Data Article

Structural parameters and physicochemical data from quantum chemical calculations of the peroxycyl nitrate derivatives RC(O)O₂NO₂

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ABSTRACT

This article present the structural parameters and physicochemical data (ΣD₀, ΔH°₂⁹₈K and ΔG°₂⁹₈K) of the methoxyformyl peroxynitrate CH₃OC(O)O₂NO₂ (MoPAN), peroxypropionyl nitrate CH₃CH₂C(O)O₂NO₂ (PPN), peroxacyrol nitrate CH₂CHC(O)O₂NO₂ (APAN), peroxy-n-butyl nitrate CH₃(CH₂)₂C(O)O₂NO₂ (PnBN), peroxycrotonyl nitrate CH₃(CH=CH)C(O)O₂NO₂ (CPAN), peroxyisobutryl nitrate (CH₃)₂CHC(O)O₂NO₂ (PiBN), peroxymethylcrotonyl nitrate CH₂=C(CH₂)C(O)O₂NO₂ (MPAN) and peroxy-n-valeryl nitrate CH₃(CH₂)₃C(O)O₂NO₂ (PnVN) peroxycyl 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 Gn 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)O₂NO₂ 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 (ΣD0, ΔH°f,0K, ΔH°f,298K and ΔG°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)O₂NO₂ (R = CH₃O-, CH₃CH₂-, CH₂CH-, CH₃(CH₂)₂-, CH₂(CH=CH)-, (CH₃)₂CH, CH₂=C(CH₃)-, CH₃(CH₂)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 C1 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 C₁, C₂, C₃, and C₄ (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 peroxycetyl nitrate derivatives RC(O)O₂NO₂ (CH₃OC(O)O₂NO₂ (MoPAN), CH₃CH₂C(O)O₂NO₂ (PPN), CH₂CHC(O)O₂NO₂ (APAN), CH₃(CH₂)₂C(O)O₂NO₂ (PnBN), CH₃(CH=CH)C(O)O₂NO₂ (CPAN), (CH₃)₂CHC(O)O₂NO₂ (PnBN), CH₃=C(CH₃)C(O)O₂NO₂ (MPAN) and CH₃(CH₂)₃C(O)O₂NO₂ (PnVN)) at level of theory B3LYP/6-311++G(3df,3pd). The distances are in Å and angles in degree.

|          | MoPAN | PPN  | APAN | CPAN | PnBN | MPAN | PnVN |
|----------|-------|------|------|------|------|------|------|
| r(N-O₁)  | 1.184 | 1.186| 1.184| 1.186| 1.186| 1.186| 1.186|
| r(O₁-N)  | 1.523 | 1.511| 1.516| 1.510| 1.514| 1.516| 1.510|
| r(O₂-O₄) | 1.392 | 1.399| 1.395| 1.399| 1.394| 1.399| 1.395|
| r(C-O₄)  | 1.393 | 1.403| 1.405| 1.405| 1.409| 1.403| 1.404|
| r(O₅=C)  | 1.189 | 1.187| 1.190| 1.187| 1.192| 1.188| 1.192|
| r(O₆-C)  | 1.319 |      |      |      |      |      |      |
| r(O₆-C₁) | 1.443 |      |      |      |      |      |      |
| D(O₆-CO₂O₃) | 104.8 |      |      |      |      |      |      |
| D(O₆-CO₂O₄) | 115.3 |      |      |      |      |      |      |

|          | MoPAN | PPN  | APAN | CPAN | PnBN | MPAN | PnVN |
|----------|-------|------|------|------|------|------|------|
| r(N-O₁)  | 1.179 | 1.180| 1.180| 1.181| 1.180| 1.180| 1.181|
| r(O₁-N)  | 1.455 | 1.449| 1.451| 1.447| 1.450| 1.447| 1.451|
| r(O₂-O₄) | 1.374 | 1.378| 1.376| 1.378| 1.375| 1.377| 1.375|
| r(C-O₄)  | 1.381 | 1.392| 1.391| 1.393| 1.396| 1.394| 1.392|
| r(O₅=C)  | 1.185 | 1.183| 1.184| 1.182| 1.186| 1.183| 1.186|
| r(O₆-C)  | 1.312 |      |      |      |      |      |      |
| r(O₆-C₁) | 1.433 |      |      |      |      |      |      |
| D(O₆-CO₂O₃) | 105.6 |      |      |      |      |      |      |
| D(O₆-CO₂O₄) | 114.4 |      |      |      |      |      |      |

Table 2
Most relevant structural parameters of the peroxycetyl nitrate derivatives RC(O)O₂NO₂ (CH₃OC(O)O₂NO₂ (MoPAN), CH₃CH₂C(O)O₂NO₂ (PPN), CH₂CHC(O)O₂NO₂ (APAN), CH₃(CH₂)₂C(O)O₂NO₂ (PnBN), CH₃(CH=CH)C(O)O₂NO₂ (CPAN), (CH₃)₂CHC(O)O₂NO₂ (PnBN), CH₃=C(CH₃)C(O)O₂NO₂ (MPAN) and CH₃(CH₂)₃C(O)O₂NO₂ (PnVN)) at level of theory M06-2X/6-311++G(3df,3pd). The distances are in Å and angles in degree.

|          | MoPAN | PPN  | APAN | CPAN | PnBN | MPAN | PnVN |
|----------|-------|------|------|------|------|------|------|
| r(N-O₁)  | 1.184 | 1.186| 1.184| 1.186| 1.186| 1.186| 1.186|
| r(O₁-N)  | 1.523 | 1.511| 1.516| 1.510| 1.514| 1.516| 1.510|
| r(O₂-O₄) | 1.392 | 1.399| 1.395| 1.399| 1.394| 1.399| 1.395|
| r(C-O₄)  | 1.393 | 1.403| 1.405| 1.405| 1.409| 1.403| 1.404|
| r(O₅=C)  | 1.189 | 1.187| 1.190| 1.187| 1.192| 1.188| 1.192|
| r(O₆-C)  | 1.319 |      |      |      |      |      |      |
| r(O₆-C₁) | 1.443 |      |      |      |      |      |      |
| D(O₆-CO₂O₃) | 104.8 |      |      |      |      |      |      |
| D(O₆-CO₂O₄) | 115.3 |      |      |      |      |      |      |

|          | MoPAN | PPN  | APAN | CPAN | PnBN | MPAN | PnVN |
|----------|-------|------|------|------|------|------|------|
| r(N-O₁)  | 1.179 | 1.180| 1.180| 1.181| 1.180| 1.180| 1.181|
| r(O₁-N)  | 1.455 | 1.449| 1.451| 1.447| 1.450| 1.447| 1.451|
| r(O₂-O₄) | 1.374 | 1.378| 1.376| 1.378| 1.375| 1.377| 1.375|
| r(C-O₄)  | 1.381 | 1.392| 1.391| 1.393| 1.396| 1.394| 1.392|
| r(O₅=C)  | 1.185 | 1.183| 1.184| 1.182| 1.186| 1.183| 1.186|
| r(O₆-C)  | 1.312 |      |      |      |      |      |      |
| r(O₆-C₁) | 1.433 |      |      |      |      |      |      |
| D(O₆-CO₂O₃) | 105.6 |      |      |      |      |      |      |
| D(O₆-CO₂O₄) | 114.4 |      |      |      |      |      |      |
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 \( \text{RC(O)O}_2\text{NO}_2 \). 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 \( (\Delta H^\circ_f_{298K}, \Delta H^\circ_f_{298K}) \) have been computed by calculating total atomization energies \( (\Sigma D^\circ) \), 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 \( \text{CH}_3\text{CH}_2\text{C(O)O}_2\text{NO}_2 \) (PPN) and peroxyacryloyl nitrate \( \text{CH}_2\text{CHC(O)O}_2\text{NO}_2 \) (APAN) have been studied previously, the values reported for \( \Delta H^\circ_f_{298K} \) 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

| RC(O)O_2NO_2 | Property | G3B3  | G3MP2B3 | G4    | G4MP2 | Mean ± Std. Dev. | Ref. |
|--------------|----------|-------|---------|-------|-------|------------------|------|
| MoPAN        | ΔS_D0    | 1054.8| 1051.5  | 1053.5| 1050.2| 1052.5 ± 2.0     |      |
|              | ΔH^°_OK  | -93.5 | -90.2   | -92.2 | -88.8 | -912 ± 2.1       |      |
|              | ΔH^0_298K| -98.0 | -94.7   | -96.8 | -93.4 | -957 ± 2.1       |      |
|              | ΔG^0_298K| -69.9 | -66.7   | -68.9 | -66.6 | -678 ± 2.0       |      |
| PPN          | ΔS_D0    | 1236.5| 1233.7  | 1235.3| 1232.4| 1234.5 ± 1.8     |      |
|              | ΔH^°_OK  | -60.9 | -58.2   | -59.7 | -56.8 | -58.9 ± 1.8      |      |
|              | ΔH^0_298K| -66.3 | -63.6   | -65.2 | -62.3 | -64.4 ± 1.8      |      |
|              | ΔG^0_298K| -37.3 | -34.5   | -36.3 | -33.4 | -35.4 ± 1.8      |      |
| APAN         | ΔS_D0    | 1103.3| 1101.1  | 1102.1| 1099.5| 1101.5 ± 1.6     |      |
|              | ΔH^°_OK  | -31.0 | -28.8   | -29.8 | -27.2 | -29.2 ± 1.6      |      |
|              | ΔH^0_298K| -34.9 | -32.7   | -33.8 | -31.2 | -32.2 ± 1.6      |      |
|              | ΔG^0_298K| -7.3  | -5.1    | -6.5  | -3.9  | -5.7 ± 1.5       |      |
| PnBN         | ΔS_D0    | 1513.4| 1510.7  | 1512.1| 1509.2| 1511.4 ± 1.8     |      |
|              | ΔH^°_OK  | -64.6 | -61.8   | -63.3 | -60.4 | -62.5 ± 1.8      |      |
|              | ΔH^0_298K| -71.4 | -68.7   | -70.3 | -67.4 | -69.5 ± 1.8      |      |
|              | ΔG^0_298K| -40.3 | -37.5   | -39.3 | -36.4 | -38.4 ± 1.8      |      |
| CPAN         | ΔS_D0    | 1383.9| 1381.6  | 1382.6| 1379.9| 1382.0 ± 1.7     |      |
|              | ΔH^°_OK  | -38.4 | -36.1   | -37.0 | -34.4 | -36.5 ± 1.7      |      |
|              | ΔH^0_298K| -43.5 | -41.2   | -42.3 | -39.6 | -41.7 ± 1.7      |      |
|              | ΔG^0_298K| -13.4 | -11.1   | -12.5 | -9.8  | -11.7 ± 1.6      |      |
| PiBN         | ΔS_D0    | 1514.1| 1511.2  | 1512.8| 1509.8| 1512.0 ± 1.9     |      |
|              | ΔH^°_OK  | -65.3 | -62.4   | -64.0 | -61.0 | -63.2 ± 1.9      |      |
|              | ΔH^0_298K| -72.2 | -69.3   | -70.9 | -67.9 | -70.1 ± 1.9      |      |
|              | ΔG^0_298K| -41.3 | -38.4   | -40.3 | -37.3 | -39.3 ± 1.8      |      |
| MPAN         | ΔS_D0    | 1383.9| 1381.7  | 1382.6| 1380.0| 1382.1 ± 1.6     |      |
|              | ΔH^°_OK  | -38.4 | -36.1   | -37.0 | -34.4 | -36.5 ± 1.7      |      |
|              | ΔH^0_298K| -43.6 | -41.3   | -42.3 | -39.7 | -41.7 ± 1.6      |      |
|              | ΔG^0_298K| -13.5 | -11.2   | -12.5 | -10.0 | -11.8 ± 1.5      |      |
| PnVN         | ΔS_D0    | 1790.4| 1787.6  | 1789.1| 1786.3| 1788.4 ± 1.8     |      |
|              | ΔH^°_OK  | -68.3 | -65.6   | -67.1 | -64.2 | -66.3 ± 1.8      |      |
|              | ΔH^0_298K| -76.6 | -73.8   | -75.4 | -72.6 | -74.6 ± 1.8      |      |
|              | ΔG^0_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 Lorette 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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