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THEORETICAL-CHEMICAL-QUANTUM ANALYSIS OF SARIN NEUROTOXICITY

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ABSTRACT

Sarin is a potent chemical weapon as a neurotoxic agent. Its dominant toxicity, ease of dispersion in the air and natural degradation allows rapid deployment by an attacking force. The objective of this very theoretical research was to find the molecular interactions of sarin vs. nine neurotransmitters (NT) that are most important for the functioning of the human nervous system. We use the hyperchem software to perform the quantum calculations, and we rely on the theory of the electron transfer coefficient to perform the calculations. We find that sarin oxidizes the nine NT investigated. For this reason, this neurotoxic it must be prohibited in all its uses. We conclude that the neurotoxic compound affects GABA, Noradrenaline, and Acetylcholine, mainly in that order.

KEYWORDS: Sarin, Neurotoxicity, Quantum Chemical.

INTRODUCTION

Sarin is a powerful chemical weapon as a neurotoxic agent.[1] This chemical compound was originally designed as an insecticide and then synthesized for military purposes. Its dominant toxicity, ease of dispersion in the air and natural degradation allows rapid deployment by an attacking force. Due to this rapid degradation, the attacking troop can enter the deployment area safely shortly after its launch.[2]

The conclusion of the Chemical Weapons Convention (CWC) in 1993 was aimed at putting an end to the threat of chemical weapons attacks. The treaty is almost universally accepted and led to the destruction of the world's most massive chemical arsenals, including countries such as Libya and Russia. However, the threats with chemical weapons have not disappeared. Residual chemical arsenals still exist in some countries. Chemical weapons have been demanded by nations at war or with threats of war. Many of these countries are widely suspected of maintaining essential arsenals of chemical weapons.[3]

MATERIAL AND METHOD

Software and parameterization

We use the hyperchem software to perform the quantum calculations, and we rely on the theory of the electron transfer coefficient to perform the calculations.[4]

Tables 1 and 2 show the parameterization of the calculations made.[5]

Table 1: Parameters used for quantum computing molecular orbitals-HUMO and LUMO.

Parameter	Value	Parameter	Value
Total charge	0	Polarizability	Not
Spin Multiplicity	1	Geometry Optimization Algorithm	Polak-Ribiere (Conjugate Gradient)
Spin Pairing	RHF	Termination condition RMS gradient of	0.1 Kcal/Amol
State Lowest Convergent Limit	0.01	Termination condition or	1000 maximum cycles
Interaction Limit	50	Termination condition or	In vacuo
Accelerate Convergence	Yes	Screen refresh period	1 cycle

Table 2: Parameters used to visualizing the map of the electrostatic potential of the molecules.

Parameter	Value	Parameter	Value
Molecular Property	Property Electrostatic Potential	Contour Grid increment	0.05
Representation	3D Mapped Isosurface	Mapped Function Options	Default
Isosurface Grid: Grid Mesh Size	Coarse	Transparency level	A criteria
Isosurface Grid: Grid Layout	Default	Isosurface Rendering: Total charge density contour value	0.015
Contour Grid: Starting Value	Default	Rendering Wire Mesh	

Quantum wells

We graph the results of the ETC calculations in quantum wells (figure 1). The dotted lines represent the pure substances that interact. The points represent the interactions of oxidation or molecular reduction because of electron transfer.

There are three probability zones. The high probability zone is shown in the background, below the last dotted line from top to bottom. The average probability zone is located between the two dotted lines. The low probability zone is located above the first dotted line. [4]

The substance to the left of the interaction is the substance that acts as a reducing agent. The substance to the right of the interaction is the substance that acts as an oxidizing agent. [6-11]

Left. Reducing agent. It is oxidized. It gives electronic cloud	A:B	Right. Oxidizing agent. It is reduced. It gets electron cloud

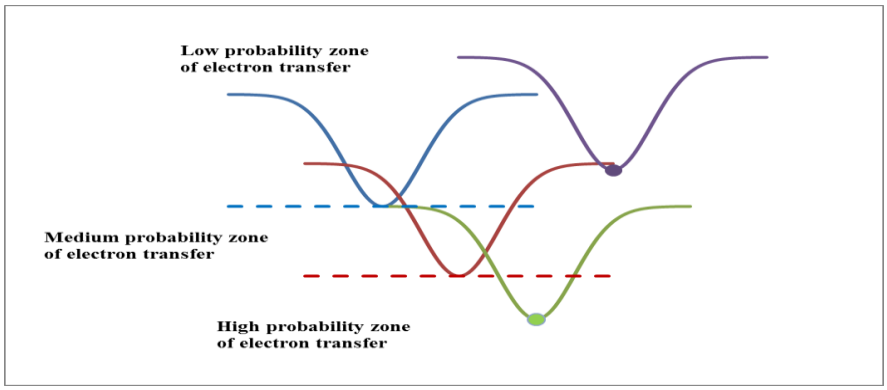

Figure 1: Graph of quantum wells. Electron transfer probability zones. The dotted lines represent the ETCs of the pure substances. The points represent the ETCs of the crossed bands between the pure substances.

RESULTS AND DISCUSSION

Table 3: NT and Sarin ETC of pure substances.

No.	Reducin agent	Ozidizin agent	HOMO	LUMO	BG	E-	E+	EP	ETC
1	***Sarin***	***Sarín***	***-10.666***	***0.464***	***11.130***	***0.032***	***0.149***	***0.117***	***95.128***
2	Acetylcholine	Acetylcholine	-9.242	1.034	10.276	-0.028	0.105	0.133	77.265
3	Noradrenaline	Noradrenaline	-9.152	-0.004	9.148	-0.083	-0.222	0.139	65.810
4	Glutamic Acid	Glutamic Acid	-10.145	0.506	10.651	-0.136	0.161	0.297	35.861
5	Glycine	Glycine	-9.853	0.874	10.727	-0.126	0.188	0.314	34.164
6	Histamine	Histamine	-9.191	0.675	9.866	-0.134	0.163	0.297	33.219
7	Gaba	Gaba	-9.562	0.939	10.500	-0.140	0.180	0.320	32.813
8	Dopamine	Dopamine	-8.868	0.199	9.067	-0.098	0.189	0.287	31.591
9	Serotonin	Serotonin	-8.948	-0.129	8.819	-0.145	0.141	0.286	30.836
10	Adrenalin	Adrenalin	-8.998	0.092	9.090	-0.117	0.198	0.315	28.858

Table 3: shows the interactions of all the pure substances involved in this research. It is observed that sarin has the highest ETC of all these substances. For this reason, we conclude that sarin is the most reactive substance of all. Because of these calculations, sarin can attack any of the nine NT.

Another critical observation is that adrenaline is the most stable substance of all due to the lower ETC in the whole table.

Table 4: NT and Sarin. ETC crossed band.

No.	Reducin agent	Ozidizin agent	HOMO	LUMO	BG	E-	E+	EP	ETC
1	Sarin	Acetylcholine	-10.666	1.034	11.700	0.032	0.105	0.073	160.273
2	Sarin	Serotonin	-10.666	-0.129	10.536	0.032	0.141	0.109	96.662
3	***Sarin***	***Sarin***	***-10.666***	***0.464***	***11.130***	***0.032***	***0.149***	***0.117***	***95.128***
4	Sarin	Glutamic Acid	-10.666	0.506	11.172	0.032	0.161	0.129	86.601
5	Sarin	Histamine	-10.666	0.675	11.341	0.032	0.163	0.131	86.573
6	Sarin	Gaba	-10.666	0.939	11.604	0.032	0.180	0.148	78.407
7	Sarin	Glycine	-10.666	0.874	11.540	0.032	0.188	0.156	73.975
8	Sarin	Dopamine	-10.666	0.199	10.864	0.032	0.189	0.157	69.201
9	Sarin	Adrenalin	-10.666	0.092	10.757	0.032	0.198	0.166	64.804
10**	Acetylcholine	Sarin	-9.242	0.464	9.706	-0.028	0.149	0.177	54.838
11***	Sarin	Noradrenaline	-10.666	-0.004	10.661	0.032	-0.222	0.254	41.974
12***	Noradrenaline	Sarin	-9.152	0.464	9.616	-0.083	0.149	0.232	41.449
13*	Dopamine	Sarin	-8.868	0.464	9.332	-0.098	0.149	0.247	37.782
14*	Glycine	Sarin	-9.853	0.464	10.317	-0.126	0.149	0.275	37.518
15*	Glutamic Acid	Sarin	-10.145	0.464	10.609	-0.136	0.149	0.285	37.225
16*	Adrenalin	Sarin	-8.998	0.464	9.463	-0.117	0.149	0.266	35.574
17*	Gaba	Sarin	-9.562	0.464	10.026	-0.140	0.149	0.289	34.692

**Substances strongly affected by sarin as an oxidizing agent. **Substance least affected by sarin as an oxidizing agent. ***Noradrenaline has a reversible oxide-reduction.*

Table 4: shows the interactions of crossed bands. As predicted in the calculations in Table 3 (pure substances), sarin oxidizes all the NT in question (crossed bands).

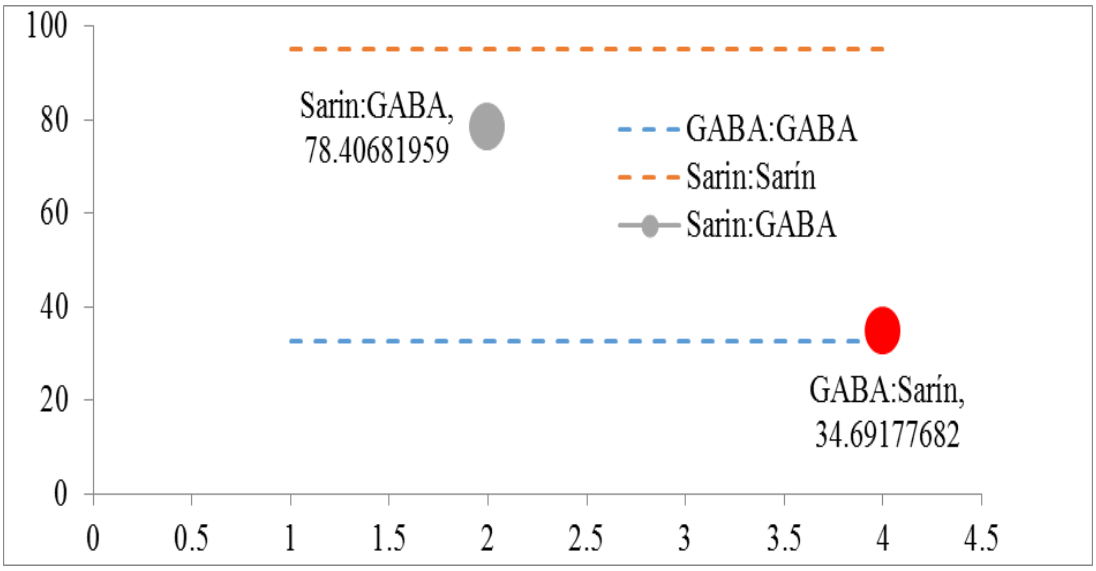

Figure 2: Representation of the extraction of crossed bands of GABA: Sarin and vice versa. The drawings of the wells were omitted.

It can also be observed that sarin attacks GABA more easily. This attack is most likely because the GABA: Sarin interaction has the lowest ETC of all (figure 2).

In this figure 2, we can see the two points that represent the crossed bands HOMO and LUMO. The red dot is located at the limit of the high probability zone and the medium probability zone. This interaction: GABA: Sarin competes with the GABA: GABA interaction. We conclude that sarin acts as an oxidizing agent of the pure substance GABA, destabilizing it.

The gray point represents the Sarin: GABA in the medium probability zone. We think that Sarin has a high probability of acting as an oxidizing agent of GABA that acts as a reducing agent of GABA.

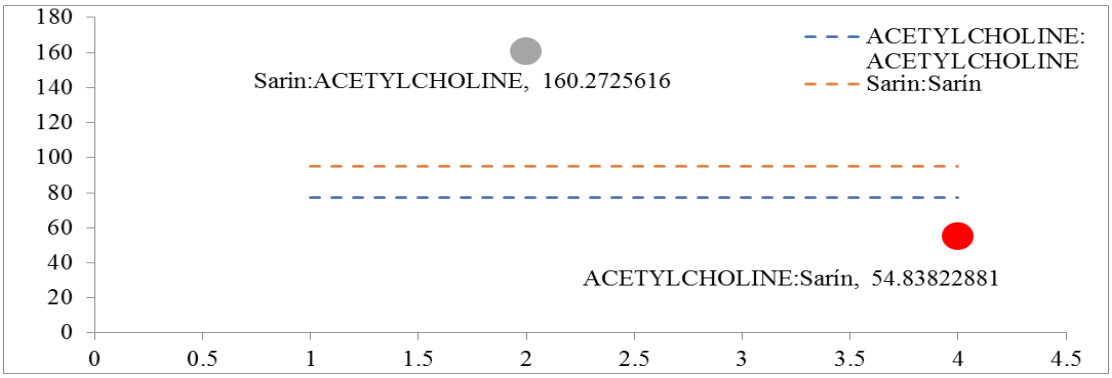

Figure 3: Quantum wells of the interaction Acetylcholine vs. Sarin and vice versa. Sarin oxidizes Acetylcholine very readily. It is observed that the Acetylcholine: sarin interaction falls in the very high probability zone of electron exchange.

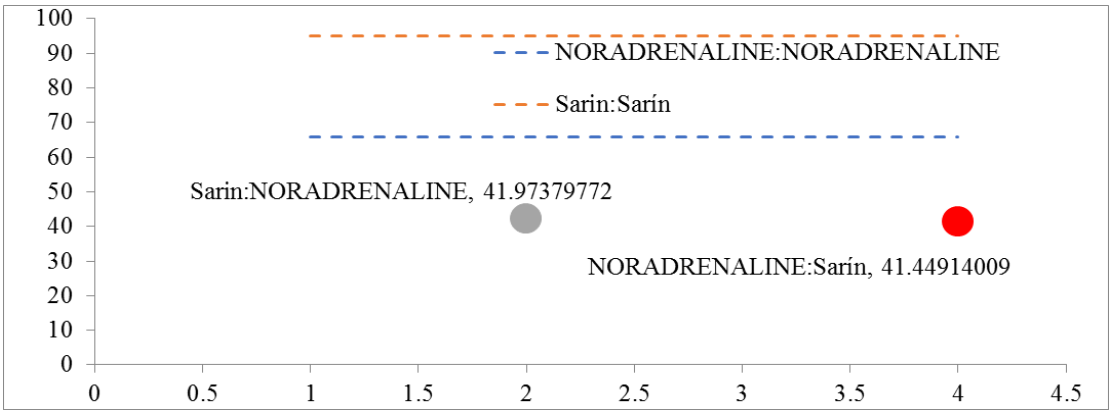

Figure 4: Quantum wells of the interaction Noradrenaline vs. Sarin and vice versa. The two interactions fall into the well of the high probability of electron exchange. It can see very delicate electron transfer equilibrium for every living thing.

Figures 3 and 4 show the quantum wells of the ETCs of Acetylcholine and Noradrenaline respectively. In these figures, it can see the red dots. In both cases the sarin with a very high probability of both compounds.

Table 5 shows the order of preferential attack of sarin. This order is related to the experimental data of the patients; but it is so fast, we cannot distinguish this order.

Table 5: NT and Sarin. ETC crossed band.

Activity	ETC	Interaction/SARIN
GABA is the most important NT inhibitor in the nervous system. It is distributed throughout the brain and spinal cord	34.69	Oxidizing (First)
NORADRENALINE acts in all regions of the brain as NT and functions as a hormone within the endocrine system.	41.45	Oxidizing (Second)
ACETYLCHOLINE has many functions: Motor control, autonomous central nervous system control, awareness and attention, pain perception.	54.83	Oxidizing (Third)

This neurotoxic compound must be banned for all use. Pacifists, scientists, ordinary people have already raised their voices.

CONCLUSIONS

We conclude that the neurotoxic compound sarin is fatal to all living beings.

1. It is an oxidizing agent for the nine NTs that we investigated.
2. The one that affects first because of a very low ETC is GABA.
3. Second, oxidize NORADRENALINE
4. Thirdly, it affects ACETILCOLINE.

Sarin gas attacks the NT directly, causing chaos in the body.

We will investigate in a future the interaction of that gas vs. amino acids and nitrogenous bases in DNA and RNA.

"All involved states and organizations should take urgent steps to ensure the protection of the most vulnerable victims of conflict, including victims of chemical weapons attacks in Syria, and to reinforce international law in the face of such serious violations". [12]

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