STUDYING THE STRUCTURE OF THE IRON BISALANINATE (Fe2+) MOLECULES USING THE GAUSSIAN 09W SOFTWARE PACKAGE

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Annotation: *The article provides information on the structure of the iron bisalaninate molecule, a chelate complex compound used in the prevention and treatment of iron deficiency anemia.*

Keywords: *Iron bisalaninate, chelate complexes, iron deficiency anemia (IDA), Gaussian 09W software package, dipole moment, total energy, atomic charge.*

Iron is one of the trace elements of the human body, which is in very small quantities, approximately 3-5 g, despite this, it plays a very significant role in the human body. It participates in many redox reactions, ensures the transport of oxygen and carbon dioxide in human cells, tissues and organs, as well as in maintaining the secondary and tertiary structure of DNA and RNA. Iron deficiency in the human body leads to a decrease in the concentration of hemoglobin in the blood, resulting in iron deficiency anemia that occurs with a variety of clinical indications in patients, such as general weakness, fatigue, dizziness, brittle nails, tachycardia and much more [1].

In modern medicine, for the prevention and treatment of IDA, a wide variety of drugs containing iron compounds, such as sulfate, iron chlorides with the addition of vitamins and excipients, are used for absorption by the body. However, they have many different side effects affecting primarily the gastrointestinal tract. [2].

Taking the above into account, scientists proposed a new iron compound bisalaninate. Iron Bisalanin is a chelate complex compound consisting of two molecules of the amino acid alanine and ferrous iron bound like a claw with alanine. This compound has the advantage of being almost completely absorbed from the intestine, as it is a familiar substance to the human body. During the decomposition of which, substances toxic to the human body are not formed. Therefore, chelate complex compounds differ from other iron compounds in the highest bioavailability and non-toxicity. [3].

To study the structure and explain such amazing properties of iron bisalaninate, we carried out quantum-chemical calculations of this molecule using the Gaussian 09W software package. [4].
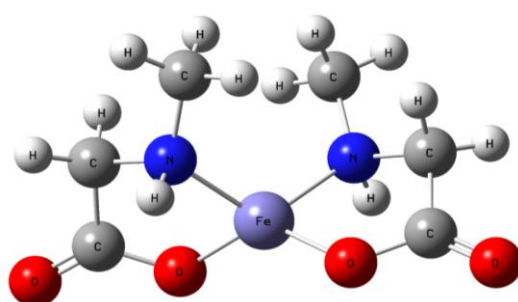
At the same time, we calculated the total energy of the molecule equal to -1900.45068297. Dipole moment = 9.4883, bond lengths between atoms, and atomic charge distribution:

№	Atoms	Charge of atoms	№	Atoms	Charge of atoms
1	Fe	0.689	14	H1	0.356
2	N1	-0.693	15	H2	0.229
3	N2	-0.693	16	H3	0.252
4	O1	-0.480	17	H4	0.215
5	O2	-0.604	18	H5	0.231
6	O3	-0.604	19	H6	0.249
7	O4	-0.480	20	H7	0.249
8	C1	0.679	21	H8	0.231
9	C2	-0.350	22	H9	0.215
10	C3	-0.428	23	H10	0.252
11	C4	-0.428	24	H11	0.229
12	C5	-0.350	25	H12	0.356
13	C6	0.679			

From the table below, one can see that the nitrogen and oxygen atoms are negatively charged, respectively, which is explained by the high electronegativity of these atoms relative to others. Iron, connected on four sides by nitrogen and oxygen atoms, is positively charged, since it gives up its electrons to these elements. Sharp differences in the charges between these atoms make it clear that the bond between them will be very strong, which will prevent this compound from decomposing in the stomach and further moving it into the intestine, which will further increase its beneficial properties in anemia. Since, in comparison with other iron compounds, this increases its absorption by the body in the right place and reduces the toxicity of iron remaining in the walls of the stomach.

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