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КВАНТОВО-ХИМИЧЕСКОЕ МОДЕЛИРОВАНИЕ ВЗАИМОДЕЙСТВИЯ АМИНОКИСЛОТ С КАРБОНАТОМ КАЛЬЦИЯ

QUANTUM-CHEMICAL SIMULATION OF THE INTERACTION OF AMINO ACIDS WITH CALCIUM CARBONATE

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Аннотация

В данной статье представлены результаты квантово-химического моделирования процесса взаимодействия аниона CO_3^{2-} с рядом протеиногенных аминокислот для выявления наиболее энергетически выгодной системы и дальнейшего сравнения с результатами лабораторного эксперимента. В результате анализа данных установлено, что все возможные взаимодействия являются оптимальными, так как обладают высокой разницей полной энергии системы, а также высоким значением химической жёсткости. Установлено, что наиболее оптимальными взаимодействиями являются взаимодействия CO_3^{2-}-аспарагин и CO_3^{2-}-серин, что обусловлено наибольшей разницей энергии системы относительно модели аминокислоты ($\Delta E = 262{,}907 \pm 0{,}088$ ккал/моль) и наибольшем значении химической стабильности ($\eta = 0{,}218$ эВ).

Ключевые слова: карбонат–анион, химическая жёсткость, квантово-химическое моделирование, аспарагин, серин

Abstract

This article presents the results of quantum chemical modeling of the interaction of the CO32-anion with a number of proteinogenic amino acids to identify the most energetically advantageous system and further compare with the results of a laboratory experiment. As a result of data analysis, it was found that all possible interactions are optimal, since they have a high difference in the total energy of the system, as well as a high value of chemical rigidity. It was found that the most optimal interactions are the interactions of CO32-asparagine and CO32-serine, which is due to the largest difference in the energy of the system relative to the amino acid model ($\Delta E = 262.907 \pm 0.088$ kcal/mol) and the highest value of chemical stability ($n = 0.218$ eV).

Key words: carbonate anion, chemical hardness, quantum chemical modeling, asparagine, serine

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Introduction

Calcium carbonate is one of the most common biominerals and, therefore, is of considerable interest in many fields of science, including medicine, as targeted drug delivery systems are increasingly being used. There are three polymorphic structures of calcium carbonate – calcite with rhombohedral symmetry, aragonite with orthorhombic symmetry, and vaterite with hexagonal symmetry.

Porous vaterite is used as a carrier in delivery systems for biologically active and medicinal compounds. In water or saline, vaterite undergoes morphological transformations. At medium temperatures, porous vaterite turns into calcite (a more thermodynamically stable structure), and at elevated temperatures (above 37-40 $^{\circ}C$) - into aragonite. Since these polymorphs are not porous, recrystallization is accompanied by the release of drugs encapsulated in vaterite [1–3].

Materials and methods

Amino acids are the main building blocks of the muscle protein structure of a living organism. More than 300 amino acids have been described in nature, only twenty of which are commonly found in human peptides. Of the twenty encoded by human DNA, ten are considered important because human metabolic pathways are insufficient to synthesize them at an adequate rate from other foods [4]. Amino acids are also used to obtain various nanomaterials [5, 6]

The main list of twenty proteinogenic amino acids can be divided into two main subgroups - essential amino acids and non-essential amino acids. An amino acid is considered essential if it cannot be synthesized by a living organism from materials normally available to cells at a rate commensurate with the needs of normal growth. There are 8 essential amino acids in the human body: isoleucine (*Ile*), leucine (*Leu*), lysine (*Lys*), methionine (*Met*), phenylalamine (*Phe*), threonine (*Thr*), tryptophan (*Trp*), valine (*Val*); and 12 non-essential amino acids: alanine (*Ala*), proline (*Pro*), glycine (*Gly*), serine (*Ser*), cysteine (*Cys*), glutamine (*Gln*), asparagine (*Asn*), glutamic acid (*Glu*), aspartic acid (*Asp*), arginine (*Arg*), histidine (*His*), tyrosine (*Tyr*) [7, 8].

Essential amino acids are amino acids that humans and other vertebrates cannot synthesize from metabolic intermediates. These amino acids must come from exogenous food, as the human body lacks the metabolic pathways necessary for the synthesis of these amino acids. Essential amino acids are necessary for the physical and mental well-being of the body, they are responsible for the amino acid stimulation of muscle protein synthesis. A complete protein, by definition, contains all the essential amino acids and is usually obtained from animal sources of nutrition, with the exception of soy. The supply of essential amino acids to the body is also available from incomplete proteins, which are usually products of plant origin [9–14].

Thus, based on the inability to independently produce and the difficult process of the entry of essential amino acids into the body, with the help of calcium carbonate, it is possible to carry out the process of targeted delivery of the necessary amino acids throughout the body. But before proceeding directly to the transportation process, you first need to make sure that these components are able to interact, and which of the communication systems will be the most beneficial. The calculation of molecular properties provides an important link to experiment. Computer quantum-chemical modeling makes it possible to calculate large-scale molecular systems, providing a visual analysis of the physico-chemical properties, in particular, and the determination of the most energetically favorable $CaCO_3$ interaction system with an amino acid.

Quantum-chemical modeling was carried out in the *IQmol* molecular editor using the *Q-Chem* software on the equipment of the *Schneider Electric* data processing center of the North Cau-

casus Federal University. Quantum-chemical calculations were performed with the following parameters:*Energy*,method:*HF*, basis: *6-31G* , *convergence* – 4, force field – *Ghemical* [15–18]. At the first stage, quantum-chemical modeling of individual amino acids was carried out. After that, the interaction of the calcium carbonate silicate anion with amino acids through the amino groups present in amino acids was considered.

To determine the most energetically favorable system of interaction CO_3^{2-}-amino acid in the process of modeling, the total energy of the system (E), the energy of the highest occupied molecular orbital (*HOMO*), the energy of the lowest free molecular orbital (*LUMO*), the energy difference between the amino acid and the interaction system (ΔE), chemical rigidity (η) [19, 20].

A complete list of proteinogenic amino acids was taken as amino acids: alanine (*Ala*), valine (*Val*), leucine (*Leu*), isoleucine (*Ile*), methionine (*Met*), proline (*Pro*), glycine (*Gly*), serine (*Ser*), threonine (*Thr*), cysteine (*Cys*), glutamine (*Gln*), asparagine (*Asn*), glutamic acid (*Gly*), aspartic acid (*Asp*), lysine (*Lys*), arginine (*Arg*), histidine (*His*), phenylalamine (*Phe*) , tyrosine (*Tyr*), tryptophan (*Trp*).

Results and discussions

The results of quantum-chemical modeling are presented in Table 1.

Table 1 - Results of computer quantum-chemical modeling

Amino acid	Interaction CO_3^{2-}-amino acid	E , kcal/mol	ΔE _	*HOMO* , eV	*LUMO* , eV	η , eV
Alanine	-	-323.545	-	-0.250	0.016	0.133
	Through the amino group of an amino acid	-584.742	261.197	-0.284	0.141	0.213
Valine	-	-402.112	-	-0.249	0.016	0.133
	Through the amino group of an amino acid	-662.834	260.722	-0.287	0.119	0.203
Leucine	-	-441.397	-	-0.260	0.006	0.133
	Through the amino group of an amino acid	-701.843	260.446	-0.282	0.146	0.214
Isoleucine	-	-441.394	-	-0.247	0.018	0.133
	Through the amino group of an amino acid	-701.689	260.295	-0.245	0.102	0.174
Methionine	-	-800.251	-	-0.232	0.006	0.119
	Through the amino group of an amino acid	-1060.301	260.050	-0.295	0.130	0.213
Proline	-	-400.906	-	-0.246	0.008	0.127
	Through the amino group of an amino acid	-661.205	260.299	-0.122	0.135	0.129
Glycine	-	-284.252	-	-0.259	0.004	0.132
	Through the amino group of an amino acid	- 545,771	261.519	-0.288	0.144	0.216
Serene	-	-398.725	-	-0.262	0.009	0.136
	Through the amino group of an amino acid	-659.624	260.899	-0.294	0.142	0.218
Threonine	-	-438.015	-	-0.248	0.006	0.127
	Through the amino group of an amino acid	-698.355	260.340	-0.202	0.122	0.162
Cysteine	-	-721.585	-	-0.254	-0.003	0.126
	Through the amino group of an amino acid	-982.265	260.680	-0.293	0.115	0.204
Glutamine	-	- 531.217	-	-0.205	-0.055	0.075
	Through the amino group of an amino acid	-791.231	260.014	-0.203	0.122	0.163
	Through the amino group in the radical	-791.393	260.176	-0.274	0.103	0.189

Asparagine	-	-489.393	-	-0.401	0.138	0.270
	Through the amino group of an amino acid	-752.212	262.819	-0.208	0.132	0.170
	Through the amino group in the radical	-752.388	262.995	-0.267	0.097	0.182
Glutamic acid	-	-551.075	-	-0.216	-0.067	0.075
	Through the amino group of an amino acid	-811.330	260.255	-0.300	0.134	0.217
Aspartic acid	-	-512.032	-	-0.263	-0.008	0.128
	Through the amino group of an amino acid	-772.307	260.275	-0.301	0.119	0.210
Lysine	-	-496.481	-	-0.177	-0.024	0.077
	Through the amino group of an amino acid	-756.541	260.060	-0.202	0.124	0.163
	Through the amino group in the radical	-756.540	260.059	-0.182	0.148	0.165
Arginine	-	-606.086	-	-0.239	-0.005	0.117
	Through the amino group of an amino acid	-865.846	259.760	-0.208	0.122	0.165
	Through the extreme amino group in the radical	-865.849	259.763	-0.199	0.149	0.174
	Through the central amino group in the radical	-865.835	259.749	-0.192	0.149	0.171
Histidine	-	-548.187	-	-0.198	-0.037	0.081
	Through the amino group of an amino acid	-808.032	259.845	-0.205	0.118	0.162
	Through the amino group in the radical	-807.989	259.802	-0.203	0.105	0.154
Phenylalanine	-	-554.424	-	-0.240	0.002	0.121
	Through the amino group of an amino acid	-814.270	259.846	-0.297	0.109	0.203
Tyrosine	-	-629.617	-	-0.221	0.002	0.112
	Through the amino group of an amino acid	-892.553	262.936	-0.293	0.121	0.207
tryptophan	-	-685.684	-	-0.195	-0.035	0.080
	Through the amino group of an amino acid	-944.639	258,955 th most common	-0.199	0.087	0.143 th most common
	Through the amino group into radicals	-944,687	259,003 th most common	-0.189	0.105	0.147 th most common

From the analysis of the data obtained, it can be concluded that all interactions of the anion CO_3^{2-} with an amino acid have a total energy value different from the energy of amino acids by 260 ± 2 kcal/mol. The interaction with the largest energy difference (ΔE = 262.995) is the CO_3^{2-}-asparagine system (Figure 1–3).

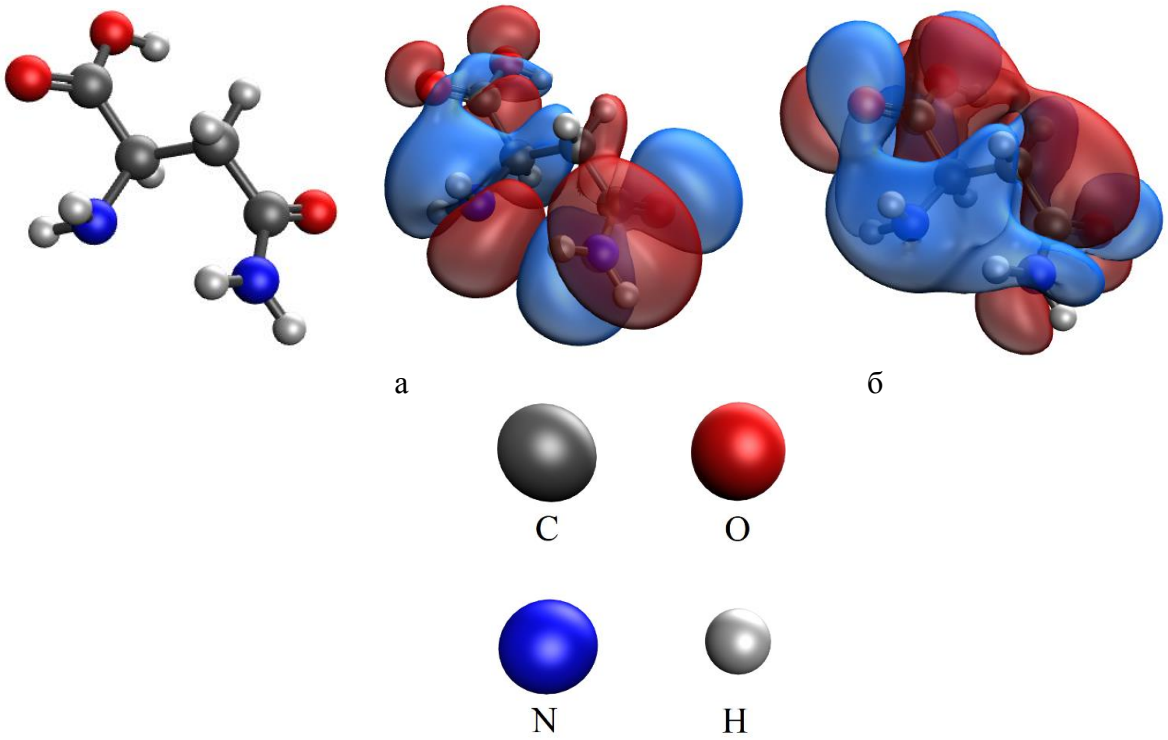

Рисунок 1 – Квантово-химическая модель молекулы аспарагина: а – модель взаимодействия, б –*HOMO*, в – *LUMO*, г – расшифровка/ **Figure 1 - Quantum-chemical model of the asparagine molecule:** a - interaction model, b - *HOMO* , c - *LUMO* , d - interpretation

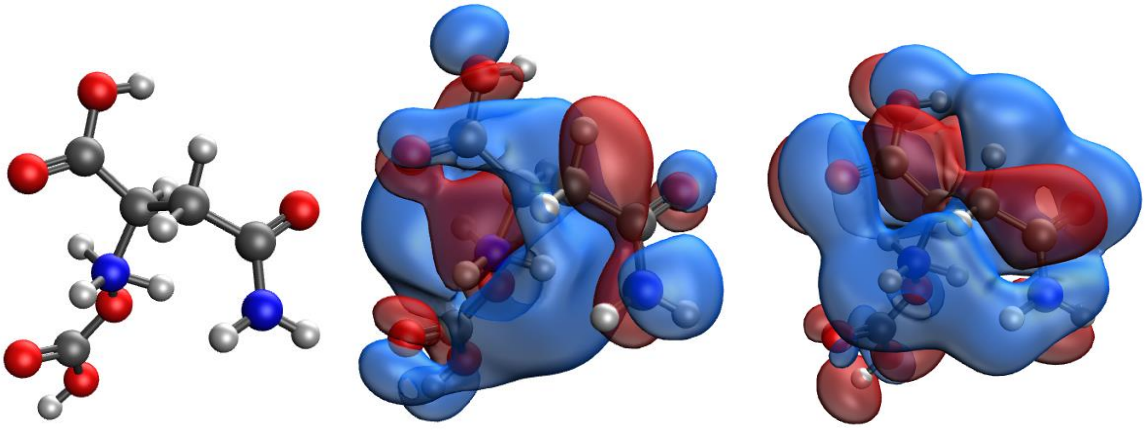

Рисунок 2 – Квантово-химическая модель молекулярной системы CO_3^{2-} -аспарагин (взаимодействия CO_3^{2-} с аминогруппой аминокислоты): а – модель взаимодействия, б –*HOMO*, в – *LUMO*, г – расшифровка/ Figure 2 - Quantum-chemical model of the molecular system CO_3^{2-} -asparagine (interactions CO_3^{2-} with the amino group of an amino acid): a - interaction model, b - *HOMO* , c - *LUMO* , d - interpretation

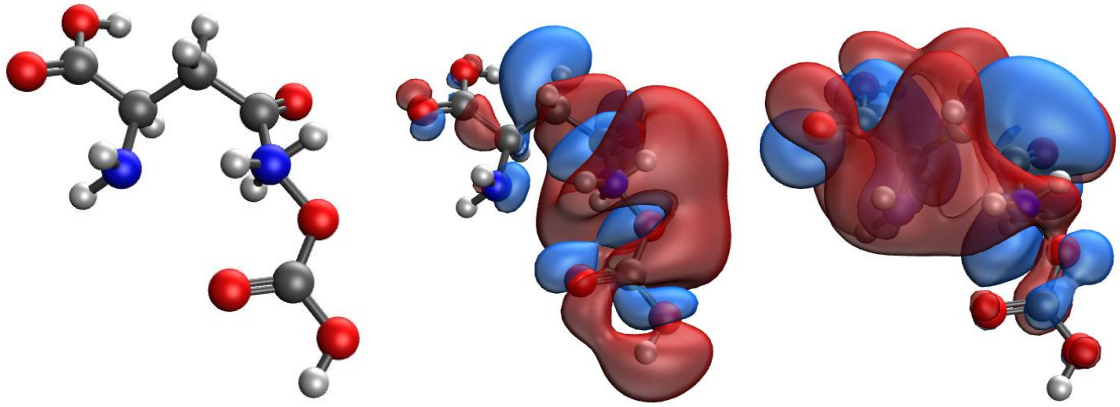

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Рисунок 3 – Квантово-химическая модель молекулярной системы CO_3^{2-} -аспарагин (взаимодействия CO_3^{2-} с аминогруппой в радикале): а – модель взаимодействия, б –*HOMO*, в – *LUMO/* Figure 3 - Quantum-chemical model of the molecular system $C\,O_3^{2-}$ -asparagine (interactions $C\,O_3^{2-}$ with an amino group in the radical): a – interaction model, b – *HOMO* , c – *LUMO*

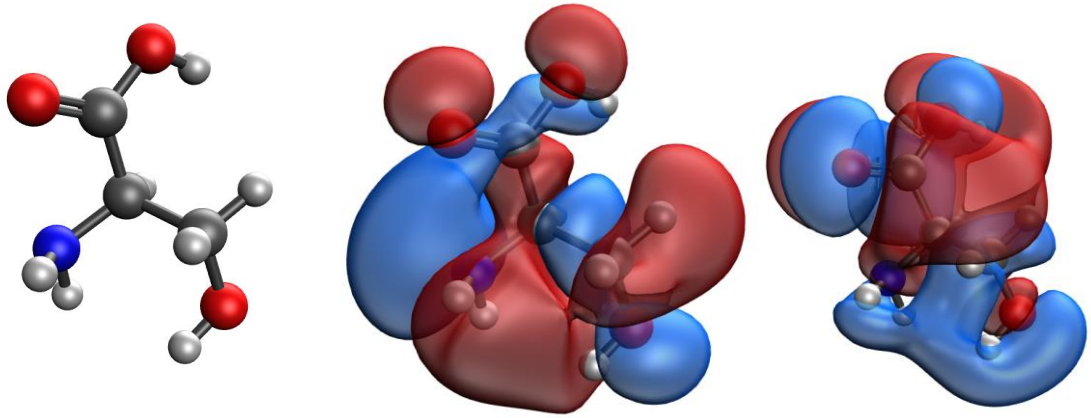

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Рисунок 4 – Квантово-химическая модель молекулы серина: а – модель взаимодействия, б –*HOMO*, в – *LUMO/* Figure 4 - Quantum-chemical model of the serine molecule: a - interaction model, b - *HOMO* , c - *LUMO*

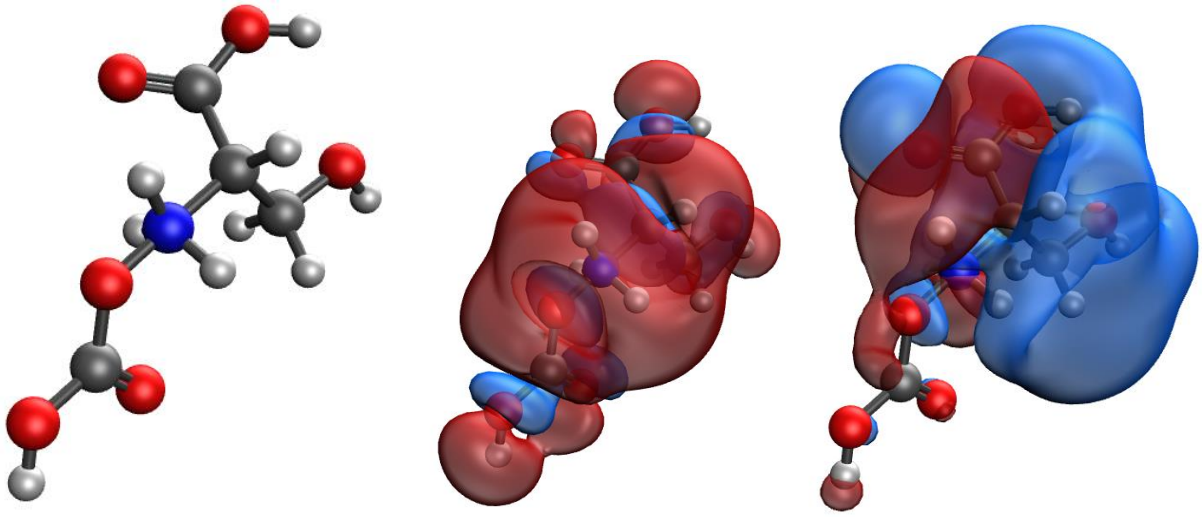

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Рисунок 5 – Квантово-химическая модель молекулярной системы CO_3^{2-}-серин (взаимодействия CO_3^{2-} с аминогруппой аминокислоты): а – модель взаимодействия, б –*HOMO*, в – *LUMO/* Figure 5 - Quantum-chemical model of the molecular system $C\,O_3^{2-}$ -serine (interactions of $C\,O_3^{2-}$ with the amino group of the amino acid): a – interaction model, b – *HOMO* , c – *LUMO*

The resulting models have a high chemical rigidity ($\eta \geq 0.129$ eV), which indicates a high stability of the systems. The CO_3^{2-}-serine system has the highest chemical rigidity ($\eta \geq 0.218$ eV) *(Figure 4–5).*

Conclusion

As a result of quantum-chemical computer modeling, it was found that all the presented interactions of calcium carbonate with a number of proteinogenic amino acids are energetically favorable. The most energetically favorable is the interaction of the carbonate anion with asparagine, the most stable is the interaction of CO_3^{2-} - serine. The study was carried out in order to further compare the analysis with laboratory test data to confirm the theoretically constructed calculations.

ЛИТЕРАТУРА

1. Matrix polyelectrolyte microcapsules: new system for macromolecule encapsulation / D.V. Volodkin, A.I. Petrov, M. Prevot, G.B. Sukhorukov // Langmuir. – 2004. – V. 20. – N. 8. – P. 3398-3406.

2. Dependence of sub-micron vaterite container release properties on pH and ionic strength of the surrounding solution / B. Parakhonskiy, F. Tessarolo, A. Haase, R. Antolini // Advances in Science and Technology. – Trans Tech Publications Ltd, 2013. – V. 86. – P. 81-85.

3. Ogino, T. The formation and transformation mechanism of calcium carbonate in water / T. Ogino, T. Suzuki, K. Sawada // Geochimica et Cosmochimica Acta. – 1987. – V. 51. – N. 10. – P. 2757-2767.

4. Reeds, P.J. Dispensable and indispensable amino acids for humans / P.J. Reeds // The Journal of Nutrition. – 2000. – V. 130. – N. 7. – P. 1835S-1840S.

5. Синтез наночастиц диоксида марганца в среде серосодержащих аминокислот / Е. Л. Малая, А. В. Блинов, Л. П. Арефьева, С. О. Крандиевский // Актуальные проблемы электроэнергетики, электроники и нанотехнологий : Материалы IV-й ежегодной научно-практической конференции Северо-Кавказского федерального университета, Ставрополь, 04–30 апреля 2016 года. – Ставрополь: Издательский дом "Тэсэра", 2016. – С. 26-28.

6. Разработка элементосбалансированного комплекса лизинаторибофлавината с эссенциальными микроэлементами / А. Б. Голик, Н. П. Оботурова, А. В. Блинов, А. А. Нагдалян // Инновационное развитие аграрно-пищевых технологий: Материалы международной научно-практической конференции, Волгоград, 17–18 июня 2021 года / Под общей редакцией И.Ф. Горлова. – Волгоград: Общество с ограниченной ответственностью "СФЕРА", 2021. – С. 221-225.

7. M.J. Lopez, S.S. Mohiuddin Biochemistry, essential amino acids. In: StatPearls. StatPearls Publishing, Treasure Island (FL); 2021.

8. Wu, G. Amino acids: metabolism, functions, and nutrition / G. Wu // Amino acids. – 2009. – V. 37. – N. 1. – P. 1-17.

9. Hou, Y. Dietary essentiality of “nutritionally non-essential amino acids” for animals and humans / Y. Hou, Y. Yin, G. Wu // Experimental Biology and Medicine. – 2015. – V. 240. – N. 8. – P. 997-1007.

10. Hou, Y. Nutritionally essential amino acids / Y. Hou, G. Wu // Advances in Nutrition. – 2018. – V. 9. – N. 6. – P. 849-851.

11. Flooding with L-[1-13C] leucine stimulates human muscle protein incorporation of continuously infused L-[1-13C] valine / K.E.N.N.E.T.H. Smith, J.M. Barua, P.W. Watt, C.M. Scrimgeour, M.J. Rennie // American Journal of Physiology-Endocrinology And Metabolism. – 1992. – V. 262. – N. 3. – P. E372-E376.

12. Effects of flooding amino acids on incorporation of labeled amino acids into human muscle protein / K. Smith, N. Reynolds, S. Downie, A. Patel, M.J. Rennie // American Journal of Physiology-Endocrinology And Metabolism. – 1998.

13. Tien Lea, D. Improving nutritional quality of plant proteins through genetic engineering / D. Tien Lea, H. Duc Chua, N. Quynh Lea // Current genomics. – 2016. – V. 17. – N. 3. – P. 220-229.

14. Aledo, J.C. Methionine in proteins: The Cinderella of the proteinogenic amino acids / J.C. Aledo // Protein Science. – 2019. – V. 28. – N. 10. – P. 1785-1796.

15. Kussmann, J. Linear- scaling self- consistent field methods for large molecules / J. Kussmann, M. Beer, C. Ochsenfeld // Wiley Interdisciplinary Reviews: Computational Molecular Science. – 2013. – V. 3. – N. 6. – P. 614-636.

16. Schaller, T. Structure of molecular tweezer complexes in the solid state: NMR experiments, X-ray investigations, and quantum chemical calculations / T. Schaller, U.P. Büchele, F.G. Klärner, D. Bläser, R. Boese, S.P. Brown, H.W. Spiess, F. Koziol, J. Kussmann, C. Ochsenfeld // Journal of the American Chemical Society. – 2007. – V. 129. – N. 5. – P. 1293-1303.

17. Pisula ,W. Helical packing of discotic hexaphenyl hexa-peri-hexabenzocoronenes: Theory and experiment / W. Pisula, Ž. Tomović, M.D. Watson, K. Müllen, J. Kussmann, C. Ochsenfeld, T. Metzroth, J. Gauss // The Journal of Physical Chemistry B. – 2007. – V. 111. – N. 26. – P. 7481-7487.

Flaig, D. Convergence of electronic structure with the size of the QM region: example of QM/MM NMR shieldings / D. Flaig, M. Beer, C. Ochsenfeld // Journal of chemical theory and computation. – 2012. – V. 8. – N. 7. – P. 2260-2271.

19. Компьютерное квантово-химическое моделирование поликомпонентных систем SiO_2-Me_xO_y / А.А. Гвозденко, А.В. Блинов, М.А. Ясная, А.Б. Голик, В.В. Раффа, В.Н. Крамаренко, Д.Г. Маглакелидзе, И.М Шевченко // Физико-химические аспекты изучения кластеров, наноструктур и наноматериалов. – 2020. – № 12. – С. 394-404.

20. Quantum-chemical simulation of copper oxide nanoparticles stabilizatio / D.M. Remizov, A.A. Gvozdenko, A.V. Blinov, V.V. Raffa, A.B. Golik, D.G. Maglakelidze, A.A. Blinova// Современная наука и инновации. – 2021. – N 1(33). – P. 29-34.

REFERENCES

1. Matrix polyelectrolyte microcapsules: new system for macromolecule encapsulation / D.V. Volodkin, A.I. Petrov, M. Prevot, G.B. Sukhorukov // Langmuir. – 2004. – V. 20. – N. 8. – P. 3398-3406.

2. Dependence of sub-micron vaterite container release properties on pH and ionic strength of the surrounding solution / B. Parakhonskiy, F. Tessarolo, A. Haase, R. Antolini // Advances in Science and Technology. – Trans Tech Publications Ltd, 2013. – V. 86. – P. 81-85.

3. Ogino, T. The formation and transformation mechanism of calcium carbonate in

water / T. Ogino, T. Suzuki, K. Sawada // Geochimica et Cosmochimica Acta. – 1987. – V. 51. – N. 10. – P. 2757-2767.

4. Reeds, P.J. Dispensable and indispensable amino acids for humans / P.J. Reeds // The Journal of Nutrition. – 2000. – V. 130. – N. 7. – P. 1835S-1840S.

5. Sintez nanochastits dioksida margantsa v srede serosoderzhashchikh aminokislot / E. L. Malaya, A. V. Blinov, L. P. Aref'eva, S. O. Krandievskii // Aktual'nye problemy ehlektroehnergetiki, ehlektroniki i nanotekhnologii : Materialy IV-i ezhegodnoi nauchno-prakticheskoi konferentsii Severo-Kavkazskogo federal'nogo universiteta, Stavropol', 04–30 aprelya 2016 goda. – Stavropol': Izdatel'skii dom "Tehsehra", 2016. – S. 26-28.

6. Razrabotka ehlementosbalansirovannogo kompleksa lizinatoriboflavinata s ehssentsial'nymi mikroehlementami / A. B. Golik, N. P. Oboturova, A. V. Blinov, A. A. Nagdalyan // Innovatsionnoe razvitie agrarno-pishchevykh tekhnologii: Materialy mezhdunarodnoi nauchno-prakticheskoi konferentsii, Volgograd, 17–18 iyunya 2021 goda / Pod obshchei redaktsiei I.F. Gorlova. – Volgograd: Obshchestvo s ogranichennoi otvetstvennost'yu "SFERA", 2021. – S. 221-225.

7. M.J. Lopez, S.S. Mohiuddin Biochemistry, essential amino acids. In: StatPearls. StatPearls Publishing, Treasure Island (FL); 2021.

8. Wu, G. Amino acids: metabolism, functions, and nutrition / G. Wu // Amino acids. – 2009. – V. 37. – N. 1. – P. 1-17.

9. Hou, Y. Dietary essentiality of "nutritionally non-essential amino acids" for animals and humans / Y. Hou, Y. Yin, G. Wu // Experimental Biology and Medicine. – 2015. – V. 240. –

N. 8. – P. 997-1007.

10. Hou, Y. Nutritionally essential amino acids / Y. Hou, G. Wu // Advances in

Nutrition. – 2018. – V. 9. – N. 6. – P. 849-851.

11. Flooding with L-[1-13C] leucine stimulates human muscle protein incorporation of continuously infused L-[1-13C] valine / K.E.N.N.E.T.H. Smith, J.M. Barua, P.W. Watt, C.M. Scrimgeour, M.J. Rennie // American Journal of Physiology-Endocrinology And Metabolism. – 1992. – V. 262. – N. 3. – P. E372-E376.

12. Effects of flooding amino acids on incorporation of labeled amino acids into human muscle protein / K. Smith, N. Reynolds, S. Downie, A. Patel, M.J. Rennie // American Journal of Physiology-Endocrinology And Metabolism. – 1998.

13. Tien Lea, D. Improving nutritional quality of plant proteins through genetic engineering / D. Tien Lea, H. Duc Chua, N. Quynh Lea // Current genomics. – 2016. – V. 17. – N. 3. – P. 220-229.

14. Aledo, J.C. Methionine in proteins: The Cinderella of the proteinogenic amino acids / J.C. Aledo // Protein Science. – 2019. – V. 28. – N. 10. – P. 1785-1796.

15. Kussmann, J. Linear-scaling self-consistent field methods for large molecules / J. Kussmann, M. Beer, C. Ochsenfeld // Wiley Interdisciplinary Reviews: Computational Molecular Science. – 2013. – V. 3. – N. 6. – P. 614-636.

16. Schaller, T. Structure of molecular tweezer complexes in the solid state: NMR experiments, X-ray investigations, and quantum chemical calculations / T. Schaller, U.P. Büchele, F.G. Klärner, D. Bläser, R. Boese, S.P. Brown, H.W. Spiess, F. Koziol, J. Kussmann, C. Ochsenfeld // Journal of the American Chemical Society. – 2007. – V. 129. – N. 5. – P. 1293-1303.

17. Pisula ,W. Helical packing of discotic hexaphenyl hexa-peri-hexabenzocoronenes: Theory and experiment / W. Pisula, Ž. Tomović, M.D. Watson, K. Müllen, J. Kussmann, C. Ochsenfeld, T. Metzroth, J. Gauss // The Journal of Physical Chemistry B. – 2007. – V. 111. –

N. 26. – P. 7481-7487.

Flaig, D. Convergence of electronic structure with the size of the QM region: example of QM/MM NMR shieldings / D. Flaig, M. Beer, C. Ochsenfeld // Journal of chemical theory and computation. – 2012. – V. 8. – N. 7. – P. 2260-2271.

19. Komp'yuternoe kvantovo-khimicheskoe modelirovanie polikomponentnykh sistem SiO2-MexOy / A.A. Gvozdenko, A.V. Blinov, M.A. Yasnaya, A.B. Golik, V.V. Raffa, V.N. Kramarenko, D.G. Maglakelidze, I.M Shevchenko // Fiziko-khimicheskie aspekty izucheniya klasterov, nanostruktur i nanomaterialov. – 2020. – № 12. – S. 394-404.

20. Quantum-chemical simulation of copper oxide nanoparticles stabilizatio / D.M. Remizov, A.A. Gvozdenko, A.V. Blinov, V.V. Raffa, A.B. Golik, D.G. Maglakelidz

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