On a possibility for analysis of the COVID-19 proteins by BSM-SG atomic models with a purpose of modification by proper drugs

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Abstract

The BSM-SG models of the atoms could be useful in understanding the COVID-19 and other viruses with the purpose of modification of the proteins involved in channel activity. The BSM-SG models are different from the quantum mechanical models while possessing a few advantages. Amongst them are the possibility to operate with real physical dimensions in the sub-nanometric scale, the visualization of directions of the chemical bonds in molecules, the magnetic field interactions between the orbiting electrons, and the nuclear magnetic moments. These features provide a new opportunity for analysis and modeling of simple and complex molecules. In proteins with the known shape, they will permit an understanding of underlined physics behind their complex three-dimensional shape and its stability. This could permit modification of their shape and properties by using proper chemical compounds as drugs.

Keywords: COVID-19, E-proteins, aminoacides, BSM-SG atomic models

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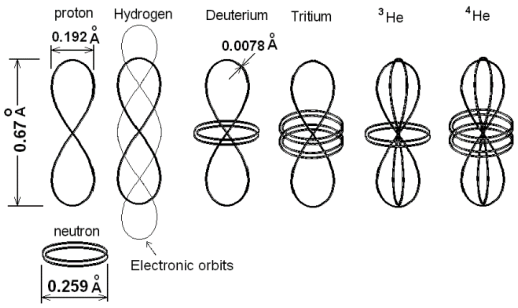

Fig. 1. First few atoms from the Periodic Table.

In the far-field, the Coulomb fields from protons are detected as a point source, but in the near field, they follow the shape of protons and neutrons, so they define the trajectories of the orbiting electrons. The near Coulomb field of the first atoms of Periodic table is illustrated in Fig. 2.

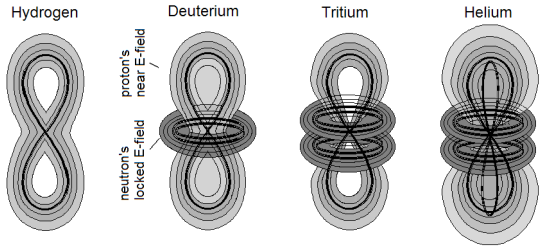

Fig. 2. Coulomb field near the nucleus

The derived nuclear structures of stable elements up to the number z = 102 are are given in the Atlas of Atomic Nuclear structures (ANS) included in the BSM-SG treatise and published separately or as appendices in other books [1,2,3,13]. In the Atlas of ANS the protons and neutrons forming the nuclear structures are shown by simplified symbols. From them, the projection views of the atomic nuclei are easily created. This is illustrated in Fig. 3 for some selected atoms.

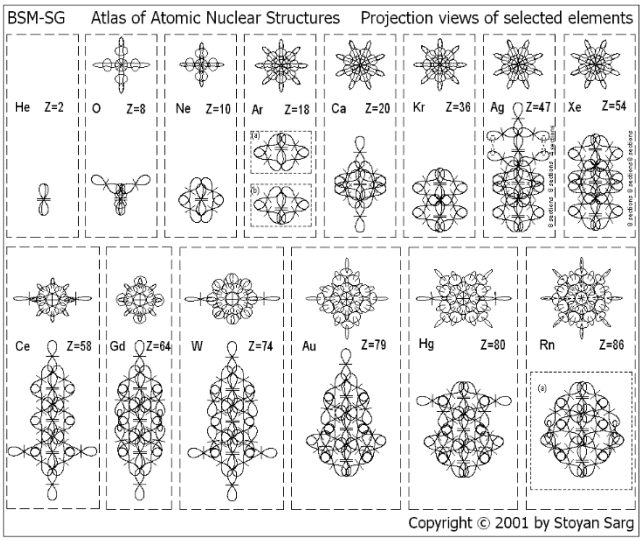

Fig. 3 Projection views of some selected atoms

1. On a possibility for analysis of some proteins in COVID-19.

For many viruses, channel proteins are essential [14]. The known channel proteins are reported to be about 100 amino acids in length. By its channel activity, the E protein interacts with host proteins of the cell and helps the S-protein spike to latch onto human cells [15]. The coronaviral genome encodes four major structural proteins: the spike (S) protein, nucleocapsid (N) protein, membrane (M) protein, and the envelope (E) protein [15]. E-protein is the smallest one. According to U.S. researchers [15,16], the spikes of E-proteins of COVID-19 are 10 to 20 times more likely to bind to human cells than the spikes from the 2002 SARS coronavirus. E-protein likely plays an essential role. This is said to make COVID-19 spread more easily from person-to-person than the earlier virus. The shape of the COVID-19 is illustrated in Fig. 4 [15]. (The illustration is provided by the Centers for Disease Control and Prevention (CDC) in January 2020 shows the 2019 Novel Coronavirus (2019-nCoV), (CDC via AP, File)). The structures of the E-proteins is shown in Fig. 5. [17].

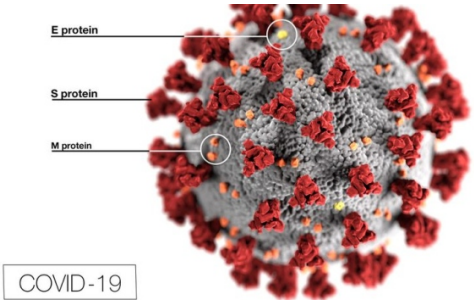

Fig. 4. Shape of COVID-19 (public domain) [15]

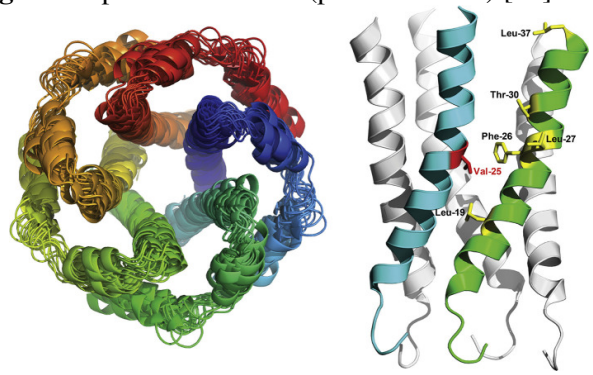

Fig. 5. Three-dimensional shape of the E-protein [17] (in public domain also)

2. Analysis of nanostructures and molecules using the BSM-SG atomic models.

Using the BSM-SG atomic models, the directions of chemical bonds of the elements are easily identifiable for molecules with known shapes. Fig. 6 illustrates the shape of some simple molecules. The calculations of chemical bond length of simple molecules are given in Chapter 9, Molecules of BSM-SG, section 9.15.2 Eq. (9.56).

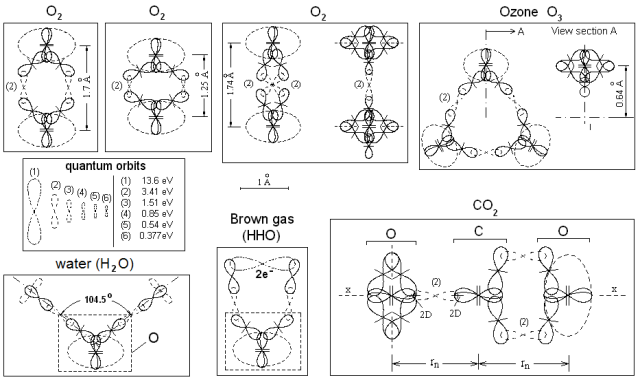

Fig. 6. Shape of some simple molecules

The BSM-SG models permit the visualizing of the magnetic fields in atoms and molecules. The energy eigenvalues of hydrogen, for example, (one-electron atom) are strongly determined by

the principal quantum number, ***n***, and less by the angular momentum, ***l***. For many-electron atoms, however, some energy levels depend stronger on ***l***, than on, ***n***. This is illustrated for the beryllium atom, shown in Fig. 7, where the magnetic field lines created by orbiting electrons are shown.

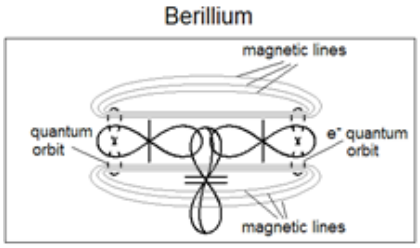

Fig. 7. Berillium atom showing the position of electronic orbits and created magnetic fields

The magnetic interactions between orbiting electrons play an important role in molecular stability. Fig. 8 shows the structure of the ozone molecule with the position of the magnetic fields created by the three chemical bonds.

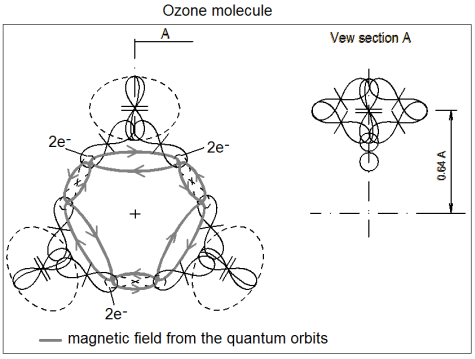

Fig. 8. Structure of the ozone molecule with the position of the magnetic fields created by the three chemical bonds.

There are many confirmations on the reality of the BSM-SG atomic models. Fig 9.a. shows the TEAM microscope image of a single carbon sheet (from a public domain), while fig. 9.b. shows the same image with a properly adjusted gamma correction of the display [18].

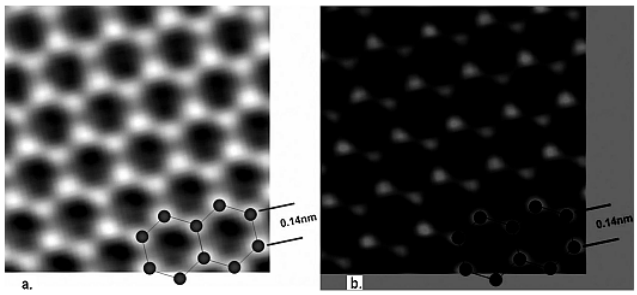

Fig. 9 a. original image, **b.** gamma correction adjusted

It is evident from the gamma-corrected image that every neighboring atom exhibits a slightly different brightness. The bright spots according to BSM-SG models are from the electrons involved in the bonds between the atoms in the graphene sheet. Fig. 10.c shows the graphene structure by the BSM-SG atomic models. The two pairs P1 and P2 in Fig. 10.b define the valence directions. They are mutually perpendicular according to BSM-SG models.

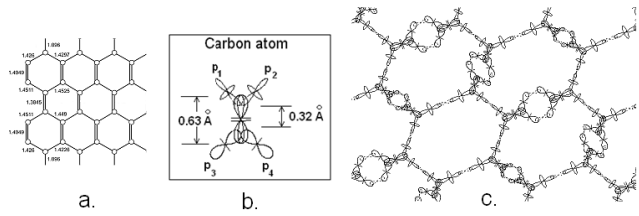

Fig. 10. Graphene structure: a. - by structural chemistry, b. - a single carbon atom with two pairs of bonds in perpendicular planes, c. - a graphene structure by BSM-SG atomic models

It is apparent from the electron microscope image of a carbon nanotube shown in Fig. 11 that the alignment of neighboring carbon atoms is not parallel to the nanotube axis. Instead, they are aligned in helixes with a large pitch. This indicates that the two pairs of valence bonds of a carbon nanotube shown in Fig. 10.b are not exactly mutual perpendicular but slightly deviate tom 90 degrees. The reason for this is that the proton shape is a twisted torus, as illustrated in Fig. 1.

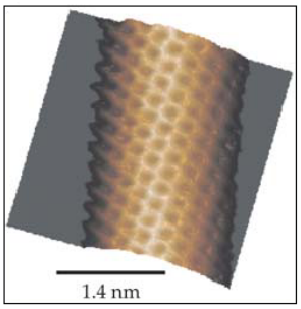

Fig. 11. The helical arrangement of the carbon atoms is an indication of the twisted shape of the protons.

The twisted shape of the protons causes twisting of the atomic nuclei of all elements. This feature plays a role in the Broglie wavelength.

The BSM-SG atomic models could provide 3-D configuration for any chemical compounds from simple non-organic to complex organic molecules and amino acids. The 3-D shape of a simple molecule as the aspirin, known by the PDB model, is shown in Fig. 12. Fig. 13 shows the same molecule by the BSM-SG atomic models.

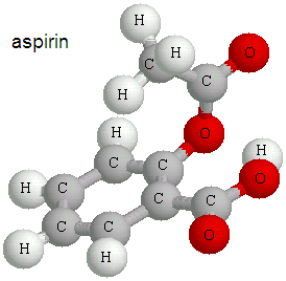

Fig. 12. Three-dimensional structure of the aspirin molecule (PDB file aspirin visualized by Chime software)

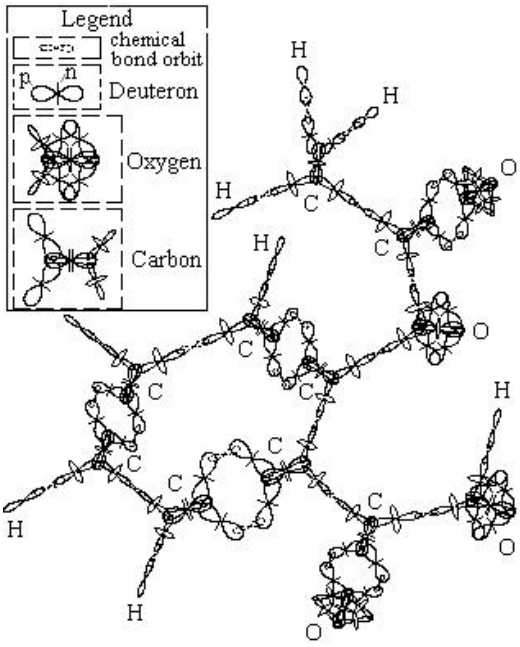

Fig. 13. Three-dimensional structure of aspirin using the BSM-SG atomic models. Electronic orbits of chemical bonds are shown by dashed lines

Multiple examples of using BSM-SG models show quite a good match of the distance between atoms with the known internuclear distances of chemical compounds. The conclusion is that the 3-dimensional shape of the proteins is also defined by the angular restrictions of the chemical bonds and the orientation of the nuclear magnetic moments of the atoms [15]. Firstly, the BSM-SG models define the 3-dimensional shapes of the amino acids. The nuclear magnetic moment has a longer range than the chemical bonds and consequently, it is important for the complex shapes of the proteins. Fig. 14. shows the configuration of the weak H-bond in a section of a DNA molecule.

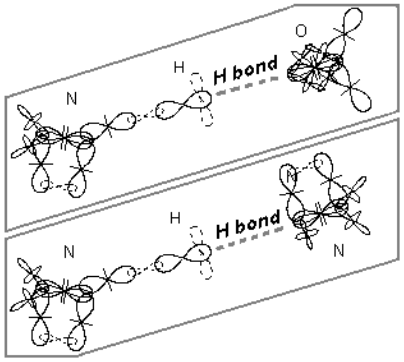

Fig. 14. Two types of hydrogen bonds, denoted by straight dashed lines. Electronic orbits involved in the magnetic interactions are curves shown by dashed lines

By using the BSM-SG models one additional feature of the ring atomic structure is unveiled. A particular same exciting energy may rotate indefinitely in the ring structure without emitting photons until some external disturbance takes place. This is a kind of energy storage mechanism at the quantum mechanical level [21]. There is an enormous number of atomic ring structures in proteins and DNA that may exhibit this feature. Fig, 15 shows the positions of such structures in the DNA strand, while fig. 16 shows a single ring structure by BSM-SG atomic models.

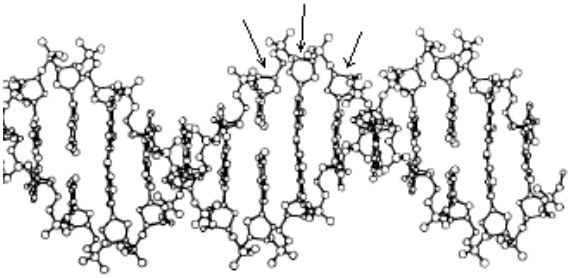

Fig. 15. Part of DNA structure showing the positions of some (O+4C) atomic rings

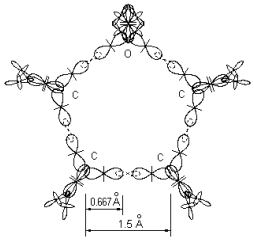

Fig. 16. Atomic ring structure from the deoxyribose molecule involved in DNA strand

Despite that these rings are formed of not the same atoms as in the aspirin, some common energy levels are possible to participate in the energy storage mechanism.

The BSM-SG models could be applied for all amino acids that build the proteins. Their configuration is well known and shown in Fig. 17. Using the Chime software, firstly the PDB model of the particular amino acid could be used to obtain its three-dimensional shape, like in the case of aspirin illustrated in Fig. 12. Then using the Atlas ANS the underlying high-resolution graphics model could be obtained like in Fig 13 for aspirin. According to the author, the complex shape of the proteins is supported by the following features of the BSM-SG atomic models: (a) the angular freedom of the interatomic bonds; (b) the nuclear magnetic state of the atoms; (c) the atomic rings embedded in the protein as a source of energy, and (d) the weak H-bonds. The twisting shape of atomic nuclei and the long-range of the nuclear magnetic spins might define the helical shape sections of the proteins. Such shape is widely persistent in many proteins, as illustrated by the shape of E-protein, shown in Fig. 5. The importance of nuclear magnetic spin is in good agreement with the study of the protein dynamics by a method based on a nuclear magnetic resonance [20]. Additional details on the usefulness of using BSM-SG models for the analysis of biomolecules are described in [12].

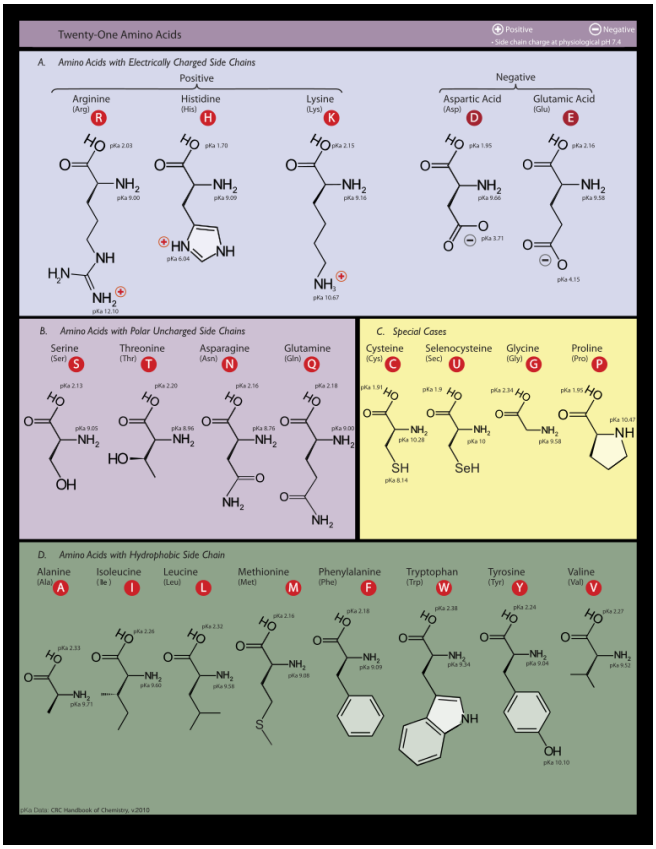

Fig. 17. Structural composition of all 21 amino acides (public domain) [22].

3. Conclusions

The E-protein of SARS-CoV according to [15] contains 76 amino acids. The number of atoms in the amino acids is well known. Using the BSM-SG models the known 3-D shape of this E-protein

could be obtained with sub-nanometric resolution and the weak sections could be identified. They could be attacked by a properly selected chemical compound that has a known 3-D shape. Even partial modification of the E-protein 3-D shape might decrease its ability for forming an intrusive ion channel into the cells.

The BSM-SG theory and the atlas of Atomic Nuclear Structures for atomic z-numbers from 1 to 102 are initially archived in the National Library of Canada [1,2] and published in books [3,13].

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