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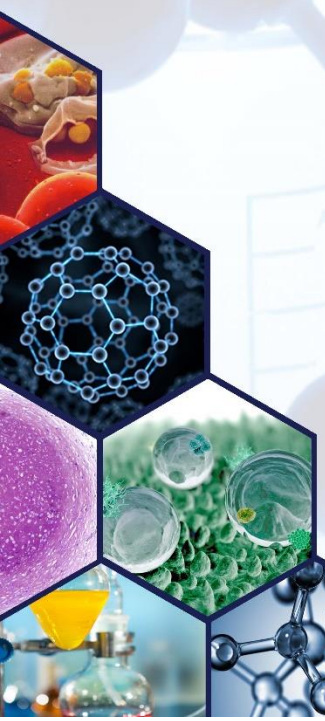

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Binding of uranyl cation to peptides: a combined quantum chemical and crystallographic study

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Interactions of uranyl cation with peptides are drawing attention of the researchers mostly because of the importance of these interactions for understanding of uranium toxicity but also because of the possible application of uranyl-peptide binding for extraction of uranium from the seawater [1]. Although structure of many complexes containing uranyl cation attached to amino acids and proteins were determined and analysed, a systematic theoretical study related to binding of uranyl cation to peptides was not performed yet [2].

Here we present theoretical study of stability of complexes containing uranyl cation and different dipeptides and tripeptides. The study was based on Density Functional Theory calculation as well as very precise CCSD(T) calculations. In the frame of this study, different bonding patterns between uranyl cation and selected peptides were proposed and analysed. Stability of structures in which uranyl cation is bonded to carboxyl group were compared to the stability of structures in which uranyl cation was bonded to atoms involved in peptide bond. In addition, crystal structures of proteins containing uranyl cation were extracted from Protein database and analysed.

Results of theoretical calculations were compared to the results of analysis of crystal structures archived in Protein databank.

References

1. R. Pardoux, S. Sauge-Merle, D. Lemaire, P. Delangle, L. Guilloreau, J-M. Adriano, C. Berthomieu, *PLoS ONE*, **2012**, 7, e41922.
2. L. Zhou, M. Bosscher, C. Zhang, S. Özçubukçu, L. Zhang, W. Zhang, C. J. Li, J. Liu, M. P. Jensen, L. Lai, C. He, *Nat. Chem.* **2014**, 6, 236.

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