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Antoine Equation Coefficients for Novichok Agents (A230, A232, and A234) via Molecular Dynamics Simulations

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Abstract: The flexible models of Novichok agents (A230, A232, and A234) from previous molecular dynamics simulations (MDSs) have been employed to create a parameter set for the Antoine equation of each of the three liquids. Furthermore, for the needs of this paper, new models of Novichok agents were created and studied via MDS due to the fact that the exact molecular structure of these compounds has been a matter of discussion in the last few years; however, recently, the literature favors a particular set of structures. Therefore, to cover our study holistically, both of the proposed molecular formulas were employed in the simulations and discussion. A range of ambient conditions was selected, and the data from the molecular dynamics simulations were employed to give the best possible fit in the selected vapor pressure range. When looking at the results for the two structures of A230, A232, and A234, we can see that, despite their differences, the A and B coefficients have the same magnitude in both cases (structures proposed by Ellison and Hoenig and structures proposed by Mirzayanov). Moving from the Ellison and Hoenig to Mirzayanov structures for substances A230 and A234 revealed a decrease (slight to major) in factors A and B of the Antoine equation. However, in the case of A232, where the Mirzayanov structure produces higher coefficients, this does not hold true. Overall, the Antoine equation of the studied agents will be an essential tool for understanding the behavior of these substances under different conditions.

Keywords: Novichok; Antoine equation; molecular dynamics

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1. Introduction

For many decades molecular dynamic (MD) simulations have helped scientists to study the properties of molecular systems, explore boundaries in terms of experimental conditions, and even propose helpful solutions to problems that arise during day-to-day experimentation. In the present study, MD simulations are employed in order to construct a low-vapor pressure-temperature reference curve for substances that present difficulties in conducting live experimentation.

It is well known that the Antoine equation is widely used in chemistry and physics. It is a semi-empirical formula used to describe the vapor pressure of a pure substance as a function of temperature. Semi-empirical equations are often used when a purely theoretical approach is not possible or practical, such as when dealing with complex systems or when experimental data are limited. By combining theoretical knowledge with empirical data, these equations can provide accurate predictions for a wide range of systems. The main specific ways in which the Antoine equation is important are the following:

- Predicting vapor pressure: The Antoine equation allows scientists to predict the vapor pressure of a substance at a given temperature. This is important in many areas of chemistry;
- Calculating the boiling point: The Antoine equation can also be used to calculate the boiling point of a substance. This is important for understanding the behavior of liquids and gases under different conditions;

- Understanding phase behavior: By using the Antoine equation, scientists can gain insight into the phase behavior of substances. This information is crucial for designing chemical processes, as well as for understanding the behavior of materials in different environments;
- Comparing chemicals: The Antoine equation can be used to compare the vapor pressures of different chemicals. For example, this is important when selecting appropriate solvents or for understanding the behavior of different substances in mixtures.

Moreover, concerning the vapor pressure of molecular liquids in a small range of temperatures, the Antoine equation [1] is a very accurate approximation of reality (Equation (1)).

$$log_{10}p = A - \frac{B}{C+T} \tag{1}$$

In Equation (1), p is the vapor pressure, i.e., the pressure of saturated vapor above the liquid in a closed container, T is the temperature, A, B, and C are the coefficients/parameters specific to each substance. For a small range of temperatures, the C parameter can be considered constant and is therefore embedded as a stable added term regarding temperature. This was the case for the August (Equation (2)) development, where the Antoine equation meets its most simplified form for a narrow range of temperatures.

$$log_{10}p = A - \frac{B}{T} \tag{2}$$

The physical meaning of the Antoine equation coefficients can be understood as follows:

A represents the constant term in the equation and is related to the vapor pressure of the liquid at its boiling point. In other words, A is the logarithm of the vapor pressure of the liquid at its boiling point and is related to the strength of the intermolecular forces between the molecules in the liquid.

B represents the coefficient for the temperature term in the equation and is related to the heat of vaporization of the liquid. In other words, B is a measure of the energy required to overcome the intermolecular forces holding the liquid together and turning it into a gas.

C represents a temperature offset term in the equation and is related to the shape of the vapor pressure curve for the liquid. Specifically, C is related to the curvature of the vapor pressure curve and can be used to determine whether the curve is concave up or down.

Since the Antoine equation cannot be employed for the whole range of temperatures of a specific liquid, many sets of parameters are usually developed, and this has been the case for this present study as well, where a low-pressure parameter set has been developed.

It is vital to mention that when T is measured in degrees of Celsius and C is set to 273.15, Antoine Equation is a semi-empirical expression of the well–known Clausius–Clapeyron equation, (Equation (3))

$$lnp\frac{p2}{p1} = -\frac{\Delta Hvap}{RT}\left(\frac{1}{T2} - \frac{1}{T1}\right) \tag{3}$$

where $\Delta Hvap$ is the heat of vaporization. It is also important to note that the A, B, and C parameters in the Antoine equation (Equation (1)) hold a not-so-strict physical meaning due to their aforementioned semi-empirical nature. They are rather used as a means of best fit in the available data in order to extrapolate in other temperatures.

The importance of the Antoine equation rises significantly in cases where vapor-liquid equilibria exist: cases such as near critical conditions, engineering calculations, and, most importantly, healthcare situations and drug administration, where each detail is of vital importance.

Chemical warfare agents (CWAs) form one of the most dangerous categories of chemical substances in the modern world since the potential risk includes harm to people and society. There should be a high level of global awareness concerning CWAs since a

small number of incidents have occurred in recent years [2,3], and many tones of these substances are still unaccounted for [4], especially after the collapse of the former Soviet Union. Novichok agents specifically belong to the general category of nerve agents and the fourth generation of CWAs [5,6]. Novichok agents are a group of nerve agents developed by the former Soviet Union in the Cold War era and Russia between 1971 and 1993 at the GosNIIOKhT state chemical research institute. They were developed under a Soviet program codenamed Foliant, and the name Novichok means "newcomer" in Russian [7]. Novichok agents were intentionally created to be challenging to identify. Experts suggest that Novichok agents were developed with four specific goals in mind: first, to avoid detection by the chemical-detection equipment used by NATO in the 1970s and 80s; second, to overcome the protective gear employed by NATO against chemical threats; third, to enhance safety during handling procedures; and fourth, to evade the list of controlled precursors outlined in the Chemical Weapons Convention. Novichok is classified as a "binary" chemical weapon, which means it utilizes two or more chemical components that are either non-toxic or less toxic on their own and only become active when combined. While this characteristic improves the safety aspects of storing, transporting, and disposing of Novichok, it also poses a challenge for detection since the precursors can be transported separately. However, there have been recent developments in the detection of Novichok agents. For example, a study published in 2023 reported on the selective colorimetric detection of Novichok agents with hydrazone chemosensors [8].

Novichok agents gained significant public awareness in the 21st century when they were utilized to poison individuals who opposed the Russian government. Notable cases include the poisoning of Sergei and Julia Skripal, as well as two other individuals in Amesbury, UK, in 2018, and the poisoning of Alexei Navalny in 2020. However, instances of civilian poisonings involving this substance have been documented as early as 1995. The Chemical Weapons Convention (CWC) of 1997 prohibits the utilization of recognized Novichok agents in warfare.

This arms control treaty imposes a set of obligations on States Parties, requiring them to abstain from activities such as the development, production, acquisition, stockpiling, retention, transfer, or use of chemical weapons. The treaty is supervised by the Organization for the Prohibition of Chemical Weapons (OPCWs), an intergovernmental organization based in The Hague, The Netherlands. States Parties are responsible for implementing and enforcing the prohibition within their respective jurisdictions. All participating nations have made a commitment to achieve chemical disarmament by disposing of their existing stockpiles of chemical weapons, dismantling production facilities, and eliminating any chemical weapons abandoned in the territories of other States Parties. Additionally, States Parties have agreed to establish a verification system to monitor specific toxic chemicals and their precursors, ensuring that these substances are solely used for purposes permitted by the Convention [9].

Moreover, the Organization for the Proliferation of Chemical Weapons (OPCWs) treaty prohibits the production of and experimentation with substances such as Novichok compounds.

Novichok agents possess an extremely high level of toxicity and can be fatal even in minuscule amounts. These agents function by interfering with the communication between nerves and muscles or the nerves within the brain. They fall into a broad category of substances known as cholinesterase inhibitors, which are utilized in various medications and poisons. Novichok disrupts the processes through which nerves transmit messages to organs by impeding the chemicals that nerve cells employ to regulate vital functions and blocking neurotransmitters. Within a matter of minutes, they induce paralysis in the muscles responsible for breathing and halt the functioning of the heart [10].

Medical professionals should approach the treatment of Novichok agent poisoning similarly to the management of other nerve agents. It is crucial for clinicians to be able to promptly identify symptoms of acute poisoning and administer appropriate antidotal

therapy as necessary to save lives. Standard antidotes, such as atropine and diazepam, can be used to treat all types of nerve agent poisoning [10].

Novichok agents are also designed to be highly persistent in the environment, which can make decontamination extremely difficult. Because of their potency and persistence, Novichok agents are considered to be a serious threat to human health and international security.

Therefore, molecular simulations might fill the gap in exploring the properties of these systems via a safe way to advance new antidote treatments and better understanding.

In the recently available scientific literature, few studies have been made concerning the relevant physical and chemical properties and toxicity [9–13]. Neponimova and Kuca reviewed a substantial amount of available data and the few available physicochemical properties [14–17].

Each time these substances are taken into consideration, an important issue that needs to be taken into account is that two forms of their molecular forms existed in the literature until recently. The first ones appeared in books published in 2008 by Ellison (revised in 2022) and Hoenig [10,11], and the subsequent ones were published by Mirzayanov in his book State Secrets: An Insider's Chronicle of the Russian Chemical Weapons Program [7]. According to the OPCWs Annex on Chemicals, Schedule 1 (16), Mirzayanov's proposed structures are enlisted as toxic chemicals and banned substances [9]. Specifically, Schedule 1 of the OPCWs substances includes the most toxic ones with no particular commercial use. However, this addition has been added after the Salisbury (Skripal) incidents and concerns this particular case of interest and has not matched the substances to the name Novichok at any point

Moreover, an interview by Nikolai Volodin, another member of the Novichok program in the Soviet regime and coworker of Mirzayanov at the time [18], seriously questioned whether the substance employed in the Salisbury incident was actually Novichok due to the serious impact when it is employed and the difficulty it possesses in being controlled.

Since the structures proposed in 2008 by Ellison and in the handbook by Hoenig have been a matter of active research in the literature, we did not opt out of studying both forms that have appeared in the literature.

However, it has to be clearly noted that in the last few years, Mirzayanov's structures are the ones that have predominantly been accepted as the ones corresponding to Novichok CWAs. In any case, in our scientific work, we tried to be inclusive of the recent and previously proposed structures.

Therefore, in all our studies, we opted to study both the proposed structures (Ellison 2008 and Hoenig structures, denoted by "eh" marked next to their name, and the Mirzayanov-proposed structures, denoted by an "m" attached to the end of their name) to be in accordance with the latest facts as well as with the studies made of both structures in previous years.

Following the collapse of the former Soviet Union, where Novichok substances were developed, many tones of the produced CWAs are still unaccounted for [14,19]. The Treaty for the Proliferation of Chemical Weapons also prohibits any production of these substances, so experimental data are scarce and rare.

During the following years, theoretical and spectrometry works confirmed the structures by Hoenig and Ellison [10,11,20–22], while other works focused on the structures proposed by Mirzayanov [12,14,15]. This work is based on both of the proposed structures in order to give a complete approach to the behavior in each case.

In our previous works [23,24], we developed the CK potential model set for all three A230, A232, and A234 Novichok substances based on the Ellison and Hoenig structures, and we explored many of their properties through extensive molecular dynamics simulations.

In this present study, continuing on from our previous studies [18,19], we further explore the properties of Novichok A230, A232, and A234 and all the proposed structures of both these agents in the literature using MDSs. Specifically, an ambient range of applied temperatures was selected for the study and extraction of the parameters. This is mainly due

to the fact that in the events where chemical warfare agents were employed, it happened in ambient temperature conditions. Therefore, a range of 15–45 degrees Celsius was selected, split into three segments, giving a set of four simulation temperatures, namely, 15, 25, 35, and 45 °C, or approximately 288, 298, 308, and 318 K when measured in Kelvin.

2. Methodology: Simulation Details

In this study, all MD simulations based on the Novichok structures proposed by Ellison and Hoenig [10,11] are denoted hereafter with symbols A230eh, A232eh, and A234eh, and the structures mentioned by Mirzayanov are denoted as A230m, A232m, and A234m. The development of the parameter set is thoroughly described in our previous work for our CK model [23,24]. The CK model is, to our knowledge, the first flexible model of the Novichok agents (A230, A232, and A234).

Our approach to the creation of reliable models for the simulations involves several sequential steps, as depicted schematically in Figure 1.

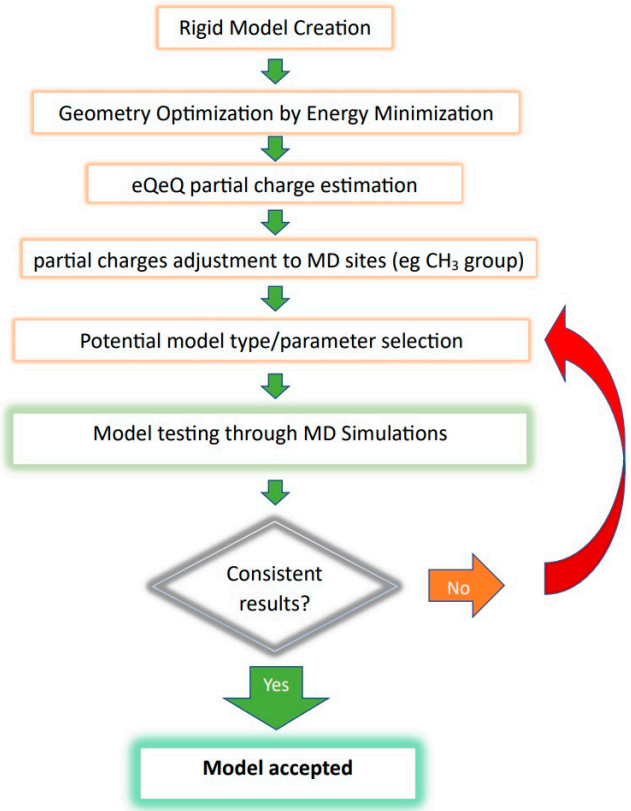


Figure 1. Model creation approach: eQeQ stands for extended charge equilibration scheme, and MD stands for molecular dynamics.

The structures used in our simulations employed unified atoms in the case of carbon groups and also are fully flexible models, so the parameters needed to be adjusted/selected in the case of each particular bond, angle, and dihedral angle. Moreover, Ellison and Hoenig's proposed study of the structures was carried out prior to the study of Mirzayanov's structure. In the Ellison and Hoenig structures, since rigid body X-ray data were not available, the model creation procedure had to start from scratch, i.e., building the rigid molecule initial model. This process was also followed by creating the Mirzayanov-proposed flexible molecular models. The latter could not have been easily created from X-ray protein data, such as 6NTO, etc., available in the literature [25,26] since, after the removal of the fluoride atom and the binding, which occurs due to the acetylcholinesterase, the interatomic interactions change substantially and affect the potential molecular model significantly since the electronegativity, partial charge, and potential model properties of the

fluoride atom differs from the ones of the attached oxygen atom in the acetylcholinesterase molecule [25,26].

The key factors in this model include:

Lennard–Jones 12–6 parameters, referring Equation (4) [27].

$$E = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] r < r_c \quad (4)$$

The bond potential parameters are representations of the harmonic bond potential, as shown in Equation (5):

$$E = K\Big(r - r_0\Big)^2 \quad (5)$$

r_0 is the distance of equilibrium calculated from the most stable rigid-body geometry, and the constant K incorporates 1/2 factor.

The angle potential parameters are also the harmonic angle potential of Equation (6):

$$E = K\Big(\theta - \theta_0\Big)^2 \quad (6)$$

θ_0 is the equilibrium angle, and the constant K incorporates the 1/2 factor.

The dihedral angle parameters are the harmonic dihedral potential of Equation (7):

$$E = K[1 + dcos(n\phi)] \quad (7)$$

where K is an energy factor, d is equal to 1, and n equals 3.

Note that, in the case of A230m, A232m, and A234m, an OPLS dihedral style potential was used, as these simulations were subsequent and improved precision was available (upgraded computing grid at the time of simulations). The OPLS dihedral potential is of the form in Equation (8).

$$E = \frac{1}{2}K_1[1 + cos(\phi)] + \frac{1}{2}K_2[1 - cos(2\phi)] + \frac{1}{2}K_3[1 + cos(3\phi)] + \frac{1}{2}K_4[1 - cos(4\phi)] \quad (8)$$

The simulations were performed using the LAMMPS software package [28]. In order to obtain dipole-moment data for an isolated molecule without periodic boundary conditions and Uvap (internal energy without any intermolecular interactions), simulations with a timestep of 0.5 fs and a duration of 500 ns were performed in an NVE statistical ensemble, following the 5 ns of the equilibration.

For the bulk calculations, 500 molecule systems were simulated for each of the three molecules under research using a timestep of 1fs and a duration of 1ns for the production runs. The cut-off radius was set to 14Å.

A 1ns NPT simulation (0.45 ns equilibration in NVT and 0.05 ns equilibration in NPT afterward and before the production runs) to verify experimental density was reproduced in a statistically accepted margin. Experimental density was found to be accurately reproduced in our previous study for EH models, so we moved onward with the same technique.

The potential energy in gas and liquid conditions: Uvap and Uliq, from 1 (500 billion independent configurations) and 500 molecule simulations, respectively, was employed to estimate the heat of vaporization $\Delta Hvap$.

3. Results and Discussion

The potential energy in gas and liquid conditions: Uvap and Uliq, from 1 and 500 molecule simulations, respectively, was employed to estimate the heat of vaporization, $\Delta Hvap$, using Equation (9):

$$\Delta H_{vap} = U_{vap} - U_{liq} + RT \quad (9)$$

After estimating the heat of vaporization from the MD simulations for all three substances: A230, A232, and A234, for all four temperatures under investigation, the Clausius–Clapeyron equation was employed to estimate the vapor pressure for the three temperatures that were not already known (15, 35, and 45 °C); we already had data for 25 °C.

Specifically, the Clausius–Clapeyron equation was transformed into the form of Equation (10):

$$p_2 = p_1 e^{\frac{\Delta H}{R}(\frac{1}{T1} - \frac{1}{T2})} \quad (10)$$

where T_1 is always 298K and p_1 equals the vapor pressure from the literature [5].

The sets of vapor pressure–temperatures are shown in Table 1.

Table 1. Vapor pressure–temperature for each of the three liquid systems.

A230eh		**A232eh**		**A234eh**	
Temperature (K)	Vapor Pressure (Pa)	Temperature (K)	Vapor Pressure (Pa)	Temperature (K)	Vapor Pressure (Pa)
288	0.72	288	0.71	288	0.47
298	2.13	298	1.48	298	1.7
308	5.71	308	3.03	308	5.74
318	12.65	318	4.56	318	21.93
A230m		**A232m**		**A234m**	
Temperature (K)	Vapor Pressure (Pa)	Temperature (K)	Vapor Pressure (Pa)	Temperature (K)	Vapor Pressure (Pa)
288	0.84	288	0.54	288	0.98
298	2.13	298	1.48	298	1.70
308	5.13	308	3.67	308	4.68
318	11.07	318	10.73	318	14.84

These sets of points were then converted to $log_{10}p$ and $-1/(C + T)$ and were subsequently plotted. In this way, we obtained a $log_{10}p$ versus $-1/(C + T)$ plot, and the Antoine equation $log_{10}p = A - B/(C + T)$ was one of the forms of Equation (11):

$$y = ax + b \quad (11)$$

This form converts the Antoine equation to the best available form for a least squares linear regression fit, where a factor of Equation (11) is equal to the B in Antoine's equation, and b is equal to the A from the same equation. In Equation (11), y equals $log_{10}(p)$, and x equals $[-1/(T + C)]$.

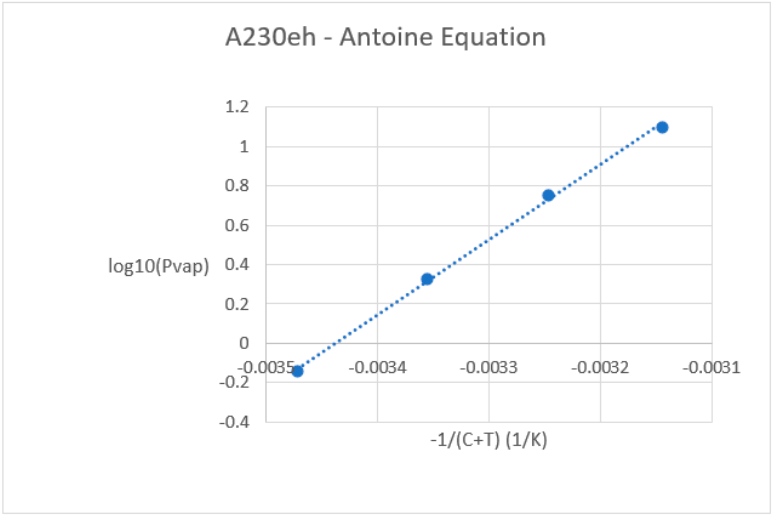
The results are shown in Figures 2–7 along with the corresponding molecular structures. The compound names are shown in the figure captions.

Linear regression lines were fitted for each structure, and the corresponding results for parameters A and B of the Antoine Equation are shown in Table 2, along with the R^2 factor for each case.

The results exhibit remarkable accuracy, as shown by the extremely close R2 regression factors; therefore, our first conclusion is that these parameters are an accurate description of the studied conditions and provide an adequate approximation of temperatures/pressures in the vicinity of the state points we studied.

In the available literature [6], there is not a clear reference as to which of the proposed Novichok structures correspond to the published vapor pressure values. So, checking the results for both available compound forms has an additional point to clarify: whether the Ellison/Hoenig or Mirzayanov structures are more consistent with the published values. It is quite clear that the results for the Mirzayanov structures in Table 2 exhibit higher cohesion among them since, in the case of results for Ellison/Hoenig structures, there is a significant drop in the predicted values for A232. It is vital to say that A230eh, A232eh, and A234eh typically differ by one or two methyl groups for the Ellison/Hoenig structures,

while for the Mirzayanov structures, A232m has an extra oxygen atom when compared to A230m and A234m has an extra methyl group when compared to A232m. Stereochemistry plays an important role in molecular attributes such as vapor pressure, and one may assert that the differences regarding the predicted simulations are, thus, to be expected.



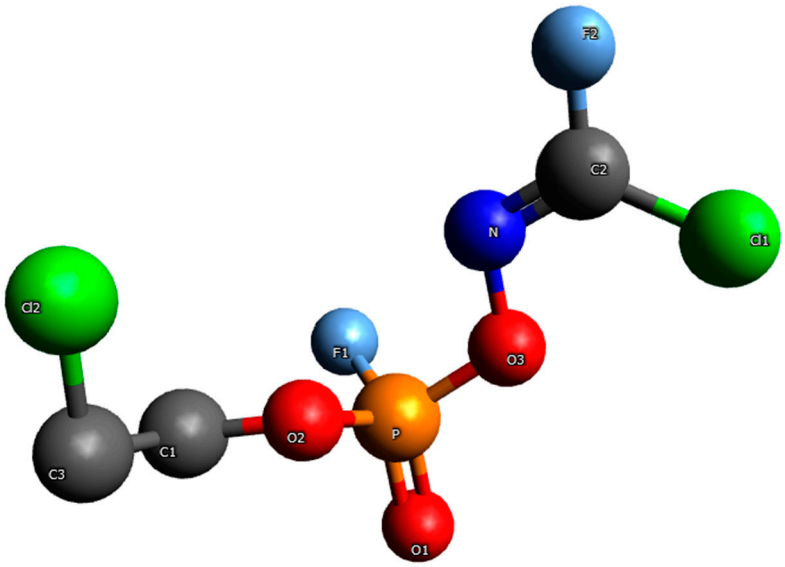


Figure 2. A230eh fit for the Antoine Equation along the A230eh structure; ([(2-chloroethoxy) fluorohydroxyphosphinyl]oxy)carbonimidic chloride fluoride [5].

Moreover, concerning the results for the two structures of A230, A232, and A234, we may observe that, in both cases (the structures proposed by Ellison and Hoenig and the structures proposed by Mirzayanov), the A and B coefficients are held in the same magnitude of scale, despite their differences. These differences are larger in the cases of A232 and A234, which is quite an expected result since, when going from A230 to A232 and to A234, the molecular mass increases, thus leading to larger differences in all molecular properties due to the change in molecular properties, such as the dipole moment, moment of inertia, total energy, etc.

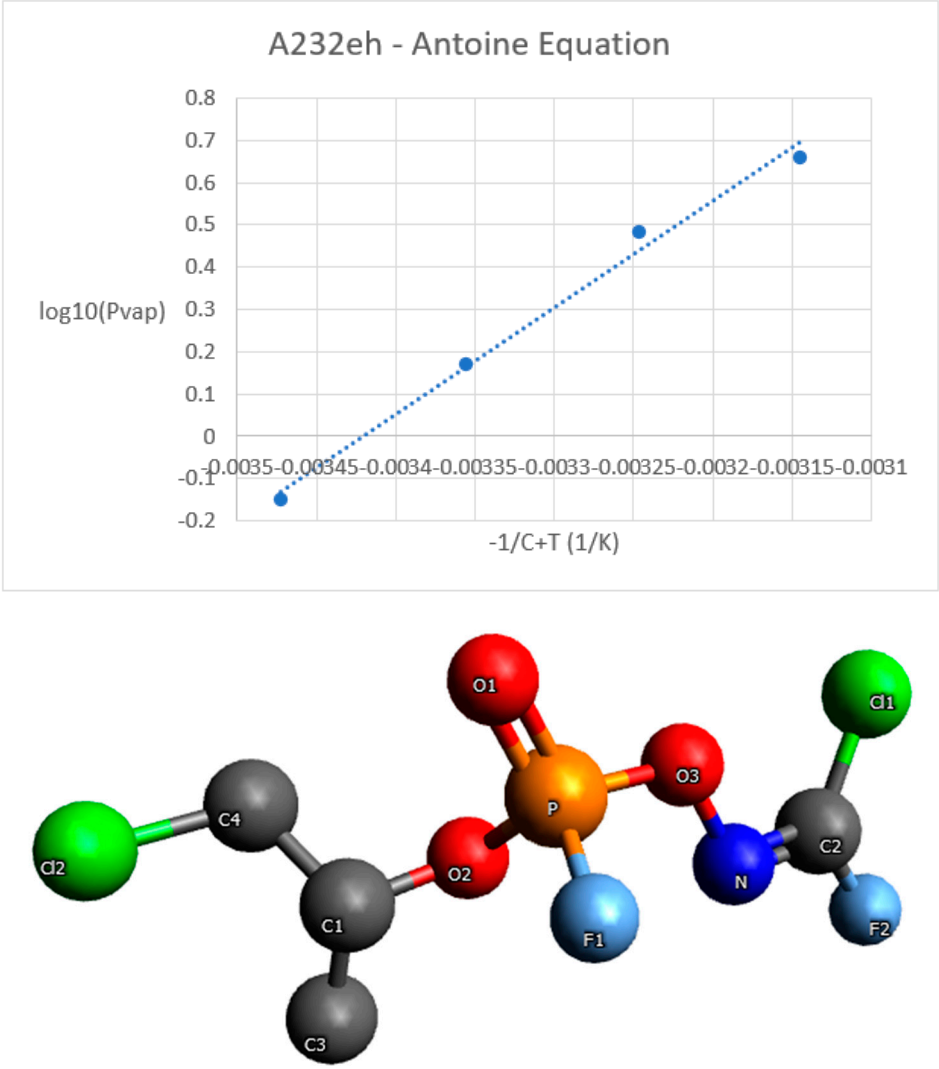


Figure 3. A232eh fit for the Antoine Equation along the A232eh structure; ([(2-chloro-1-methylethoxy) fluorohydroxyphosphinyl]oxy)carbonimidic chloride fluoride [5].

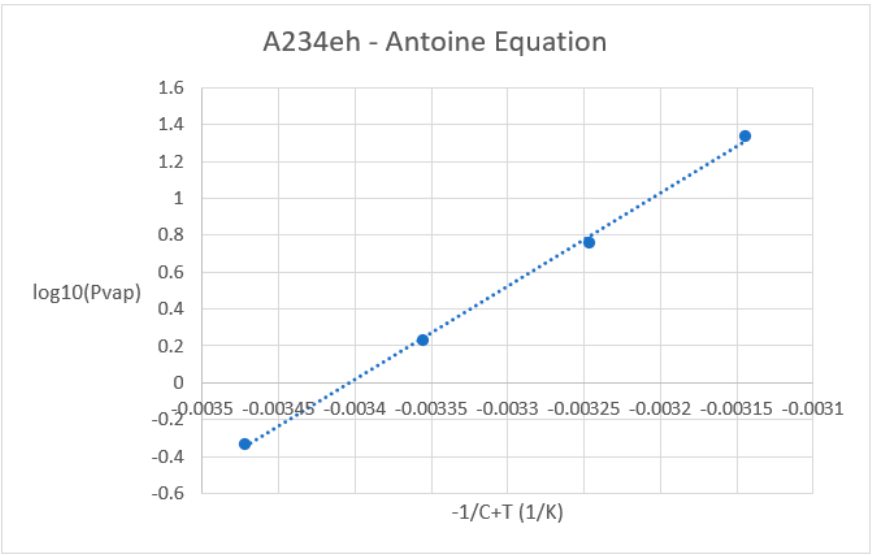


Figure 4. *Cont.*

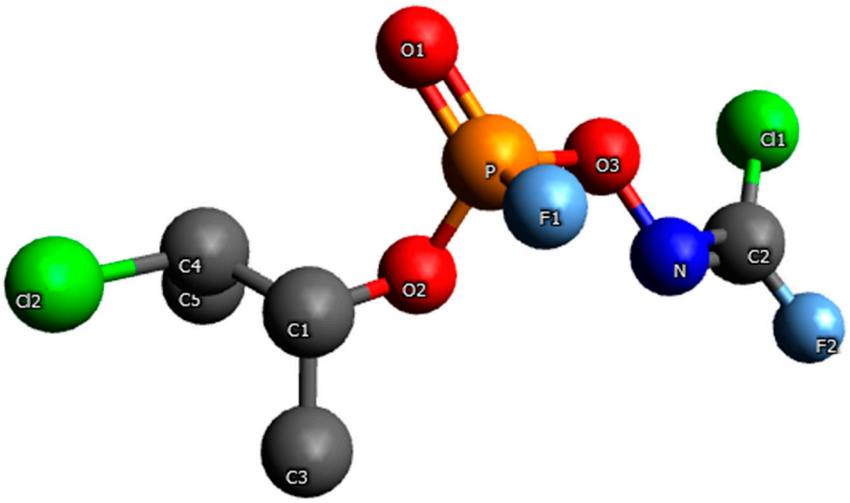
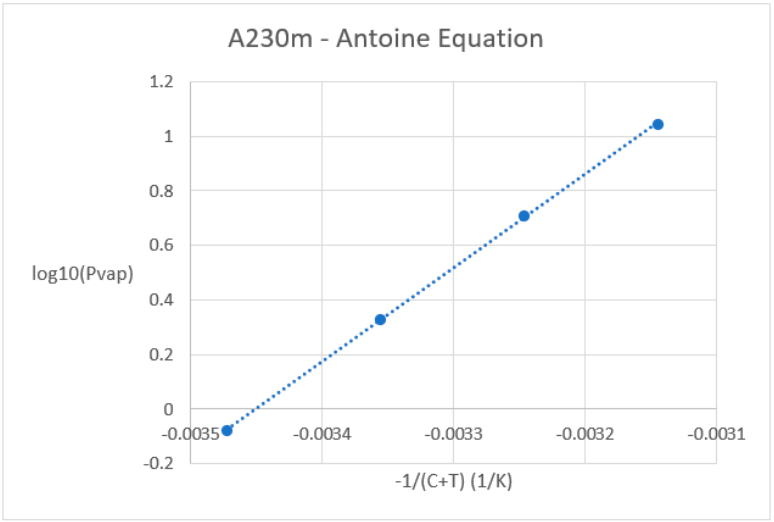


Figure 4. A234eh fit for the Antoine Equation along the A234eh structure; ([(2-chloro-1-methylpropoxy) fluorohydroxyphosphinyl]oxy)carbonimidic chloride fluoride [5].



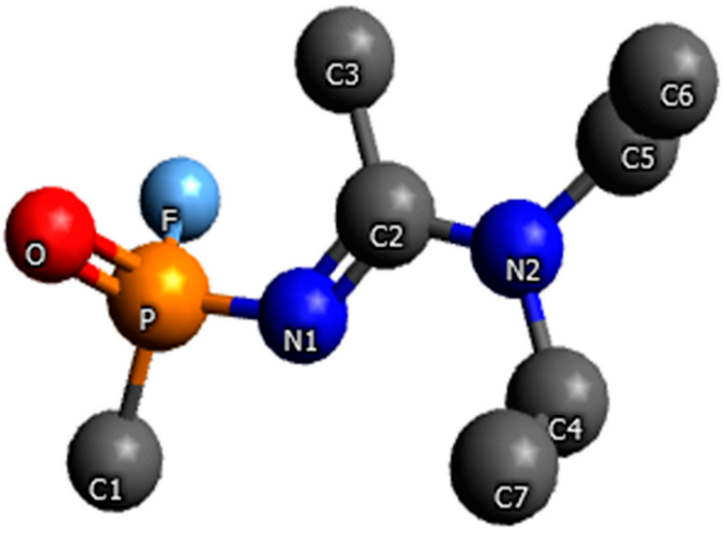


Figure 5. A230m fit for the Antoine Equation along the A230m structure; methyl-(1-(diethylamino) ethylidene)phosphonamidofluoridate [16].

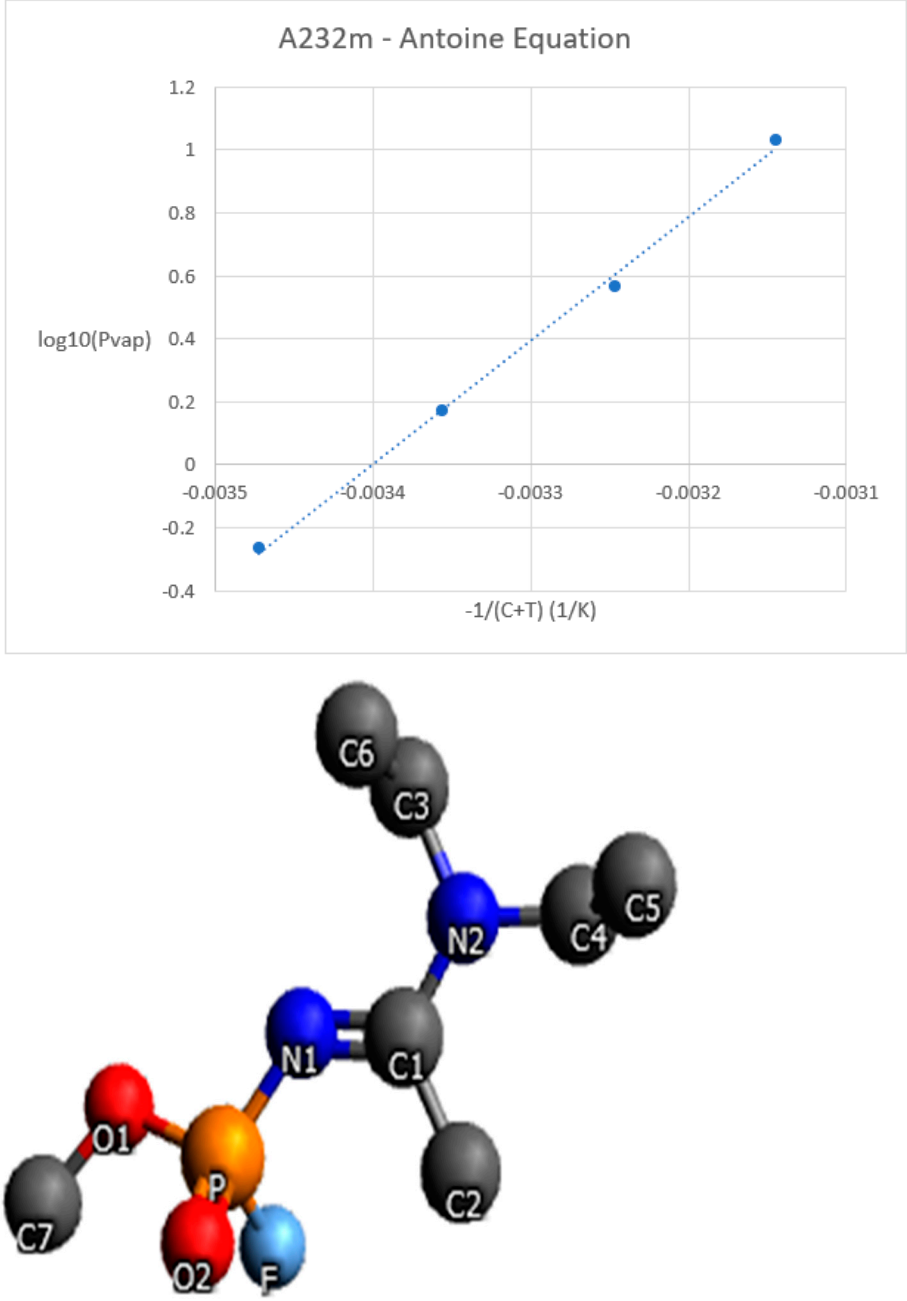


Figure 6. A232m fit for the Antoine Equation along the A232m structure; methoxy-(1-(diethylamino) ethylidene)phosphoramidofluoridate [16].

Concerning substances A230 and A234, when moving from the Ellison and Hoenig to the Mirzayanov structures, we see a decrease (slight to major) in factors A and B of the Antoine equation. On the other hand, this does not apply to A232, where the Mirzayanov structure yields higher coefficients. This should be noted and is probably a factor of the quite different intermolecular forces, affecting vapor pressure and, consequently, the Antoine equation coefficients.

Overall, in each case studied, parameters A and B and the regression represent a good indication that the selected state points are covered by the Antoine equation semi-empirical description.

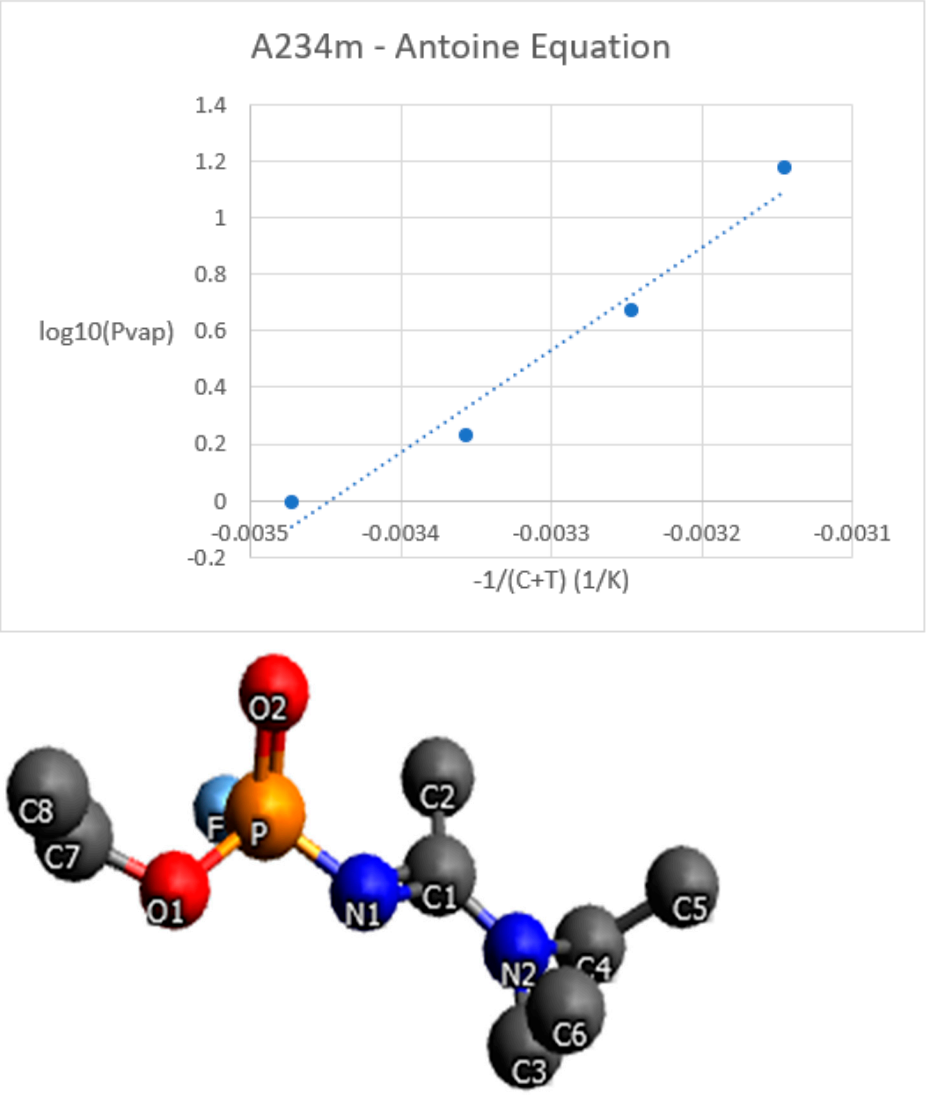


Figure 7. A234m fit for the Antoine Equation along the A234m structure; ethyl N-[(1E)-1-(diethylamino) ethylidene]-phosphoramidofluoridate [16].

Table 2. Antoine equation parameters for Novichok A230, A232, and A234 liquids; C = 273.15K; "eh" denotes Ellison and Hoenig structures; "m" denotes Mirzayanov structures.

A230eh		**A232eh**		**A234eh**	
Temperature Range 15–45 °C		Temperature Range 15–45 °C		Temperature Range 15–45 °C	
Vapor Pressure Range (0.7–12.65 Pa) R^2 = 0.9985		Vapor Pressure Range (0.7–4.56 Pa) R^2 = 0.9904		Vapor Pressure Range (0.47–21.93 Pa) R^2 = 0.9983	
A	B	A	B	A	B
13.12	3815.6	8.61	2517.5	17.26	5071.1
A230m		**A232m**		**A234m**	
Temperature Range 15–45 °C		Temperature Range 15–45 °C		Temperature Range 15–45 °C	
Vapor Pressure Range (0.83–11.07 Pa) R^2 = 0.9998		Vapor Pressure Range (0.54–10.73 Pa) R^2 = 0.9974		Vapor Pressure Range (0.98–14.84 Pa) R^2 = 0.9686	
A	B	A	B	A	B
11.84	3432.3	13.34	3923.9	12.52	3630.9

4. Conclusions

The Antoine equation is an essential tool for understanding the behavior of chemical compounds in different environments and is widely used in various fields of physical chemistry.

Previously developed molecular models and new versions were employed in this MDS study in order to create a set of parameters for the Antoine equation for three substances. Novichok A230, A232, and A234 were the investigated models, and 15, 25, 35, and 45 °C represent the range of temperatures under the pressure of 1 atmosphere. Both structures proposed in the literature were used for all three substances. An estimation of the heat of vaporization, a calculation of the vapor pressure under different conditions, and the linear regression fits of the estimated points in relation to the Antoine equation parameters yielded remarkable accuracy in estimating the low-pressure equation for all three molecular liquid systems.

The estimated Antoine equation parameters will be useful for calculations concerning the vapor pressure over the liquid surface of these dangerous CWAs, substances that, when deployed in the smallest amount, can prove fatal. Therefore, knowing the behavior of their vapor is of vital importance in order to create mechanisms and means of protection. Furthermore, the Antoine equation can also be used to estimate thermodynamic properties, such as enthalpy, entropy, and Gibbs's free energy, and, in environmental research, to estimate the evaporation rate of these agents from water and soil.

In organic synthesis, the Antoine equation can be used to predict the boiling point and vapor pressure of a solvent or reagent at different temperatures. This information is important because it allows chemists to select the appropriate solvents and conditions for reactions, as well as to design and optimize distillation and purification processes.

By using the Antoine equation to predict the vapor pressure of a substance, chemists can design reactions that operate at the desired temperature and pressure conditions. This can improve the efficiency and yield of the reaction, as well as reduce the risk of unwanted side reactions or product degradation.

The properties of volatile liquids, such as Novichok compounds, need to be calculated in order to facilitate treatment in events of possible terrorist incidents. Determining the airborne amount of these particular liquids can be critical to estimating the degree that human subjects have been exposed to these dangerous CWAs in an event. Afterward, this can lead to decisions by emergency medical professionals concerning the treatment of the aforementioned exposure.

As time passes, new threats and forms of terrorism using CWAs might emerge. The scientific community should be prepared as much as possible to prevent or minimize the damage in each of these scenarios. Molecular dynamics simulations can provide a vast amount of data to researchers across the globe since producing and experimenting with these substances is prohibited and extremely dangerous. These data, piece by piece, can form a complete picture for understanding behavior, possible threats, and, of course, means of treatment and deactivation.

It is of vital importance and our greatest hope that the work in the present study, along with all the previous work on this matter, would be used for the benefit of humanity against any possible threats and for the development of accurate antidotes and countermeasures.

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Data Availability Statement: For all MD simulations, LAMMPS version 29-Sept-2021 Stable was used [28]. LAMMPS is open-source software distributed under the GNU General Public License Version 2. The procedure followed is described in detail in the section "Methodology: Simulation Details" in the present paper (Figure 1).

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