

# New 1,2,4-triazole based cationic surfactants in the synthesis of silver and gold nanoparticles



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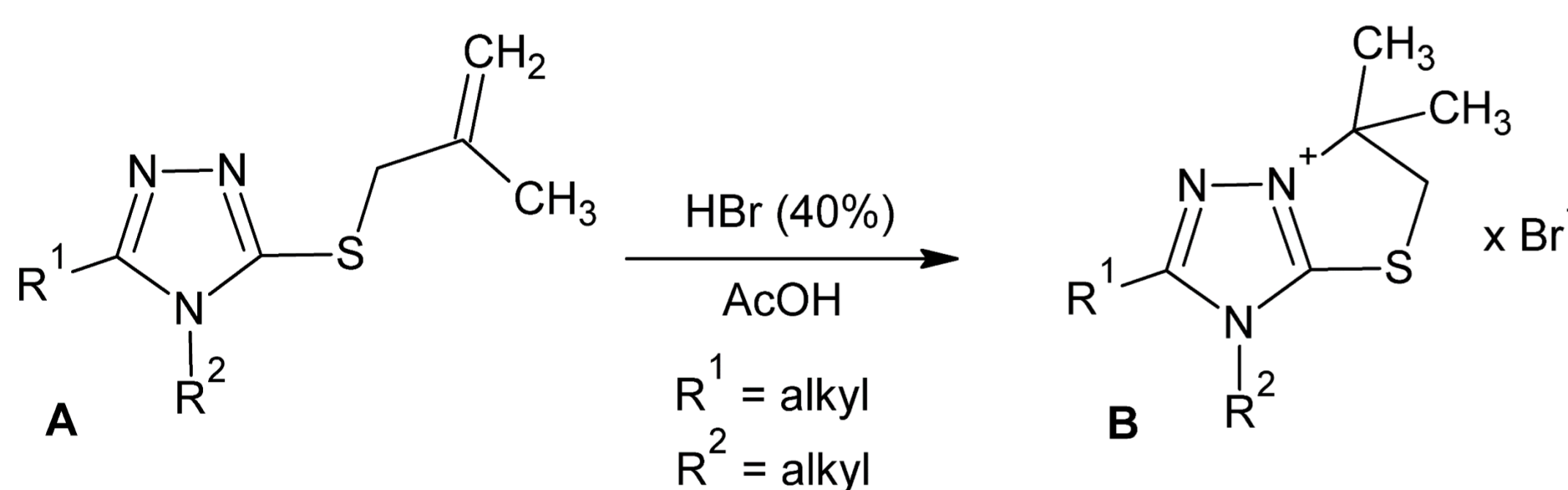
## Introduction / Objectives / Aims

The synthesis of metal nanoparticles (NPs) is a fast developing trend in modern nano-science [1]. It should be noted that surfactants play an important role in the synthesis of metal NPs. The relationship between surfactant compounds structure and the NPs' morphology should be studied in detail. The recent work of Song et al. discusses the role of surfactants in NPs synthesis, and authors have suggested that the review can open up new avenues for the synthesis of nanocrystals [2].

In the present work, we have focused on the improvement of the synthesis of Ag-NPs via the reaction of silver nitrate with hydroxylamine hydrochloride in the presence of new surfactants **B** (see Scheme 1) in basic medium. The theoretical explanation of the silver surface with the surfactant cation has been given in terms of the quantum chemical density functional theory (DFT) calculations.

## Results

Synthesis of the new surfactants has been performed starting from methylthio-1,2,4-triazoles under the action of hydrobromic acid in acetic acid. NMR spectra confirmed the formation of the thiazoline ring. For example, in the case of 2-heptadecyl-3,6,6-trimethyl-5,6-dihydro-3H-[1,3]thiazolo[3,2-b][1,2,4]triazol-7-ium bromide ( $R^1 = C_{17}H_{35}$ ,  $R^2 = CH_3$ ), singlet peak at 1.57 ppm with the relative intensity 6 corresponds to the formation of the two same methyl groups bonded with the thiazoline cycle. The singlet at 4.14 ppm was caused by the endocyclic methylene group of the thiazoline cycle. At 3.66 ppm a signal of the N-methyl group. Other peaks correspond to the heptadecyl chain. For the synthesis of Ag-NPs, as the main reducing agent, we have decided to use hydroxylamine. The choice is dictated by numerous successful protocols described in modern papers.



Scheme 1. Synthesis of the new surfactants **B**.

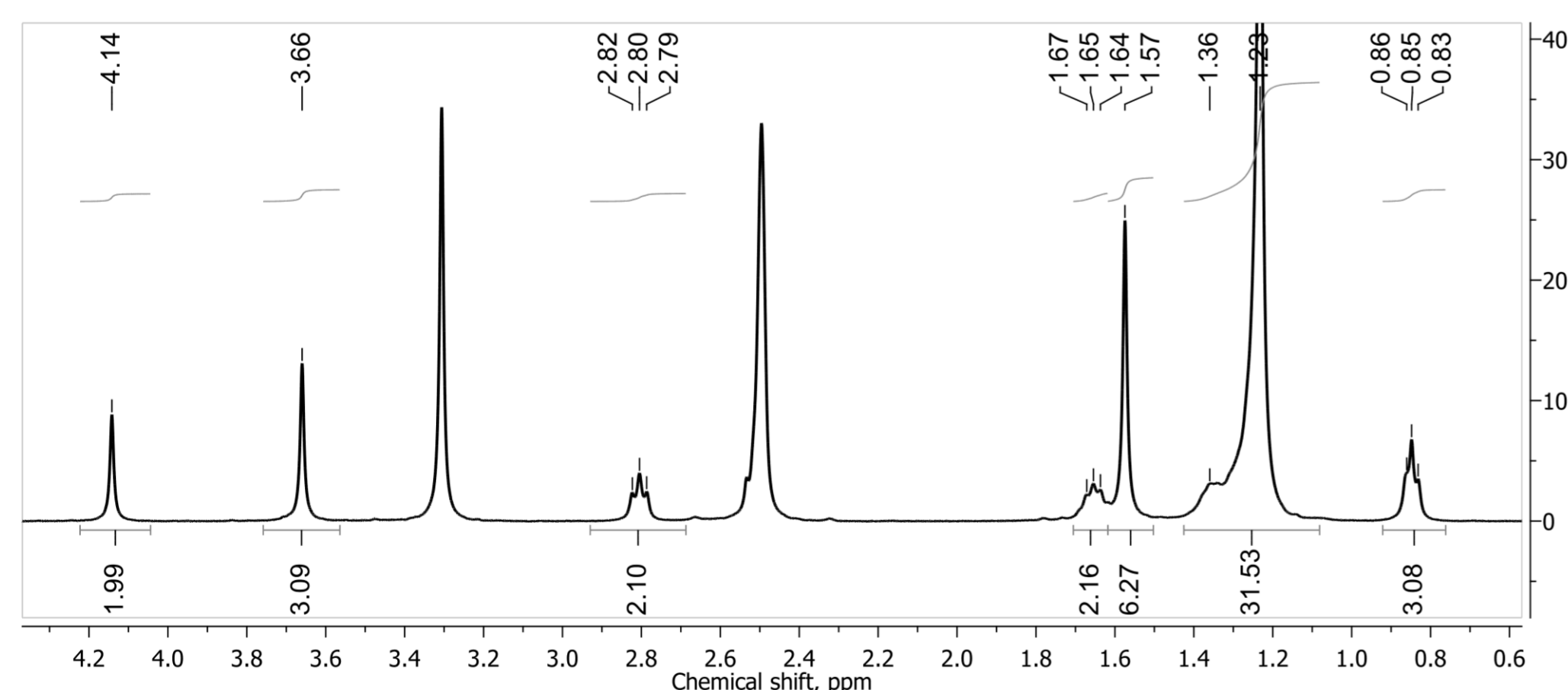


Figure 1. 2-heptadecyl-3,6,6-trimethyl-5,6-dihydro-3H-[1,3]thiazolo[3,2-b][1,2,4]triazol-7-ium bromide ( $R^1 = C_{17}H_{35}$ ,  $R^2 = CH_3$ ).

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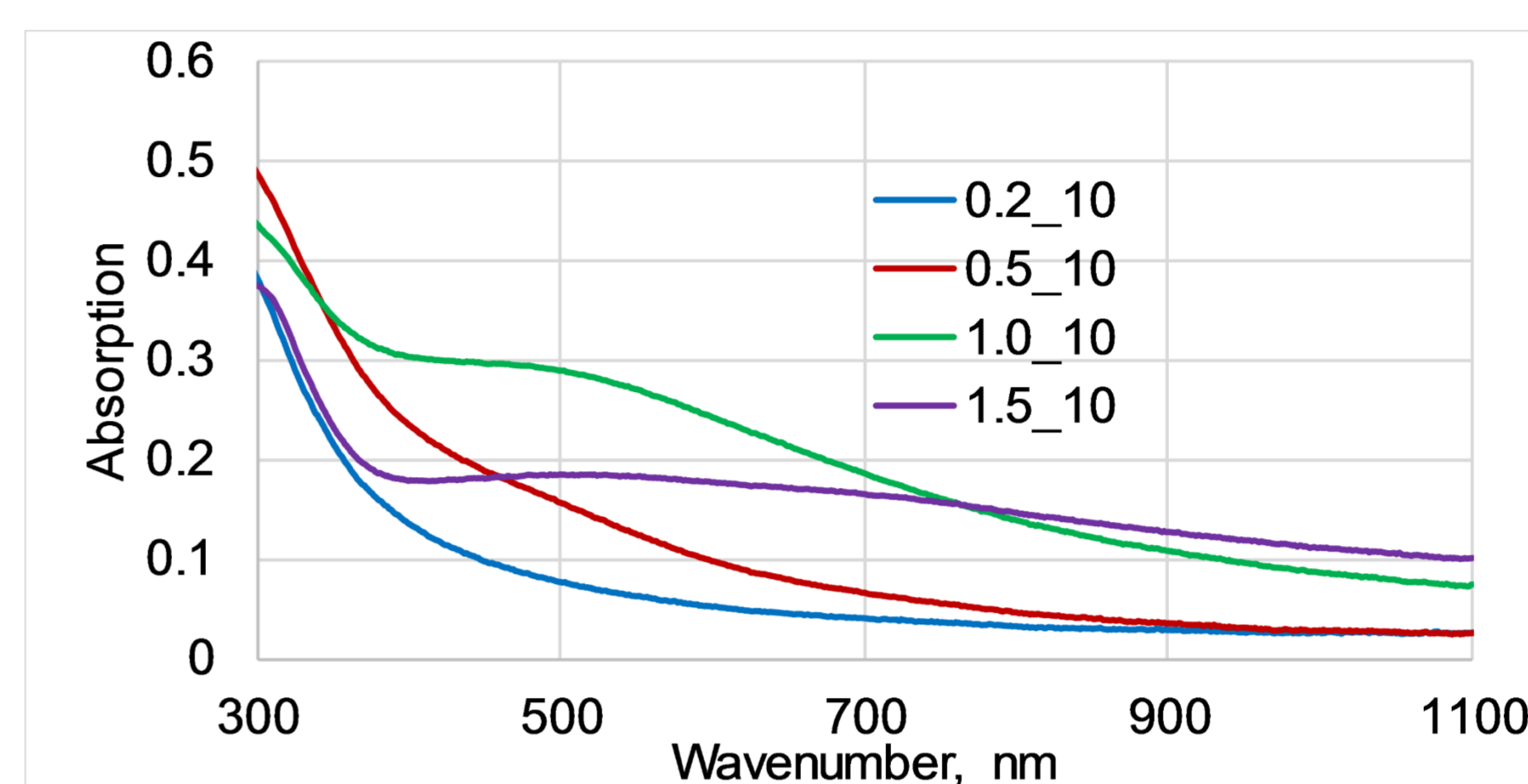


Figure 2. UV-VIS spectra of four solutions with different starting concentration of silver nitrate, mmol/L: 0.19 (blue), 0.46 (red), 0.92 (green), 1.23 (purple).

Varying the experimental conditions, we have succeeded in developing new simple methods for the synthesis of Ag-NPs with using of new triazole surfactants. Corresponding UV-VIS spectra presented in Figure 2. A relatively high baseline in the case of 1.23 and 0.92 mmol/L concentration solutions can be explained by partial precipitation of silver bromide in the reaction mixture. The absorption maxima are in the range of 420-550 nm, which correspond to the formation of classical spherical silver nanoparticles. Absorption at the lower wavelength range of 300-340 nm corresponds to the absorption of the triazole itself.

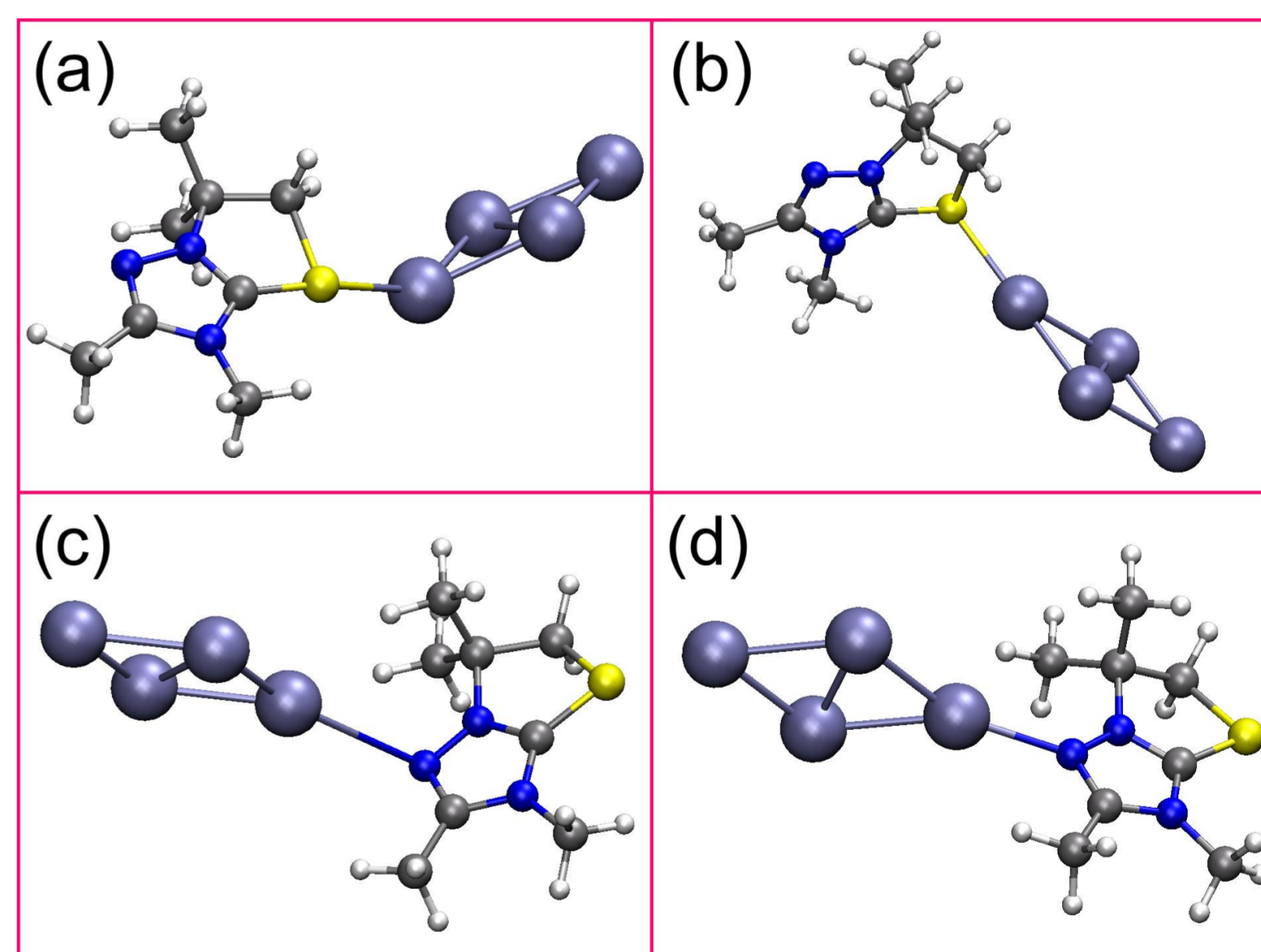


Figure 3. DFT calculations of model **B** core coordination with the model  $Ag_4$  cluster. N-coordinated structures are more stable.

## Conclusions

It was determined that the new [1,3]thiazolo[3,2-b][1,2,4]triazol-7-ium cationic surfactants can be used in stabilization of silver (gold) nanoparticles. According to DFT calculations, the coordination of the cationic surfactants takes place over the nitrogen atom.

## Acknowledgements

This study was partially supported by the National Scholarship Programme of the Slovak Republic [Grant ID 32706].

## References

- [1] Appl. Nanosci. 2019, <https://doi.org/10.1007/s13204-019-00990-x>.
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