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УСОВЕРШЕНСТВОВАНИЕ РАСЧЕТОВ ТЕПЛА СГОРАНИЯ ФОСФОРСОДЕРЖАЩИХ ОГНЕЗАЩИТНЫХ ВЕЩЕСТВ: СОЧЕТАНИЕ ЭФФЕКТИВНОСТИ МЕТОДА GFN2-XTB С ТОЧНОСТЬЮ DFT/B3LYP С ИСПОЛЬЗОВАНИЕМ КОРРЕКТИРУЮЩИХ ФАКТОРОВ

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Теплота сгорания фосфорсодержащих соединений была исследована с использованием двух широко применяемых вычислительных методов: самосогласованного метода квантовой химии (GFN2-xTB) и теории функционала плотности (DFT) на уровне B3LYP/6-311G(d,p). Оба метода были использованы для оптимизации молекулярных структур и расчета колебательных частот для ряда стандартных образцов, включая алканы, альдегиды, спирты и арены, что позволило провести их оценку и сравнение эффективности. Результаты показали, что метод DFT/B3LYP, как и ожидалось, дает более точные предсказания теплоты сгорания по сравнению с методом GFN2-xTB. Однако одним из ключевых преимуществ GFN2-xTB является значительно более короткое время вычислений, что особенно важно для работы с большими системами, где вычислительная эффективность имеет решающее значение. Кроме того, была замечена устойчивая закономерность отклонений между двумя методами, особенно для фосфорсодержащих соединений. Эта закономерность позволила вывести корректирующие факторы, которые были использованы для калибровки результатов GFN2-xTB для реакций сгорания фосфорных огнезащитных веществ, таких как бис(дифенилфосфат) и бисфенол А бис(дифенилфосфат). Применяя эти корректирующие факторы, удалось сохранить вычислительную эффективность GFN2-xTB, при этом сохраняя высокую точность, характерную для метода DFT/B3LYP. Этот подход представляет собой сбалансированное решение для изучения сложных процессов сгорания, особенно в тех случаях, когда речь идет о больших и сложных молекулах. Он позволяет проводить быструю аналитику для более крупных систем, не теряя точности, необходимой для глубокого понимания химических реакций. Метод имеет большой потенциал для оптимизации исследований в области сгорания, материаловедения, экологической химии и разработки передовых огнезащитных материалов.

Ключевые слова: резорцин бис(дифенилфосфат), бисфенол А бис(дифенилфосфат), GFN2-xTB, B3LYP, огнезащитное средство

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ENHANCING COMBUSTION HEAT CALCULATIONS OF PHOSPHORUS-CONTAINING FLAME RETARDANTS: COMBINING GFN2-XTB EFFICIENCY WITH DFT/B3LYP ACCURACY THROUGH ADJUSTMENT FACTORS

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The heat of combustion for phosphorus-containing compounds was investigated using two widely employed computational methods: the self-consistent tight-binding quantum chemical method (GFN2-xTB) and density functional theory (DFT) at the B3LYP/6-311G(d,p) level. Both methods were applied to optimize the molecular structures and calculate the vibrational frequencies of a series of standard samples, including alkanes, aldehydes, alcohols, and arenes, to benchmark their performance. The results indicated that DFT/B3LYP, as expected, provided more accurate predictions of the combustion heat compared to GFN2-xTB. However, one of the key advantages of GFN2-xTB is its significantly shorter computational time, which is especially useful for large systems where computational efficiency is critical. In addition, a consistent pattern of deviation ratios between the two methods was observed specifically for phosphorus-containing compounds. This consistency allowed for the derivation of adjustment factors, which were used to calibrate the GFN2-xTB results for the combustion reactions of specific phosphorus-based flame retardants, such as bis(diphenyl phosphate) and bisphenol A bis(diphenyl phosphate). By applying these adjustment factors, the computational efficiency of GFN2-xTB could be preserved, while still benefiting from the high accuracy of DFT/B3LYP. This approach offers a balanced solution for studying complex combustion processes, particularly those involving large and intricate molecules. It enables rapid analysis of larger systems without sacrificing the precision required for understanding detailed chemical reactions. The method has the potential to streamline the study of combustion in materials science, environmental chemistry, and the development of advanced flame retardants.

Keywords: resorcinol bis (diphenyl phosphate), bisphenol A bis (diphenyl phosphate), GFN2-xTB, B3LYP, flame retardant

INTRODUCTION

Phosphorus-containing flame retardants (PCFRs) are increasingly replacing halogen-containing counterparts due to their more environmentally benign properties [1]. These PCFRs are now extensively employed in various engineering plastics, such as polycarbonate/acrylonitrile-butadiene-styrene composites. Among the wide array of PCFRs, aryl phosphorus additives are particularly prominent in applications involving plastics, wood, and paper materials. Resorcinol bis(diphenyl phosphate) (RDP – $C_{30}H_{24}O_8P_2$) and bisphenol A bis(diphenyl phosphate) (BDP – $C_{39}H_{34}O_8P_2$) are the most commonly utilized within this category, prized for their superior thermal stability, low volatility, and effective flame retardancy [2]. Despite their widespread use as flame retardants, RDP and BDP are themselves susceptible to combustion under high-temperature conditions [3]. The heat released during their combustion can pose significant safety hazards, making it imperative to understand and quantify this heat release. Such knowledge would contribute to a more comprehensive understanding of the safety and effectiveness of PCFRs.

Currently, no experimental studies have been conducted to determine the heat released during the combustion of BDP and RDP. This gap in the literature underscores the necessity of conducting such research. Experimental approaches to measure the heat of combustion, such as the use of calorimetric bombs, are often complex and costly [4]. Consequently, theoretical methods based on quantum mechanics offer a valuable alternative. These computational approaches can provide estimates of combustion heat and other thermodynamic properties with a high degree of accuracy, often closely aligning with experimental values, while also offering significant savings in both time and cost [5].

Computing the combustion heat of RDP, BDP, and other PCFRs requires extensive calculations and efficient computational techniques to assess a broad range of substances. Density Functional Theory (DFT) is the standard method for calculating electronic structures and material properties. However, the DFT method is constrained by high computational demands and struggles with large-scale systems. To address these challenges, alternative approaches such as Density Functional Tight-Binding (DFTB) and Self-Consistent Tight-Binding Quantum Chemical Methods (SC-TBQC), including GFN2-xTB, have been developed. GFN2-xTB is designed for large-scale systems, encompassing thousands of atoms, while balancing accuracy and computational efficiency. It accounts for anisotropic second-order density fluctuations through short-range interactions of atomic multipole moments and eliminates the requirement for classical halogen or hydrogen bonding corrections, relying instead on global and element-specific parameters up to radon (Z = 86). Additionally, it incorporates the D4 London dispersion model, which depends on atomic partial charges and is naturally derived from second-order density fluctuations within a tight-binding framework. The method provides fully analytical and numerically accurate gradients. GFN2-xTB's accuracy has been validated across various systems and compared with other semiempirical computational methods, demonstrating its capability to handle large-scale simulations effectively while maintaining computational efficiency [6-8].

The primary objective of this study is to evaluate and compare the effectiveness of two computational techniques – GFN2-xTB and DFT/B3LYP – in predicting the heat of combustion for phosphorus-containing compounds, specifically focusing on BDP and RDP. This research aims to determine the relative accuracy of these methods by validating their predictions against experimental data and assessing their computational efficiency. Given that DFT/B3LYP is known for its high accuracy but also its substantial computational cost, and GFN2-xTB is recognized for its speed but with potentially less precision, this study seeks to balance these aspects. It is important to note that certain functionals, such as M06-2X, are specifically parameterized for thermochemical accuracy [9]. Nevertheless, B3LYP generally provides more accurate results than GFN2-xTB. By deriving adjustment factors between the two methods, this research aims to enhance the reliability of GFN2-xTB results while leveraging its computational efficiency. The choice of DFT/B3LYP for comparison with GFN2-xTB is based on its well-established reliability in calculating optimized molecular geometries, bond vibrational frequencies, and thermodynamic functions for organic compounds without requiring extensive parameterization, as demonstrated in several previous studies [10-11].

Ultimately, the goal is to provide a robust framework for rapid and accurate analysis of combustion reactions in larger systems, thus supporting improved safety measures for handling and storing flame retardant chemicals.

COMPUTATINONAL DETAILS

To conduct a comparative study of the GFN2-xTB and DFT computational techniques, we first optimized the geometric structures of several “standard samples”, including small molecules such as alkanes, aldehydes/alcohols, and arenes/phenols. We then calculated their vibrational frequencies using both approaches.

Additionally, we performed calculations for oxygen and the combustion products associated with these samples. From these vibrational frequency calculations, the standard enthalpy changes in combustion at temperature T (K) were determined using Equation 1 [9]. This approach allowed us to systematically assess and compare the performance of the two computational techniques in predicting combustion properties.

$$\Delta_r H_T^o = \sum_{i=1}^{n}(E_{tot}+H_{corr})_{i,T}^{product} - \sum_{j=1}^{m}(E_{tot}+H_{corr})_{j,T}^{reactant} \quad (1)$$

where E_{tot} is total electronic energy at $0K$ of each molecule, H_{corr} is enthalpy correction at temperature T.

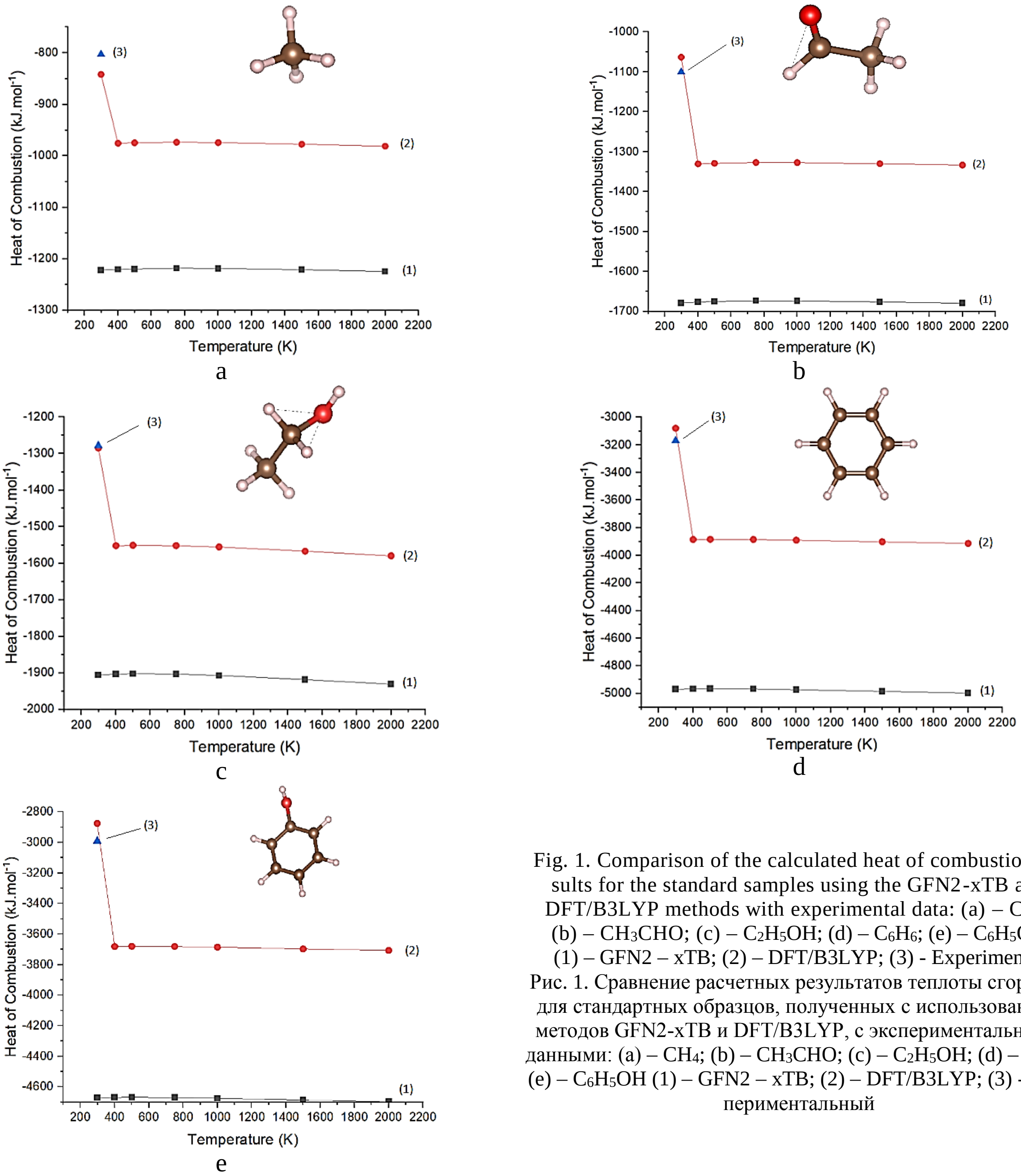
Subsequently, the results for the "standard samples" were compared with experimental data to evaluate the accuracy of both the DFT and GFN2-xTB methods. Following this, calculations for the "test samples" of phosphorus-containing compounds were performed using both GFN2-xTB and DFT methods. In the absence of experimental data for most of these compounds, the results were interpreted by referencing the more accurate DFT method. Finally, the combustion reactions of RDP and BDP were computed exclusively using the GFN2-xTB method, with adjustment factors (f_{adj}) derived from the results obtained for the test samples. This approach allowed for the utilization of GFN2-xTB's computational efficiency while refining the results through calibration based on the DFT method.

The DFT calculations were performed using the hybrid B3LYP functional and the 6-311G(d,p) basis set. DFT calculations were carried out using the Gaussian 09 software [12]. The B3LYP exchange-correlation functional is used because it has been proven sufficiently accurate for various systems, including those containing phosphorus [13,14]. The GFN2-xTB calculations were conducted using the open-source xTB software at an electron temperature of 300K, with energy convergence criteria set at 0.1×10^{-5} Hartree, and wavefunction convergence at 0.1×10^{-3} e.

RESULTS AND DISCUSSIONS

Heat of combustion of "standard samples"

After optimizing the structures and calculating the vibrational frequencies for several compounds: CH_4, CH_3CHO, C_2H_5OH, C_6H_6, and C_6H_5OH using both the GFN2-xTB and DFT-B3LYP/6-311G(d,p) methods, the heat of combustion of the standard samples at various temperatures ranging from 298.15 K to 2000 K is summarized in Table 1. The comparison of discrepancies between the two methods and the deviations from experimental data are presented in Fig. 1.



a

b

c

d

e

Fig. 1. Comparison of the calculated heat of combustion results for the standard samples using the GFN2-xTB and DFT/B3LYP methods with experimental data: (a) – CH_4; (b) – CH_3CHO; (c) – C_2H_5OH; (d) – C_6H_6; (e) – C_6H_5OH (1) – GFN2 – xTB; (2) – DFT/B3LYP; (3) - Experimental

Рис. 1. Сравнение расчетных результатов теплоты сгорания для стандартных образцов, полученных с использованием методов GFN2-xTB и DFT/B3LYP, с экспериментальными данными: (a) – CH_4; (b) – CH_3CHO; (c) – C_2H_5OH; (d) – C_6H_6; (e) – C_6H_5OH (1) – GFN2 – xTB; (2) – DFT/B3LYP; (3) - Экспериментальный

Table 1

Heat of combustion (kJ/mol) of standard compounds at temperatures ranging from 298.15 K to 2000 K

***Таблица 1.* Теплота сгорания (кДж/моль) стандартных соединений при температурах от 298,15 К до 2000 К**

T/K	CH_4		CH_3CHO		C_2H_5OH		C_6H_6		C_6H_5OH	
	B3LYP	GFN2-xTB	B3LYP	GFN2-xTB	B3LYP	GFN2-xTB	B3LYP	GFN2-xTB	B3LYP	GFN2-xTB
298.15	-841.888	-1221.943	-1063.170	-1678.807	-1284.536	-1905.554	-3079.349	-4969.003	-2875.356	-4671.094
400	-975.478	-1220.771	-1330.458	-1676.704	-1551.949	-1903.543	-3885.114	-4966.766	-3681.069	-4668.791
500	-974.617	-1219.776	-1328.949	-1675.124	-1550.956	-1902.441	-3884.165	-4965.717	-3680.127	-4667.721
750	-973.659	-1218.525	-1327.113	-1673.308	-1551.686	-1903.108	-3885.560	-4967.422	-3681.416	-4669.309
1000	-974.200	-1218.771	-1327.277	-1673.556	-1555.512	-1906.947	-3890.161	-4972.589	-3685.682	-4674.147
1500	-977.400	-1221.308	-1330.019	-1676.309	-1566.964	-1918.284	-3902.119	-4985.462	-3696.515	-4685.977
2000	-981.241	-1224.501	-1333.333	-1679.454	-1579.606	-1930.647	-3914.039	-4997.812	-3707.117	-4697.128
Exp.[a]	-802.53		-1099.94		-1277.65		-3169.42		-2990.13	

Note: a The experimental data on the heat of combustion of the compounds were calculated using the experimental standard enthalpy of formation values of the reactants and products at 298.15K from the database: https://cccbdb.nist.gov/exp1x.asp

Примечание: а Экспериментальные данные по теплоте сгорания соединений рассчитаны с использованием экспериментальных стандартных значений энтальпии образования реагентов и продуктов при 298,15 К из базы данных: https://cccbdb.nist.gov/exp1x.asp

Table 2

Calculation duration (s) for each standard molecule using the GFN2-xTB and DFT/B3LYP Methods

***Таблица 2.* Длительность вычислений (с) для каждой стандартной молекулы с использованием методов GFN2-xTB и DFT/B3LYP**

Molecules	Methods	Structure Optimization Calculation Time (s)	Total calculation time of vibrational frequencies and thermodynamic functions	Total time (s)*
CH_4	GFN2-xTB	N/I	N/I	0.071
	DFT/B3LYP	8	62	70
CH_3CHO	GFN2-xTB	N/I	N/I	0.239
	DFT/B3LYP	101	634	735
C_2H_5OH	GFN2-xTB	N/I	N/I	0.278
	DFT/B3LYP	164	930	1094
C_6H_6	GFN2-xTB	N/I	N/I	0.270
	DFT/B3LYP	916	6312	7228
C_6H_5OH	GFN2-xTB	N/I	N/I	0.534
	DFT/B3LYP	4094	8693	12787

Note: * All calculations were performed on a computer system with 4 processing cores and 8GB of RAM

Примечание: * Все расчеты проводились на компьютерной системе с 4 ядрами процессора и 8 ГБ оперативной памяти

Based on the calculated combustion enthalpies for phosphorus-free compounds using both the GFN2-xTB and DFT/B3LYP methods, it is clear that the DFT/B3LYP method yields results that are significantly closer to experimental values compared to those obtained with GFN2-xTB. This is not unexpected, as DFT/B3LYP is a well-established method known for its reliability in calculating properties of small to moderately sized molecules [15]. Although GFN2-xTB lacks high accuracy in thermodynamic calculations, its computational speed offers a significant advantage over traditional DFT methods, including DFT/B3LYP. The computation times for structure optimization and vibrational frequency calculations for each molecule using both methods are summarized in Table 2.

The GFN2-xTB method offers extremely rapid computation, with total time for structure optimization, vibrational frequency calculations, and thermodynamic functions calculations at temperatures ranging from 298.15 K to 2000 K being under 1 second. Moreover, as the molecular size increases, the computation time for GFN2-xTB remains relatively stable, with a factor of approximately 7.5 between CH_4 and C_6H_5OH. In contrast, the DFT/B3LYP method requires significantly more time, with a factor of about 182.7 between CH_4 and C_6H_5OH.

These results illustrate that GFN2-xTB is considerably faster than DFT/B3LYP, with speed improvements ranging from about 1000 to about 24000 times. This disparity is expected to grow with increasing molecular size, making the computational cost of DFT/B3LYP increasingly prohibitive. Consequently, using GFN2-xTB for rapid calculations, combined with adjusting results for accuracy using DFT/B3LYP, appears to be an effective approach for studying the combustion reactions of PCFRs with large molecules.

Heat of combustion of "test samples"

The standard phosphorus-containing compounds selected for this study include formyl phosphinate (CH_3O_4P), phenyl phosphate ($C_6H_7O_4P$), diphenyl phosphate ($(C_6H_5)_2HPO_4$), and triphenyl phosphate ($(C_6H_5)_3PO_4$). These compounds were chosen to represent both aromatic and non-aromatic phosphates, with a particular emphasis on aromatic phosphates, as the primary substances of interest – RDP and BDP – are aromatic phosphates with multiple rings. The combustion heats of these phosphorus-containing compounds were calculated using the GFN2-xTB and DFT/B3LYP methods across a range of temperatures, as presented in Table 3. Furthermore, Fig. 2 illustrates the discrepancies between the results obtained from the two computational methods.

Table 3

Heat of combustion (kJ/mol) of standard phosphorus-containing compounds at temperatures ranging from 298.15 K to 2000 K

Таблица 3. **Теплота сгорания (кДж/моль) стандартных фосфорсодержащих соединений при температурах от 298,15 К до 2000 К**

T/K	CH_3O_4P		$C_6H_7O_4P$		$(C_6H_5)_2HPO4$		$(C_6H_5)_3PO_4$	
	B3LYP	GFN2-xTB	B3LYP	GFN2-xTB	B3LYP	GFN2-xTB	B3LYP	GFN2-xTB
298.15	-534.922	-878.147	-2878.262	-4645.210	-5755.059	-9285.416	-8630.499	-13930.397
400	-669.959	-879.120	-3685.422	-4645.006	-7369.324	-9284.298	-11051.914	-13928.413
500	-670.172	-879.969	-3685.645	-4645.819	-7369.739	-9285.180	-11052.554	-13929.397
750	-670.542	-882.218	-3689.366	-4651.737	-7377.143	-9295.059	-11063.705	-13943.287
1000	-671.036	-884.776	-3695.775	-4660.712	-7389.937	-9310.989	-11082.926	-13966.188
1500	-672.181	-890.182	-3710.693	-4680.705	-7419.755	-9346.866	-11127.683	-14017.933
2000	-673.178	-895.425	-3725.348	-4700.020	-7449.050	-9381.361	-11171.639	-14067.577

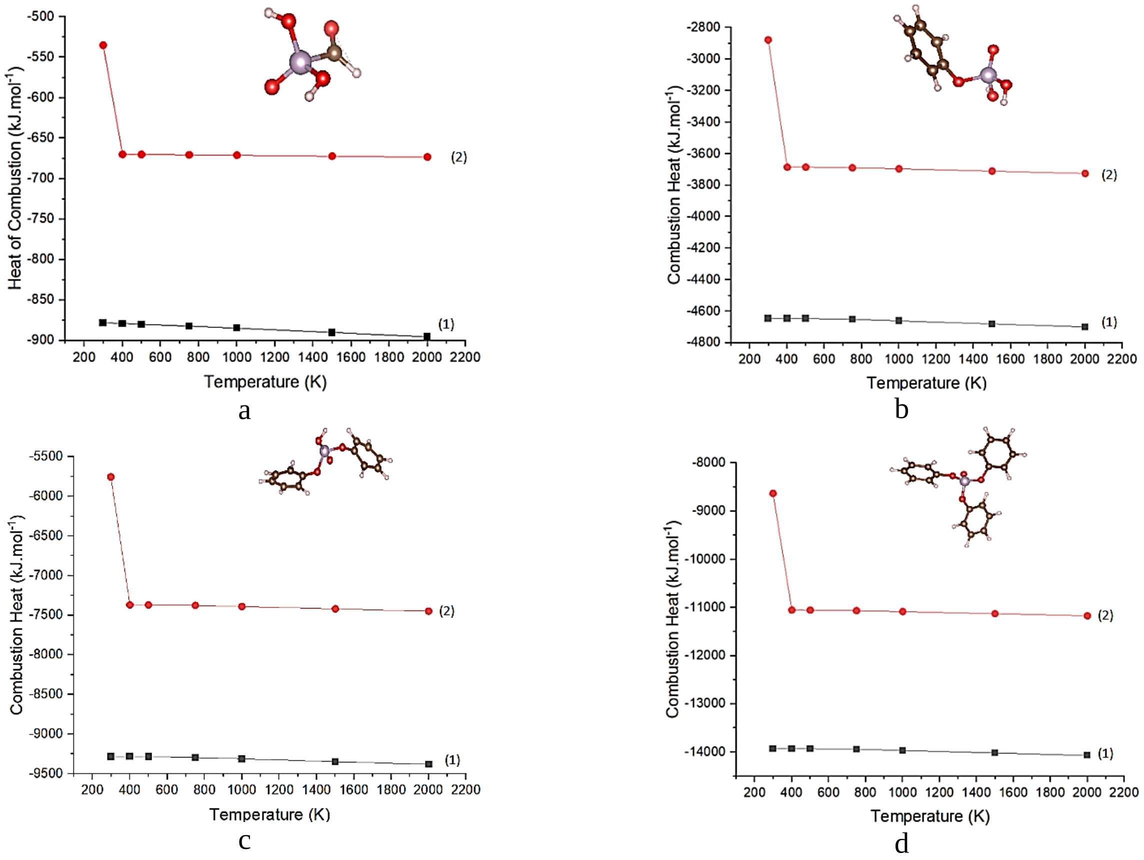


Fig. 2. Comparison of the results of calculating the heat of combustion of standard phosphorus-containing compounds using the GFN2-xTB and DFT/B3LYP methods: (a) - CH_3O_4P; (b) - $C_6H_7O_4P$; (c) - $(C_6H_5)_2HPO_4$; (d) - $(C_6H_5)_3PO_4$ (1) – GFN2 – xTB; (2) – DFT/B3LYP

Рис. 2. Сравнение результатов расчетов теплоты сгорания для стандартных фосфорсодержащих соединений, полученных с использованием методов GFN2-xTB и DFT/B3LYP: (a) - CH_3O_4P; (b) - $C_6H_7O_4P$; (c) - $(C_6H_5)_2HPO_4$; (d) - $(C_6H_5)_3PO_4$ (1) – GFN2 – xTB; (2) – DFT/B3LYP

Table 4

Ratio of combustion heats of phosphorus-containing compounds calculated using GFN2-xTB and DFT/B3LYP

***Таблица 4.* Соотношение теплот сгорания фосфорсодержащих соединений, вычисленных с использованием методов GFN2-xTB и DFT/B3LYP**

T/K	**Ratio between GFN2-xTB and DFT/B3LYP**				**Average results**
	CH_3O_4P	$C_6H_7O_4P$	$(C_6H_5)_3PO_4$	$(C_6H_5)_2HPO4$	
298.15	1.641636	1.613894	1.614089	1.613435	1.6207636
400	1.312199	1.260373	1.260272	1.259857	1.2731754
500	1.31305	1.260517	1.260288	1.259906	1.2734403
750	1.315679	1.26085	1.260273	1.259981	1.2741957
1000	1.318522	1.261092	1.260154	1.259955	1.318522
1500	1.32432	1.26141	1.259735	1.259727	1.32432
2000	1.330146	1.261632	1.259222	1.259404	1.330146

Table 5

Heat of combustion (kJ/mol) of RDP and BDP at temperatures ranging from 298.15 K to 2000 K

***Таблица 5.* Теплота сгорания (кДж/моль) RDP и BDP при температурах от 298,15 К до 2000 К**

	GFN2-xTB			**Refined values**	
T/K	RDP	BDP	f_{adj}	RDP	BDP
298.15	-22878.547	-30353.051	1.6207636	-14115.906	-18727.624
400	-22876.763	-30349.800	1.2731754	-17968.273	-23837.878
500	-22879.743	-30353.137	1.2734403	-17966.875	-23835.540
750	-22905.765	-30387.146	1.2741957	-17976.646	-23848.100
1000	-22946.383	-30441.782	1.3185220	-17403.110	-23087.807
1500	-23036.996	-30565.689	1.3243200	-17395.339	-23080.290
2000	-23123.942	-30685.894	1.3301460	-17384.514	-23069.568

The calculated combustion heats indicate that discrepancies between the two computational methods persist and are comparable to those observed for standard non-phosphorus-containing compounds. The most pronounced discrepancy occurs at 298.15 K, where the ratio of values obtained using the GFN2-xTB method to those from DFT/B3LYP is approximately 1.6. At other temperatures, this ratio ranges from about 1.2 to 1.3 (see Table 4). Despite these variations, the ratios are relatively close, which may be attributed to the influence of the phosphate group. Among the compounds studied, CH_3O_4P exhibits the largest discrepancy, with a ratio of approximately 1.64 at 298.15 K, while the discrepancies for the remaining compounds are nearly identical, around 1.61. This variation may be due to the opposing effects of different substituent groups (carbon-containing frameworks) on the phosphate group, with CH_3O_4P containing a formyl group and the other compounds containing phenyl groups.

The ratio of discrepancies in combustion heat calculated using the GFN2-xTB and DFT/B3LYP methods for phosphorus-containing compounds was averaged, as these ratios are relatively similar. This average value is used as an adjustment factor (f_{adj}) to extrapolate results from GFN2-xTB to DFT/B3LYP.

Heat of combustion of RDP and BDP

The combustion heats of RDP and BDP were calculated using the GFN2-xTB method. These values were then refined using the adjustment factor determined in section 3.2, according to the following formula:

$$\Delta_r H_T^o = \frac{\Delta_r H_T^o\,(\text{GFN2-xTB})}{f_{adj}^T} \qquad (2)$$

The resulting refined values of combustion heats for RDP and BDP are presented in Table 5, and the values, normalized to one mole of oxygen, are shown in Table 6. The combustion reaction equations of RDP and BDP are respectively:

$$C_{30}H_{24}O_8P_2 + 34.5O_2 \rightarrow$$
$$\rightarrow 30CO_2 + 9H_2O + 2H_3PO_4 \qquad (3)$$
$$C_{39}H_{34}O_8P_2 + 46O_2 \rightarrow$$
$$\rightarrow 39CO_2 + 14H_2O + 2H_3PO_4 \qquad (4)$$

Table 6

Heat of combustion (kJ/mol) of RDP and BDP at temperatures ranging from 298.15 K to 2000 K

***Таблица 6.* Теплота сгорания (кДж/моль) RDP и BDP при температурах от 298,15 К до 2000 К**

T/K	**RDP**	**BDP**
298.15	-409.157	-407.122
400	-520.82	-518.215
500	-520.779	-518.164
750	-521.062	-518.437
1000	-504.438	-501.909
1500	-504.213	-501.745
2000	-503.899	-501.512

The combustion heat values per mole of oxygen for RDP and BDP at 298.15 K are -409.157 kJ/mol and -407.122 kJ/mol, respectively. These values are relatively close to the average combustion heat per mole of oxygen for organic compounds in general, which is approximately 418 kJ/mol oxygen [16], demonstrating the validity of applying GFN2-xTB with the adjustment factor. It should be noted that BDP and RDP have combustion heat values per unit mass comparable to highly flammable chemicals such as acetone, butanol, and aniline [17-19]. This indicates that BDP and RDP could significantly impact safety considerations for their use, storage, and production, in accordance with the fire and explosive hazard classification methods for warehouses and production facilities as outlined in QCVN06:2022 [20].

CONCLUSIONS

Theoretical studies utilizing GFN2-xTB and DFT/B3LYP were conducted to investigate the heat of combustion and to compare the performance of these two computational techniques. The results indicate that DFT/B3LYP provides more accurate predictions compared to GFN2-xTB when validated against experimental data. However, GFN2-xTB demonstrates significantly shorter computation times relative to DFT/B3LYP. The deviation ratios between the results obtained by two methods at the same temperatures are consistent across phosphorus-containing compounds. From these ratios, adjustment factors were derived to calibrate the GFN2-xTB results for the combustion reactions of BDP and RDP. This approach capitalizes on the computational efficiency of GFN2-xTB while adjusting the results based on DFT/B3LYP, thereby facilitating the rapid analysis of larger systems without compromising accuracy. The calculated combustion heats for RDP and BDP reveal that, despite their efficacy as flame retardants in plastics, these substances can still combust and release a significant amount of heat. Consequently, it is imperative to implement safety measures to ensure proper handling and storage of these chemicals.

The authors declare the absence of a conflict of interest warranting disclosure in this article.

Авторы заявляют об отсутствии конфликта интересов, требующего раскрытия в данной статье.

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