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Data Article

Structural parameters and physicochemical data from quantum chemical calculations of the peroxyacyl nitrate derivatives $RC(O)O_2NO_2$

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ABSTRACT

This article present the structural parameters and physicochemical data (ΣD_0, $\Delta H°_{f,298K}$ and $\Delta G°_{f,298K}$) of the methoxyformyl peroxynitrate $CH_3OC(O)O_2NO_2$ (MoPAN), peroxypropionyl nitrate $CH_3CH_2C(O)O_2NO_2$ (PPN), peroxyacryloyl nitrate $CH_2CHC(O)O_2NO_2$ (APAN), peroxy-*n*-butyryl nitrate $CH_3(CH_2)_2C(O)O_2NO_2$ (PnBN), peroxycrotonyl nitrate $CH_3(CH{=}CH)C(O)O_2NO_2$ (CPAN), peroxyisobutyryl nitrate $(CH_3)_2CHC(O)O_2NO_2$ (PiBN), peroxymethacryloyl nitrate $CH_2{=}C(CH_3)C(O)O_2NO_2$ (MPAN) and peroxy-*n*-valeryl nitrate $CH_3(CH_2)_3C(O)O_2NO_2$ (PnVN) peroxyacyl nitrate derivatives. The equilibrium structures have been performed using the B3LYP and M06-2X functionals combined with the 6-311++G(*3df,3pd*) basis set. The physicochemical data were calculated using several G*n* methods, G3B3, G3MP2B3, G4 and G4MP2. Computational calculations were carried out with GAUSSIAN09 program.

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Specifications Table

Subject area	Chemistry
More specific subject area	Physical chemistry and Theoretical Chemistry
Type of data	Tables and Gaussian output files
How data was acquired	Quantum chemical computation on Gaussian 09
Data format	Both raw and analyzed
Parameters for data collection	B3LYP/6-311++G(*3df,3pd*), M06-2X/6-311++G(*3df,3pd*), G3B3, G3MP2B3, G4 and G4MP2.
Description of data collection	Structural parameters and energetic data from quantum chemical calculations of peroxyacyl nitrates $RC(O)O_2NO_2$ were generated by quantum chemical computation.
Data source location	Antonio Nariño University – Bogotá/Colombia - Latitude and longitude: 4.634977, -74.056385
Data accessibility	With the article

Value of the Data

- Data of the equilibrium geometries of 8 peroxyacyl nitrates of environmental interest reported, these information are important for both theoretical and experimental work involving these pollutants, particularly for electronic structure theory and spectroscopy.
- Physicochemical data such as atomization energies, enthalpies of formation and Gibbs free energies ($\Sigma D0$, $\Delta H°f,0K$, $\Delta H°f,298K$ and $\Delta G°f,298K$) can be used as a reference due to experimental values are not available for peroxyacyl nitrates studied here. Also, these data can be used in atmospheric studies.
- High accurate quantum chemical composite Gaussian-n methods have been employed to derive energies of the peroxyacyl nitrates these values can be used for understand relative stability of these gaseous compounds and estimate other properties. These values can provide further insights into development of future experiments.
- Raw data are provided so that interested researchers can reproduce our data and perform calculation at other levels of theory or for other relevant classes of compounds. Vibrational spectrum, rotational constants, Mulliken charges, and other detailed information can be extracted from output files as needed.

1. Data Description

The equilibrium structures of the peroxyacyl nitrate derivatives $RC(O)O_2NO_2$ (R = CH_3O-, CH_3CH_2-, CH_2CH-, $CH_3(CH_2)_2$-, $CH_3(CH{=}CH)$-, $(CH_3)_2CH$, $CH_2{=}C(CH_3)$-, $CH_3(CH_2)_3$-) have been optimized at the B3LYP and M06-2X functionals from Density Functional of Theory (DFT) combined with the extensive 6-311++G(*3df,3pd*) basis set under C_1 symmetry (see Fig. 1). Most relevant structural parameters are reported in Tables 1 and 2, the C-C, C=C, and C-H bonds and angles for peroxyacyl nitrate derivatives with label C_1, C_2, C_3, and C_4 (see Fig. 1, Tables 1 and 2) present characteristic values. The complete structural parameters data are available in the output files (see supplementary material) which include vibrational spectrum calculated at the same level of theory. The output files can be viewed in any visualizer software compatible.

The following associated files are provided in Supplementary material.

- Raw Gaussian output files (.txt) for equilibrium structure, vibrational frequencies, rotational constants, Mulliken charges, and other detailed information for all compounds at B3LYP/6-311++G(3df,3pd) and M06-2X/6-311++G(3df,3pd) levels of theory.
- Raw Gaussian output files (.txt) for energetic values for all compounds at G3B3, G3MP2B3, G4 and G4MP2 levels of theory.

Table 1
Most relevant structural parameters of the peroxyacyl nitrate derivatives $RC(O)O_2NO_2$ ($CH_3OC(O)O_2NO_2$ (MoPAN), $CH_3CH_2C(O)O_2NO_2$ (PPN), $CH_2CHC(O)O_2NO_2$ (APAN), $CH_3(CH_2)_2C(O)O_2NO_2$ (PnBN), $CH_3(CH{=}CH)C(O)O_2NO_2$ (CPAN), $(CH_3)_2CHC(O)O_2NO_2$ (PiBN), $CH_2{=}C(CH_3)C(O)O_2NO_2$ (MPAN) and $CH_3(CH_2)_3C(O)O_2NO_2$ (PnVN)) at level of theory B3LYP/6-311++G(*3df,3pd*). The distances are in Å and angles in degree.

	MoPAN	PPN	APAN	PnBN	CPAN	PiBN	MPAN	PnVN
$r(N\text{-}O_1)$	1.184	1.186	1.184	1.186	1.185	1.186	1.185	1.186
$r(O_3\text{-}N)$	1.523	1.511	1.516	1.510	1.514	1.510	1.516	1.510
$r(O_3\text{-}O_4)$	1.392	1.399	1.395	1.399	1.394	1.399	1.395	1.399
$r(C\text{-}O_4)$	1.393	1.403	1.405	1.405	1.409	1.403	1.404	1.405
$r(O_5{=}C)$	1.189	1.187	1.190	1.187	1.192	1.188	1.192	1.187
$r(O_6{-}C)$	1.319							
$r(O_6{-}C_1)$	1.443							
$r(C_1{-}C)$		1.506	1.476	1.506	1.467	1.515	1.486	1.506
$r(C_1{-}C_2)$		1.524	1.328	1.527	1.334	1.536	1.502	1.527
$r(C_2{-}C_3)$				1.527	1.490			1.529
$r(C_1{-}C_3)$						1.536	1.333	
$r(C_3{-}C_4)$								1.528
$\angle(O_4CO_6)$	104.8							
$\angle(CO_6C_1)$	115.3							
$\angle(O_4CC_1)$		107.8	107.5	107.8	110.8	109.0	111.2	107.8
$\angle(CC_1C_2)$		112.4	120.2	112.9	125.7	111.7	121.7	112.8
$\angle(C_1C_2C_3)$				112.0	124.5			112.3
$\angle(C_2C_3C_4)$								112.8
$\angle(C_2C_1C_3)$						112.1	124.1	
$D(O_5CO_4O_3)$	−5.4	−4.5	−4.8	−4.2	−6.2	−5.3	−7.1	−5.0
$D(O_6CO_4O_3)$	174.9							
$D(C_1CO_4O_3)$		175.9	175.6	176.3	174.3	174.9	173.4	111.9

Table 2
Most relevant structural parameters of the peroxyacyl nitrate derivatives $RC(O)O_2NO_2$ ($CH_3OC(O)O_2NO_2$ (MoPAN), $CH_3CH_2C(O)O_2NO_2$ (PPN), $CH_2CHC(O)O_2NO_2$ (APAN), $CH_3(CH_2)_2C(O)O_2NO_2$ (PnBN), $CH_3(CH{=}CH)C(O)O_2NO_2$ (CPAN), $(CH_3)_2CHC(O)O_2NO_2$ (PiBN), $CH_2{=}C(CH_3)C(O)O_2NO_2$ (MPAN) and $CH_3(CH_2)_3C(O)O_2NO_2$ (PnVN)) at level of theory M06-2X/6-311++G(*3df,3pd*). The distances are in Å and angles in degree.

	MoPAN	PPN	APAN	PnBN	CPAN	PiBN	MPAN	PnVN
$r(N\text{-}O_1)$	1.179	1.180	1.180	1.181	1.180	1.181	1.180	1.181
$r(O_3\text{-}N)$	1.455	1.449	1.451	1.447	1.450	1.447	1.451	1.447
$r(O_3\text{-}O_4)$	1.374	1.378	1.376	1.378	1.375	1.377	1.375	1.378
$r(C\text{-}O_4)$	1.381	1.392	1.391	1.393	1.396	1.394	1.392	1.393
$r(O_5{=}C)$	1.185	1.183	1.184	1.182	1.186	1.183	1.186	1.182
$r(O_6{-}C)$	1.312							
$r(O_6{-}C_1)$	1.433							
$r(C_1{-}C)$		1.499	1.477	1.500	1.469	1.506	1.485	1.500
$r(C_1{-}C_2)$		1.532	1.324	1.522	1.330	1.527	1.328	1.521
$r(C_2{-}C_3)$				1.523	1.490			1.524
$r(C_1{-}C_3)$						1.534	1.498	
$r(C_3{-}C_4)$								1.524
$\angle(O_4CO_6)$	105.6							
$\angle(CO_6C_1)$	114.4							
$\angle(O_4CC_1)$		108.8	108.2	108.5	111.0	109.2	111.6	108.5
$\angle(CC_1C_2)$		109.5	119.1	112.0	124.7	108.0	113.8	112.0
$\angle(C_1C_2C_3)$				111.4	124.0			112.0
$\angle(C_2C_3C_4)$								112.1
$\angle(C_2C_1C_3)$						111.7	124.9	
$D(O_5CO_4O_3)$	−3.9	−5.1	−4.2	−2.9	−3.9	−0.6	−4.8	−2.5
$D(O_6CO_4O_3)$	176.4							
$D(C_1CO_4O_3)$		173.0	176.3	177.9	176.7	177.6	175.7	178.4

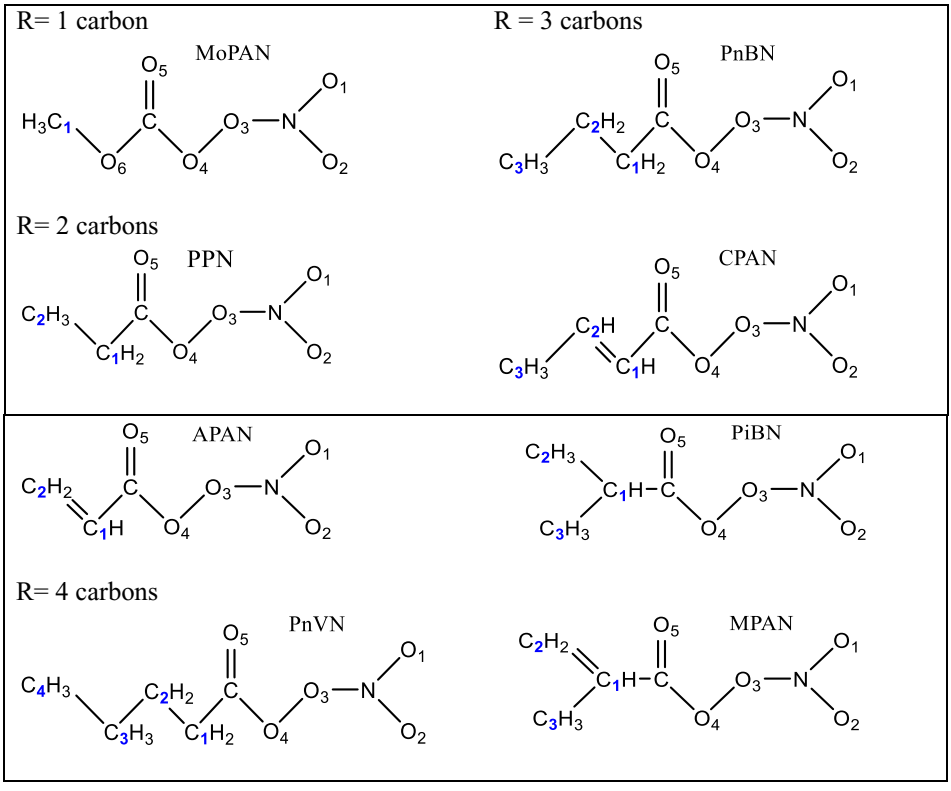

Fig. 1. Geometries of peroxyacyl nitrate derivatives $RC(O)O_2NO_2$, ($CH_3OC(O)O_2NO_2$ (MoPAN), $CH_3CH_2C(O)O_2NO_2$ (PPN), $CH_2CHC(O)O_2NO_2$ (APAN), $CH_3(CH_2)_2C(O)O_2NO_2$ (PnBN), $CH_3(CH{=}CH)C(O)O_2NO_2$ (CPAN), $(CH_3)_2CHC(O)O_2NO_2$ (PiBN), $CH_2{=}C(CH_3)C(O)O_2NO_2$ (MPAN) and $CH_3(CH_2)_3C(O)O_2NO_2$ (PnVN)) with atom labeling, numbers in color blue indicates different derivatives studied in this work. R indicates the quantities of carbon atoms of the peroxyacyl nitrate derivatives.

2. Experimental Design, Materials and Methods

Gaussian input files (.inp) were generated by using Gaussview 5 [1]. The *ab initio* calculations were performed using the Gaussian 09 program package [1] to optimize the structures at B3LYP/6-311++G(*3df,3pd*) and M06-2X/6-311++G(*3df,3pd*) levels of theory. Frequency calculations confirm that structures are minima on the electronic potential energy surface for all peroxyacyl nitrate derivatives $RC(O)O_2NO_2$. The output files were processed using Gaussview 5 [1] to extract geometric and energetic data of all the compounds studied. The enthalpies of formation and Gibbs free energies ($\Delta H°_{f,0K}$, $\Delta H°_{f,298K}$ and $\Delta G°_{f,298K}$) have been computed by calculating total atomization energies (ΣD_0), see Table 3, for further details see the Gaussian Software web site and our previous publications [1–3]. Physicochemical data recommended have been presented by means of the composed methods G3B3, G3MP2B3, G4 and G4MP2, see Table 3 in Mean ± Std. Dev. [4–7].

The thermochemical values for peroxypropionyl nitrate $CH_3CH_2C(O)O_2NO_2$ (PPN) and peroxyacryloyl nitrate $CH_2CHC(O)O_2NO_2$ (APAN) have been studied previously, the values reported for $\Delta H°_{f\ 298K}$ are −66.5 and −34.8 kcal mol^{-1} respectively [8–9]. These values are consistent with our values at G3B3 level of theory reported. The dataset reported in this paper used composited methods most accurate compared to other previously published results on these compounds.

Table 3
Atomization energies, enthalpies of formation, and Gibbs free energies (ΣD_0, $\Delta H°_{f,0K}$, $\Delta H°_{f,298K}$ and $\Delta G°_{f,298K}$) physicochemical data calculated from Gaussian-*n* composited methods for the peroxyacyl nitrate derivatives $RC(O)O_2NO_2$ ($CH_3OC(O)O_2NO_2$ (MoPAN), $CH_3CH_2C(O)O_2NO_2$ (PPN), $CH_2CHC(O)O_2NO_2$ (APAN), $CH_3(CH_2)_2C(O)O_2NO_2$ (PnBN), $CH_3(CH{=}CH)C(O)O_2NO_2$ (CPAN), $(CH_3)_2CHC(O)O_2NO_2$ (PiBN), $CH_2{=}C(CH_3)C(O)O_2NO_2$ (MPAN) and $CH_3(CH_2)_3C(O)O_2NO_2$ (PnVN)). Values are reported in kcal mol^{-1}.

$RC(O)O_2NO_2$	Property	G3B3	G3MP2B3	G4	G4MP2	Mean ± Std. Dev.	Ref.
MoPAN	ΣD_0	1054.8	1051.5	1053.5	1050.2	1052.5 ± 2.0	
	$\Delta H°_{f\,0K}$	−93.5	−90.2	−92.2	−88.8	−91.2 ± 2.1	
	$\Delta H°_{f\,298K}$	−98.0	−94.7	−96.8	−93.4	−95.7 ± 2.1	
	$\Delta G°_{f\,298K}$	−69.9	−66.7	−68.9	−65.6	−67.8 ± 2.0	
PPN	ΣD_0	1236.5	1233.7	1235.3	1232.4	1234.5 ± 1.8	
	$\Delta H°_{f\,0K}$	−60.9	−58.2	−59.7	−56.8	−58.9 ± 1.8	
	$\Delta H°_{f\,298K}$	−66.3	−63.6	−65.2	−62.3	−64.4 ± 1.8	−66.5* [8]
	$\Delta G°_{f\,298K}$	−37.3	−34.5	−36.3	−33.4	−35.4 ± 1.8	
APAN	ΣD_0	1103.3	1101.1	1102.1	1099.5	1101.5 ± 1.6	
	$\Delta H°_{f\,0K}$	−31.0	−28.8	−29.8	−27.2	−29.2 ± 1.6	
	$\Delta H°_{f\,298K}$	−34.9	−32.7	−33.8	−31.2	−33.2 ± 1.6	−34.8* [9]
	$\Delta G°_{f\,298K}$	−7.3	−5.1	−6.5	−3.9	−5.7 ± 1.5	
PnBN	ΣD_0	1513.4	1510.7	1512.1	1509.2	1511.4 ± 1.8	
	$\Delta H°_{f\,0K}$	−64.6	−61.8	−63.3	−60.4	−62.5 ± 1.8	
	$\Delta H°_{f\,298K}$	−71.4	−68.7	−70.3	−67.4	−69.5 ± 1.8	
	$\Delta G°_{f\,298K}$	−40.3	−37.5	−39.3	−36.4	−38.4 ± 1.8	
CPAN	ΣD_0	1383.9	1381.6	1382.6	1379.9	1382.0 ± 1.7	
	$\Delta H°_{f\,0K}$	−38.4	−36.1	−37.0	−34.4	−36.5 ± 1.7	
	$\Delta H°_{f\,298K}$	−43.5	−41.2	−42.3	−39.6	−41.7 ± 1.7	
	$\Delta G°_{f\,298K}$	−13.4	−11.1	−12.5	−9.8	−11.7 ± 1.6	
PiBN	ΣD_0	1514.1	1511.2	1512.8	1509.8	1512.0 ± 1.9	
	$\Delta H°_{f\,0K}$	−65.3	−62.4	−64.0	−61.0	−63.2 ± 1.9	
	$\Delta H°_{f\,298K}$	−72.2	−69.3	−70.9	−67.9	−70.1 ± 1.9	
	$\Delta G°_{f\,298K}$	−41.3	−38.4	−40.3	−37.3	−39.3 ± 1.8	
MPAN	ΣD_0	1383.9	1381.7	1382.6	1380.0	1382.1 ± 1.6	
	$\Delta H°_{f\,0K}$	−38.4	−36.1	−37.0	−34.4	−36.5 ± 1.7	
	$\Delta H°_{f\,298K}$	−43.6	−41.3	−42.3	−39.7	−41.7 ± 1.6	
	$\Delta G°_{f\,298K}$	−13.5	−11.2	−12.5	−10.0	−11.8 ± 1.5	
PnVN	ΣD_0	1790.4	1787.6	1789.1	1786.3	1788.4 ± 1.8	
	$\Delta H°_{f\,0K}$	−68.3	−65.6	−67.1	−64.2	−66.3 ± 1.8	
	$\Delta H°_{f\,298K}$	−76.6	−73.8	−75.4	−72.6	−74.6 ± 1.8	
	$\Delta G°_{f\,298K}$	−43.3	−40.6	−41.6	−38.8	−41.1 ± 1.9	

* Theoretical value reported.

Ethics Statement

This article conforms to Elsevier's standards of ethical publishing.

Declaration of Competing Interest

The authors declare no conflict of interest.

CRediT Author Statement

Cristian Buendía-Atencio: Conceptualization, Methodology, Data curation, Formal analysis, Writing – original draft, Funding acquisition; **Darcy Parra Correa:** Methodology, Data curation, Writing – review & editing, Funding acquisition; **Miguel Ángel Delgado Gómez:** Writing –

review & editing, Funding acquisition; **Javier Alonso Pérez Cubides:** Writing – review & editing, Funding acquisition; **Vaneza Paola Lorett Velásquez:** Writing – review & editing, Funding acquisition.

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Supplementary Materials

Supplementary material associated with this article can be found in the online version at doi:10.1016/j.dib.2021.107350.

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