>	O(1)–C=O(2)	125.7(25)
N=O(2',3') <sup>c)</sup>	1.193(2)	O(1)–C–C	107.7(16)
C–C	1.505 <sup>b)</sup>	O(2')=N=O(3')	135.1(56)
O(1)–C(1)	1.395(12)	$\Delta(\text{ONO})$ <sup>d)</sup>	7.2 <sup>c)</sup>
O(1')–N	1.492(7)	O(1')–O(1)–C	107.3(13)
O(1)–O(1')	1.418(12)	O(1)–O(1')–N	108.6(20)
C–H <sup>c)</sup>	1.090 <sup>c)</sup>	H–C–H	109.4 <sup>c)</sup>
		$\tau_1$ <sup>f)</sup>	–3.0 <sup>c)</sup>
		$\tau_2$ <sup>g)</sup>	2.0 <sup>c)</sup>
		$\tau_3$ <sup>h)</sup>	84.7(13)



The molecule was found to exist as the *syn* conformer with C(1)=O(2) bond in the *syn* position with respect to the O(1)–O(1') bond. Local C<sub>3v</sub> symmetry was assumed for the methyl group. The nozzle was at room temperature.

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

<sup>b)</sup> Constrained to the value for similar molecules.

<sup>c)</sup> Mean value.

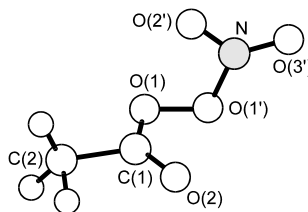
<sup>d)</sup> [O–N=O(2')] – [O–N=O(3')].

<sup>e)</sup> Assumed at the value from B3PW91/6-311+G\* or MP2/6-31G\* calculations.

<sup>f)</sup> Torsional angle O(1')–O(1)–C(1)=O(2).

<sup>g)</sup> Torsional angle O(1)–O(1')–N=O(2').

<sup>h)</sup> Torsional angle C(1)–O(1)–O(1')–N.



Hermann, A., Niemeyer, J., Mack, H.-G., Kopitzky, R., Beuleke, M., Willner, H., Christen, D., Schäfer, M., Bauder, A., Oberhammer, H.: Inorg. Chem. **40** (2001) 1672.