Short Communication

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A Translational Biomedical Approach to Structural Arrangement of Amino Acids' Complexes: A Combined Theoretical and Computational Study

A Heidari

Faculty of Chemistry, California South University, 14731 Comet St. Irvine, CA 92604, USA

Corresponding author: A Heidari, Faculty of Chemistry, California South University (CSU), 14731 Comet St. Irvine, CA 92604, USA, Tel: +1 (775) 410-4974; E-mail: Scholar.Researcher.Scientist@gmail.com

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In this short communication, respectively bonding among Boron (B^{3+}), Aluminum (Al^{3+}), Gallium (Ga^{3+}), Indium (In^{3+}) and Thallium (Tl^{3+}) cations and Alanine, Arginine, Asparagine, Aspartic Acid, Cysteine, Glutamic Acid, Glutamine, Glycine, Proline, Selenocysteine, Serine, Tyrosine, Histidine, Isoleucine, Leucine, Lysine, Methionine, Phenylalanine, Threonine, Tryptophan and Valine ligands and also structural arrangement of the present compounds were studied, theoretically and computationally [1-16]. Calculations were done via HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP computational methods with 31G, 6-31G*, 6-31+G*, 6-31G(3df,3pd), 6-311G, 6-311G* and 6–311+G* basis sets, respectively. Alanine, Arginine, Asparagine, Aspartic Acid, Cysteine, Glutamic Acid, Glutamine, Glycine, Proline, Selenocysteine, Serine, Tyrosine, Histidine, Isoleucine, Leucine, Lysine, Methionine, Phenylalanine, Threonine, Tryptophan and Valine ligands are bonded to Boron (B^{3+}), Aluminum (Al^{3+}), Gallium (Ga^{3+}), Indium (In^{3+}) and Thallium (Tl^{3+}) cations via Oxygen (O) and Nitrogen (N) atoms. It is evident that if Alanine, Arginine, Asparagine, Aspartic Acid, Cysteine, Glutamic Acid, Glutamine, Glycine, Proline, Selenocysteine, Serine, Tyrosine, Histidine, Isoleucine, Leucine, Lysine, Methionine, Phenylalanine, Threonine, Tryptophan and Valine ligands form complexes with Boron (B^{3+}), Aluminum (Al^{3+}), Gallium (Ga^{3+}), Indium (In^{3+}) and Thallium (Tl^{3+}) cations, different isomers will be obtained. Energy of each of the isomers was optimized via HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP computational methods with 31G, 6-31G*, 6-31+G*, 6-31G(3df,3pd), 6-311G, 6-311G* and 6-311+G* basis sets, respectively. The most stabilized isomers are complexes in which Boron (B^{3+}), Aluminum (Al^{3+}), Gallium (Ga^{3+}), Indium (In^{3+}) and Thallium (Tl^{3+}) cations are bonded to Oxygen (O) in Carbonyl (C=O) group and Nitrogen (N) in Amide (R-CO-NR'R") group in Alanine, Arginine, Asparagine, Aspartic Acid, Cysteine, Glutamic Acid, Glutamine, Glycine, Proline, Selenocysteine, Serine, Tyrosine, Histidine, Isoleucine, Leucine, Lysine, Methionine, Phenylalanine, Threonine, Tryptophan and Valine ligands. Then, numbers of Alanine, Arginine, Asparagine, Aspartic Acid, Cysteine, Glutamic Acid, Glutamine, Glycine, Proline, Selenocysteine, Serine, Tyrosine, Histidine, Isoleucine, Leucine, Lysine, Methionine, Phenylalanine, Threonine, Tryptophan and Valine ligands surrounding Boron (B^{3+}), Aluminum (Al^{3+}), Gallium (Ga^{3+}), Indium (In^{3+}) and Thallium (Tl^{3+}) cations are increased. Energy of each of the resulting complexes was optimized via HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP computational methods with 31G, 6-1G*, 6-31+G*, 6–31G(3df, 3pd), 6-311G, 6-311G* and 6–311+G* basis sets as mentioned above, respectively. Furthermore, stability energy of the complexes, bond lengths and also bond angles were investigated.

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