



A DFT Study of a Novel $C_{12}H_{12}Cl_{12}O_{12}$ Crystal as a Promising Anti-Virus

M Barhoumi*; M Said

Department of Physics, Faculty of Sciences of Monastir, Avenue de l'Environnement, 5019 Monastir, Tunisia

***Corresponding Author(s): M Barhoumi**

Laboratory of Condensed Matter and Nanosciences (LMCN), University of Monastir, Tunisia.

Tel: +21696812087; Email: med.ferrybn@gmail.com

Abstract

Coronaviruses (CoVs) such as α -CoVs, β -CoVs, and COVID-19 are a wide group of viruses that include viruses that can cause a group of disorders in humans, ranging from a common cold to severe acute respiratory syndrome. Given the difficulties the world is experiencing in the face of the Coronavirus, which has spread from China, everyone is trying to find an antibiotic and reduce its spread, but to the extent that there is no effective vaccine. Crystals have widely employed to increase medication properties. Using density functional theory, we investigate the structural properties of a novel crystal, i.e., $C_{12}H_{12}Cl_{12}O_{12}$ as a promising antibiotic to destroy Coronavirus. Using AIMD calculations, we show that this compound is dynamically stable. We believe that this new crystal can kill one of the membranes present in the COVID-19 in the first stage. This allows entering the rest of the crystal components and destroying the ribose of this pandemic as the second stage.

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Introduction

In the final months of 2019 [1,2], a deadly virus was discovered in Wuhan, Hubei Province, China. The World Health Organization (WHO) has called it the Coronavirus (COVID-19), due to the symptoms that appear in people with it. The virus might be bat origin [3], and the transmission of the virus might be linked to a seafood market [4,5]. The current reference name for the virus is severe acute respiratory syndrome Coronavirus 2 (SARS-CoV-2) [6,7]. Through deep studied, we have noticed that COVID-19 never reproduces outside the body (unlike the germs that reproduce outside the body). Nevertheless, it remains susceptible to infection. In order to proliferate, it must enter into

a cell (each virus loves a type of cell), and the COVID-19 is specialized in the cells of the lungs, so its only goal is to enter the cells of the lungs. Therefore, the first thing that comes through inhalation from the injured spray is and settles in the throat as a first station, here the body tries to prevent it from entering the respiratory system, and takes it to the digestive system to get rid of it in the stomach, but the virus tries to hold onto the throat which leads to a dry throat. Here we have to drink a lot of water and liquid to take the virus to the stomach and dispose of it. But this is not enough, especially for those with weak immunity, such as the elderly. Note that the COVID-19 driving the current



pandemic can survive on plastic and stainless steel surfaces for several days. Many types of research have been published examining the epidemiology, causes, clinical manifestation and diagnosis, and prevention and control of the novel CoVs (i.e., COVID-19). For instance, Prof. Yong-Zhen Zhang et al. [6] have studied the first genome of COVID-19, on 10 January 2020. Many studies give further insight into the person-to-person transmission [8-12]. Also, Sasmita et al. [13] have investigated the epidemiology, causes, clinical manifestation and diagnosis, prevention and control of coronavirus disease (COVID-19) during the early outbreak period. Koo et al. [14] have studied the interventions to mitigate early spread of SARS-CoV-2 in Singapore. COVID-19 has spread to several other countries around the world, e.g., European countries such as Italy, Germany, and Spain. Many of the dead and infected by this virus in Italy, the authorities concerned no longer want to count the dead, perhaps until at least a little morale remains for the Italian people. This pandemic has become worse also in Iran, thousands of dead, and large numbers infected. This virus brought terror and fear into people, e.g., in Tunisia, we witnessed a great fear among the general population, with the increasing number of infected and deaths. Furthermore, Thousands of dead and infected in the united states of america. However, since late June 2020, the number of deaths has decreased. A second wave of the virus is expected in the fall of 2020. This prompted us to think well about finding a counter to get out of this catastrophe and eradicate this pandemic. In fact, there are many antidotes to kill various types of CoVs such as $C_9H_{12}N_2O_6$ Uridine [15], $C_8H_{12}N_4O_5$ Ribavirin [16], 2,4,6-TRIS-[(3,3-DINITRO)-1-AZETIDINYL]-1,3,5-TRIAZINE ($C_{12}H_{12}N_{12}O_{12}$) [17], and other [17]. However, these antagonists did not result in eliminating this pandemic and could not reduce it. Therefore, it is urgent to develop and find new material to reduce the seriousness of this pandemic that afflicts mankind. In this present work, we study the structural properties of a novel material, i.e., $C_{12}H_{12}Cl_{12}O_{12}$ crystal, which can kill the COVID-19. We think that the presence of Cl atom in this compound can destroy the COVID-19 membranes. The present paper is organized as follows: In Sec. 2 we present our computational details. We discuss our results in Sec. 3, and we conclude in Sec. 4.

Methods

We have performed Density Functional Theory (DFT) [18] calculations with the Projector-Augmented Wave (PAW) [19] scheme as implemented in the Vienna Ab-initio Simulation Package (VASP) [20] code. Exchange and correlation were approximated using the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) [21] with a plane wave cutoff of 500 eV and a 12 12 12 k-point mesh for structures. The atomic positions were relaxed until the change in total energy was less than 10^{-6} eV and the force on each atom less than 5×10^{-3} eV/Å.

Results

The goal of the virus is to enter a cell to multiply in it because the virus is not a living being, because it lacks two elements of life. As mentioned in Refs. [22,23], CoV does not consist of cells, but it is DNA and RNA covered with a protein membrane. Indeed, the coronaviral genome encodes four major structural proteins: The spike (S) protein, nucleocapsid (N) protein, membrane (M) protein, and the envelope (E) protein, all of which are required to offer a structurally complete viral particle [24]. Besides, RNA is a linear polymer made up of a sequence of nucleotides. Each nucleotide contains a phosphate group, a sugar (ribose) and a nucleic base, or a nitrogenous base. Note that the

main part of the RNA is ribose. To eradicate this pandemic, it is necessary to kill the ribose, which is the primary nucleus in it. Otherwise, this virus will return to life because it can with great ability to recover its current components in a form it manages.

In Figure 1, we show the ribose part, which is present in all virus, e.g., Coronaviruses, which are enveloped viruses with a positive sense, single-stranded RNA genome. We also see the ribose formula is very strong. The bond between the atoms of this body is very strong, especially between carbon (C) and hydrogen (H) atoms, but this body can be destroyed. Note that CoVs have the largest genomes for RNA viruses (where the genome sizes ranging from 26 to 32 kilobases (kb) in length) [25]. The eradicate the CoV requires two stages, the first is the destruction of the virus membrane, which is a protein, which allows antidote to enter for destroying the ribose as the second stage. And thus the virus is completely eradicated. Before using our suggestion, we advise employing the $C_{12}H_{12}N_{12}O_{12}$ crystal as a first stage. Note that the $C_{12}H_{12}N_{12}O_{12}$ crystal is a fragment of the family of composites known as pyrimidine nucleosides. In this direction, we show the geometric structure of this compound in different directions in Figure 2. As mentioned before in Ref. [15], the $C_{12}H_{12}N_{12}O_{12}$ crystal contains by two molecules in the asymmetric unit. The carbon atoms are shown in brown, the nitrogen atoms in gray, the oxygen atoms in red, and the hydrogen atoms in pink. Our GGA calculations show that the structure has not changed before and after relaxation. We found that the nitrogen (N) atoms interact well with carbon and hydrogen atoms, which make up a protein (O=C-N-H) later with oxygen (O) atoms. At the edge of the $C_{12}H_{12}N_{12}O_{12}$ structure, there are only the oxygen atoms. Thus, when using this crystal, the O atoms, that will first interact with the virus membranes (i.e, S-protein, N-protein, M-protein, and the E-protein). Here, we assume that the oxygen atoms are not able to interact positively with the virus membrane (consisting of protein) because they made of protein with other atoms in the crystal. Thus this structure will serve as food for the COVID-19 membranes. Because of the ineffectiveness of the $C_{12}H_{12}N_{12}O_{12}$ crystal. We suggested changing nitrogen atoms with chlorine (Cl) atoms to get rid of the protein present in the previous structure. The geometric structure of $C_{12}H_{12}Cl_{12}O_{12}$ crystal in different directions is illustrated in Figure 3, which their structure belong to the monoclinic space group $P2_1$. Note that the carbon atoms are shown in brown, the chlorine atoms in green, the oxygen atoms in red, and the hydrogen atoms in pink. Upon relaxation by GGA-PBE functional, the C-C, Cl-H, O-H, C-O, and Cl-C bond lengths of $C_{12}H_{12}Cl_{12}O_{12}$ are 1.52, 1.35, 1.37, 1.22, and 2.52 Å. Furthermore, the Cl-C-O, C-C-O, and Cl-H-O bond angles are 106.44, 111.45, and 180. After relaxation, we found that the chlorine atoms destroyed the basic structure, at the same time creating a new crystal (As seen in Figure 3). In this structure, we see that some of the Cl atoms interact perfectly with a strong bond with the H atoms surrounding the Cl-C-O-H bond length, which is what we want. We think that the ClH molecules in the vicinity of the Cl-C-O-H structure will interact with the protein on the surface of the Coronavirus. The ClH molecule will attracts with the protein (S, M, and E) atoms. Upon reaction, the ClH molecules will attract the virus protein to the top and thus get rid of it. If the mist succeeds in opening the membrane, which we believe will happen. The crystal will fully enter at the virus and will also destroy the ribose for this epidemic. As Ribavirin, the $C_{12}H_{12}Cl_{12}O_{12}$ crystal is a water-soluble broad-spectrum antiviral. We have also performed ab-initio molecular dynamics calculations (AIMD) using time steps of 10^{-15} seconds at a temperature of 300 K to further

confirm the stability of this crystal, i.e., $C_{12}H_{12}Cl_{12}O_{12}$. In these calculations, we have used a 3 X 3 X 3 supercell to permit mutilation which isn't conceivable in the crude cell. After calculations, we obtained the geometry is not destroyed, confirming the dynamical stability of this compound.

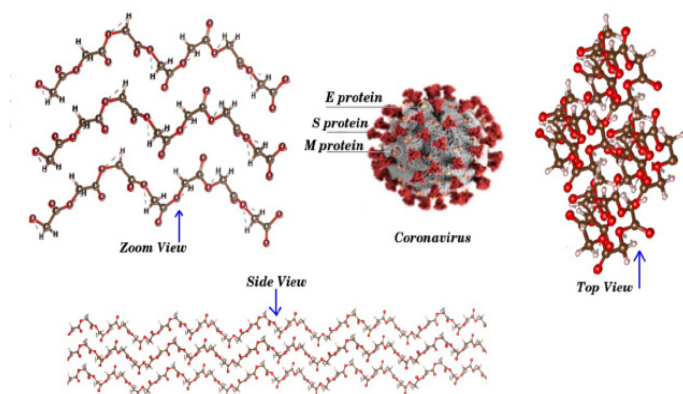


Figure 1: Top and side views of ribose. The carbon atoms are shown in brown, the oxygen atoms in red, and the hydrogen atoms in pink.

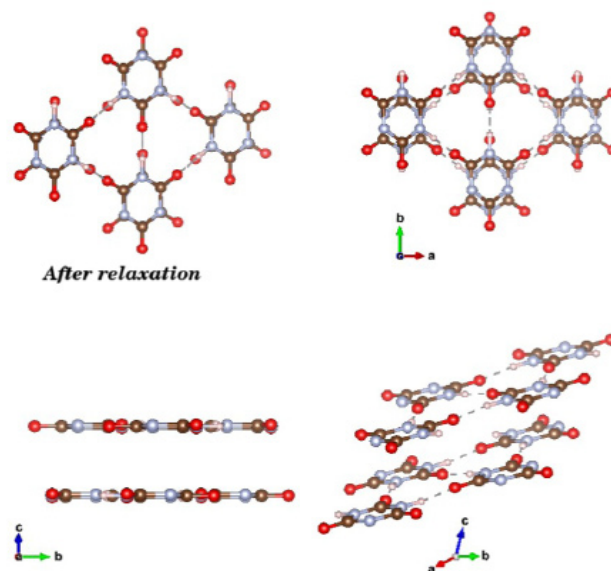


Figure 2: The geometric structure of the $C_{12}H_{12}N_{12}O_{12}$ crystal in different directions.

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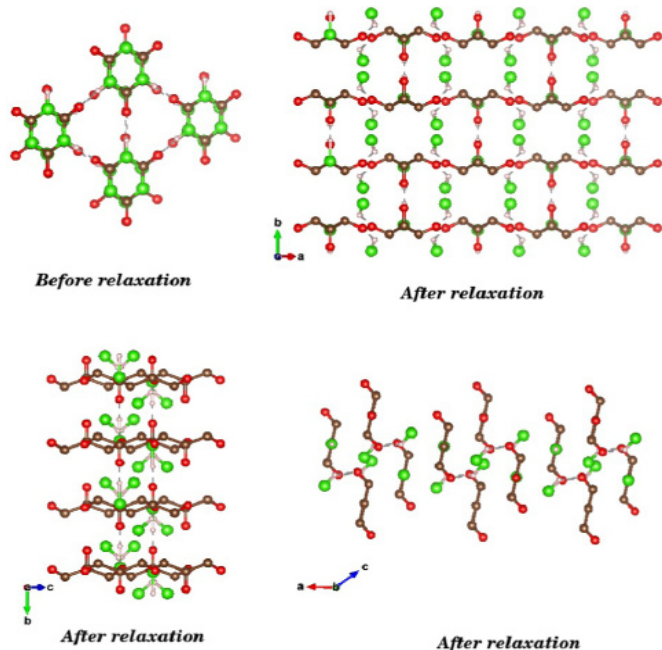


Figure 3: The geometric structure of the $C_{12}H_{12}Cl_{12}O_{12}$ crystal in different directions before and after relaxation.

Conclusion

In summary, we suggested a novel crystal, which is $C_{12}H_{12}Cl_{12}O_{12}$, to destroy the COVID-2019, since the crystals have widely employed to increase medication properties. We have studied their structural properties, using GGA functional. We have shown that this compound is dynamically stable. We believe that this crystal is a water-soluble broad-spectrum antiviral. We hope that researchers can make this crystal despite its difficulty and thus try it on clinical cases. We also hope that this antagonist will succeed in order to reduce the risk of this virus, which seeks to destroy the world. Everyone should be careful because the virus enters by inhalation or mouth and stops at the throat. Where the body is trying to take it to the digestive system. While the virus tries to stick to the throat and cause a drought. Which requires drinking warm water frequently because it helps the body.

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