

Molecular modeling of protein structures and metal salts interaction



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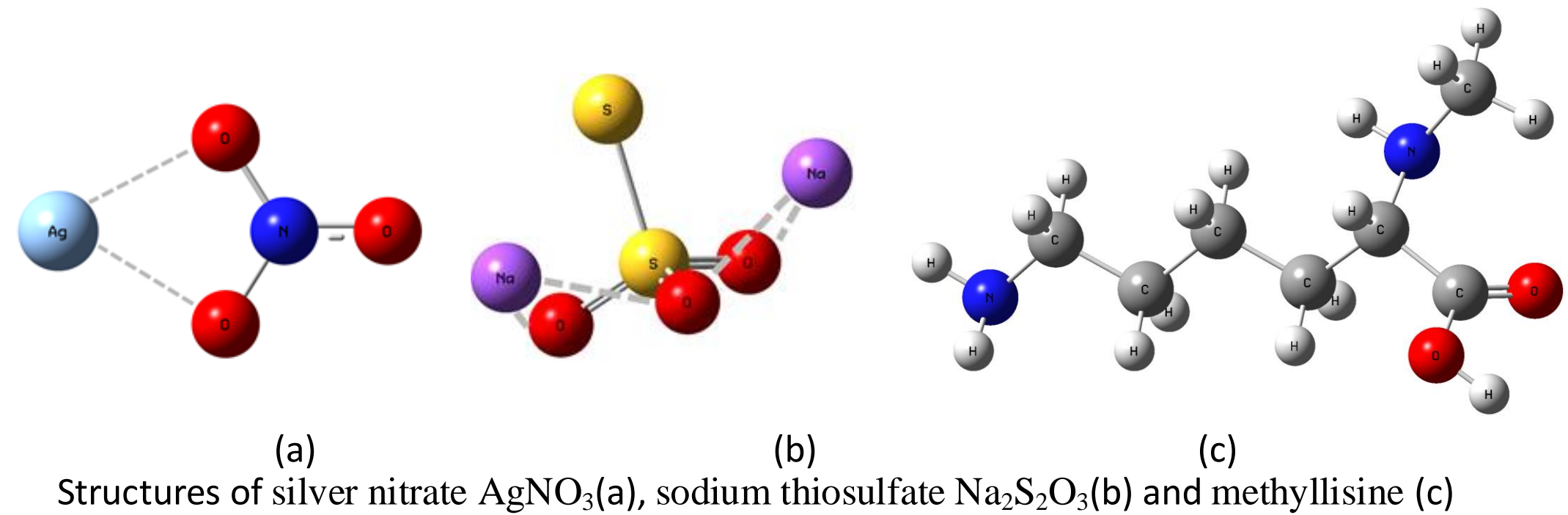
ABSTRACT

The aim of this work is to study the molecular mechanisms of bacterial synthesis of a promising material for nanoelectronics – silver sulfide nanoparticles. A special feature of obtaining silver sulfide nanoparticles by biosynthesis [1] using *Bacillus subtilis* 168 bacteria is that the only protein involved in the synthesis process and adsorbed on the surface of the particles is the flagellin protein. Silver nitrate and sodium thiosulfate, as well as the non-standard amino acid methyllisine, which is part of the flagellin protein, are considered as the objects under study. The IR spectra, structure, and parameters of the resulting hydrogen bonds of the molecular complexes silver nitrate, sodium thiosulfate, and the non-standard amino acid methyllisine were calculated.

MOLECULAR MODELING:

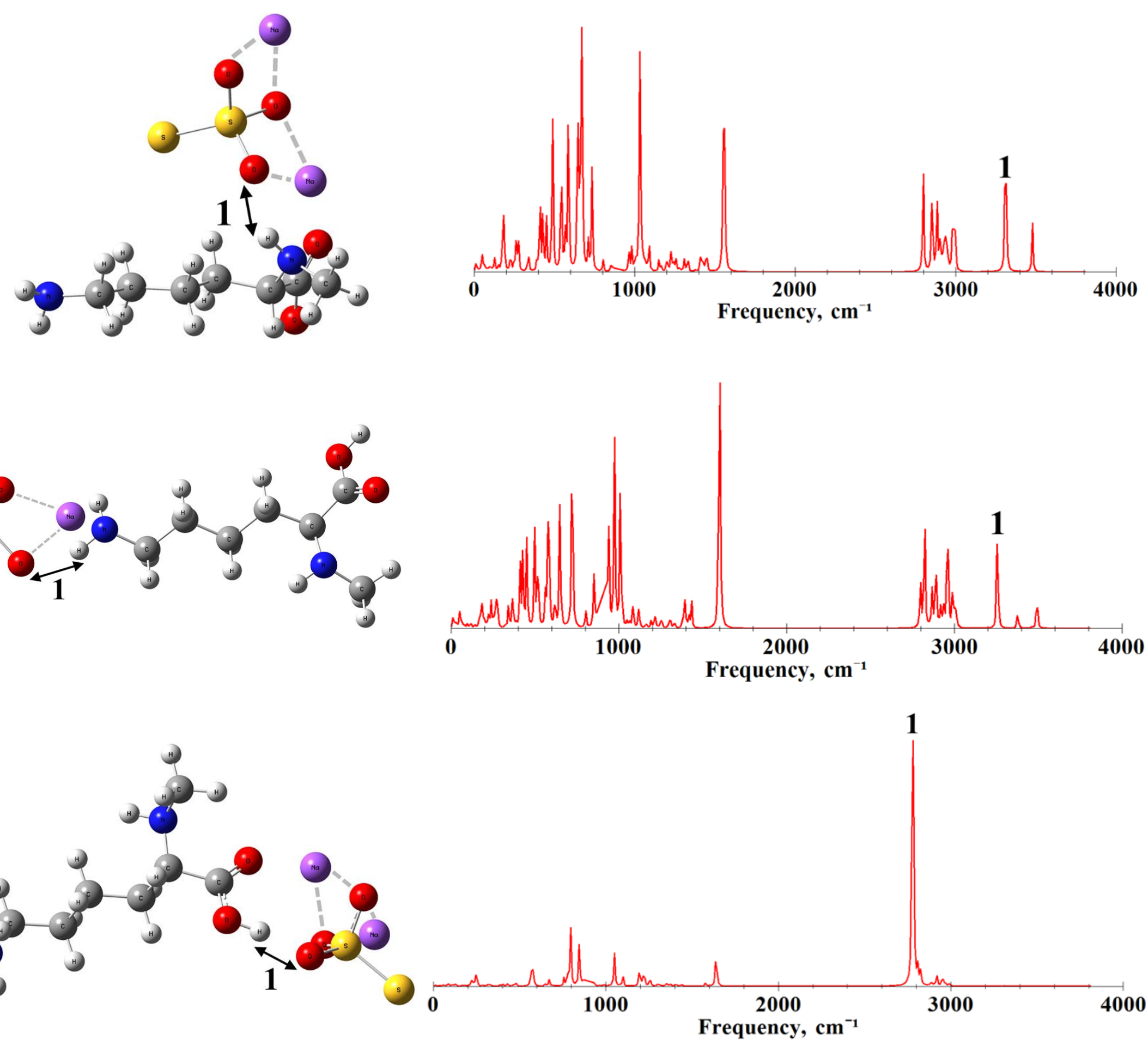
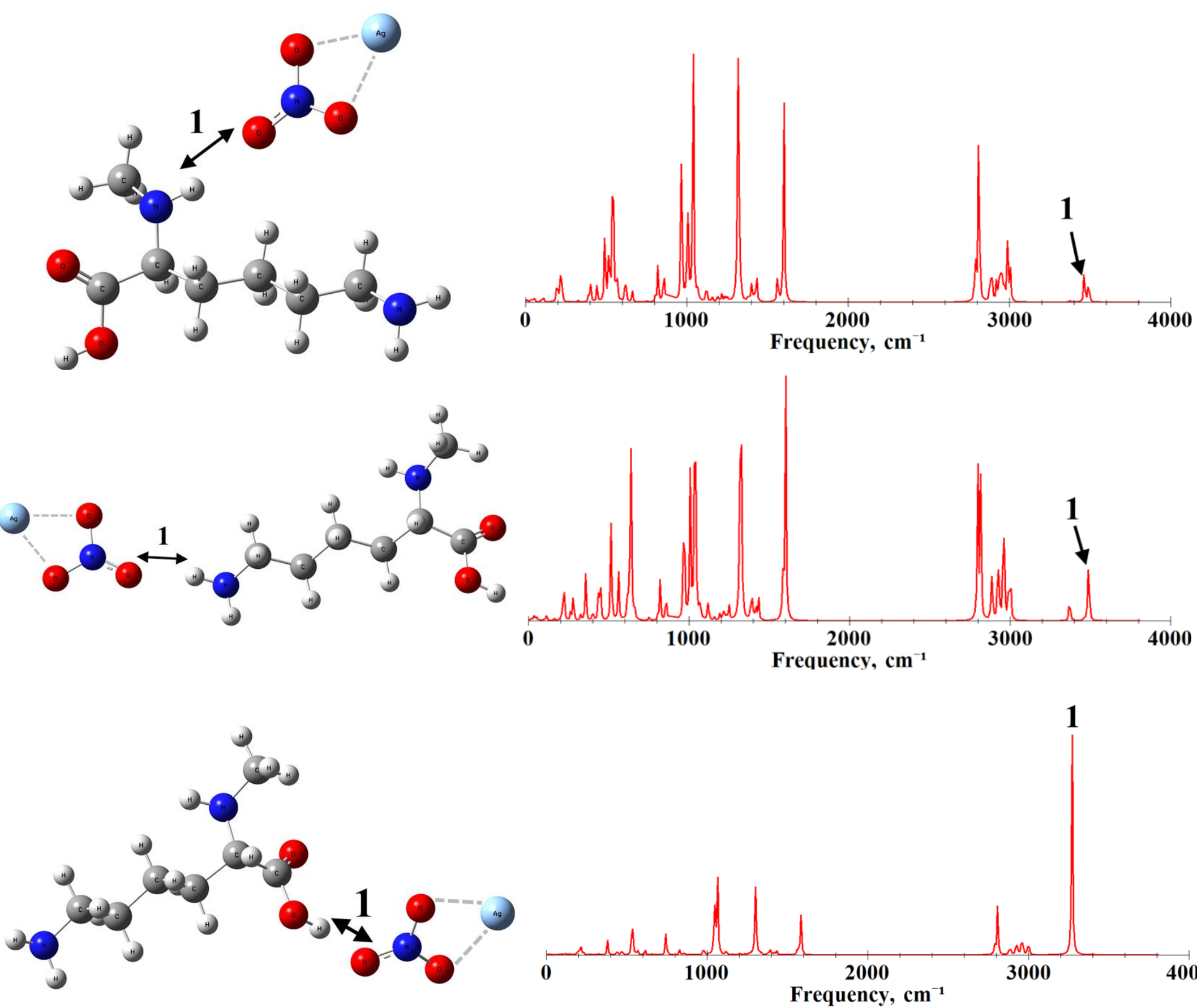
Modeling based on the density functional theory using the B3LYP functional and the LANL2DZ basis using the Gaussian 09 software package.

RESEARCH OBJECTS

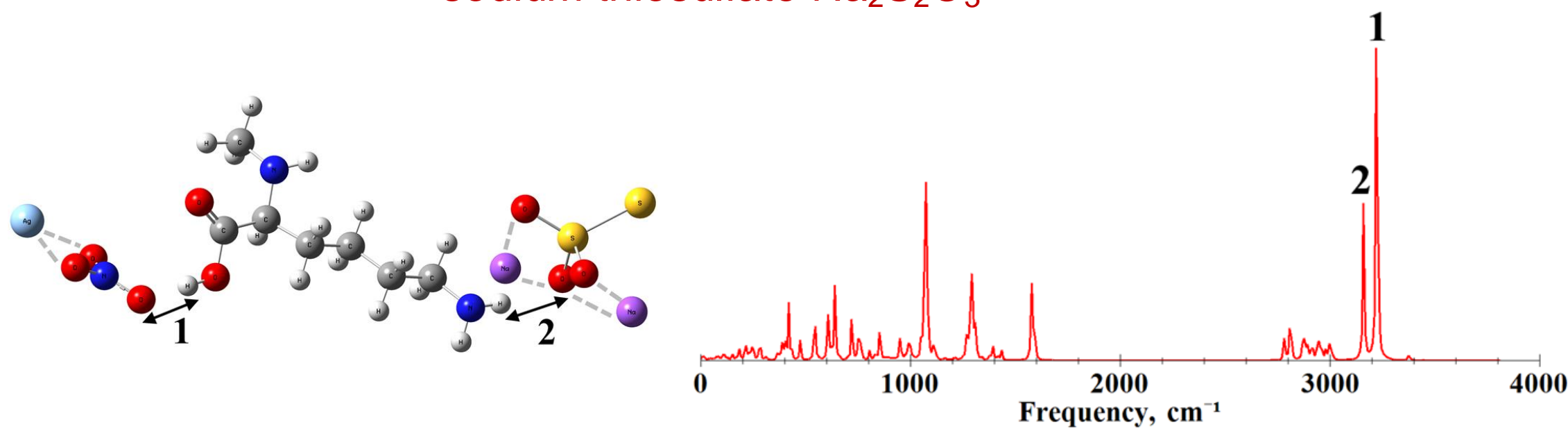


Structure and IR spectrum of methyllisine and sodium thiosulfate $\text{Na}_2\text{S}_2\text{O}_3$

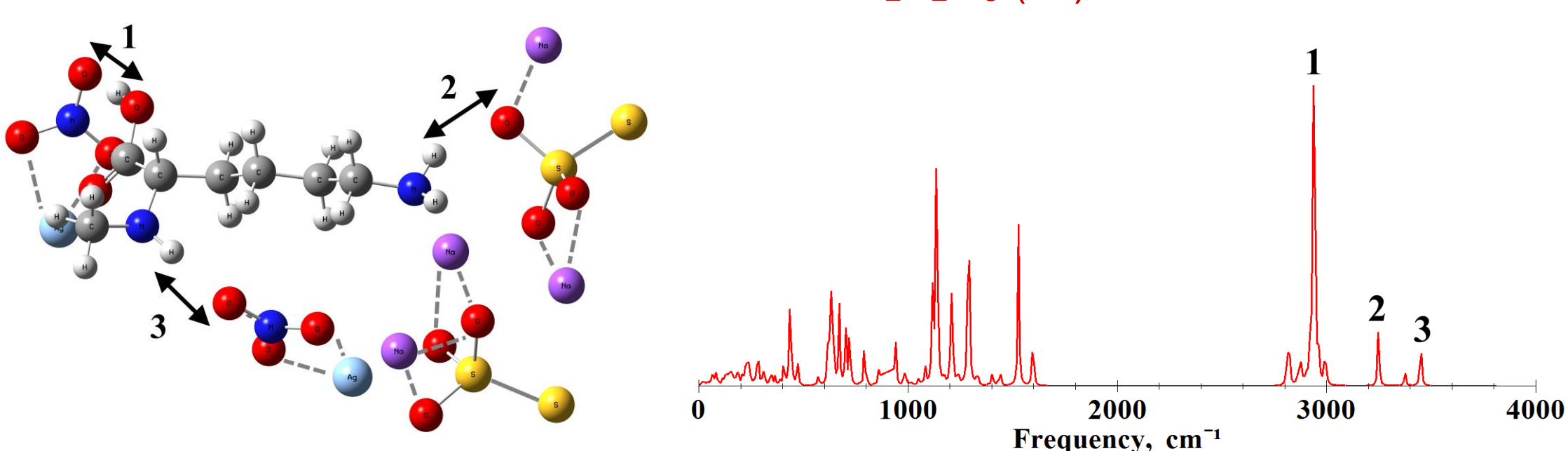
Structure and IR spectrum of methyllisine and silver nitrate AgNO_3



Structure and IR spectrum of Methyllisine, silver nitrate AgNO_3 and sodium thiosulfate $\text{Na}_2\text{S}_2\text{O}_3$



Structure and IR spectrum of Methyllisine, silver nitrate AgNO_3 (x2) and sodium thiosulfate $\text{Na}_2\text{S}_2\text{O}_3$ (x2)



Calculated H-bonds parameters in four cases of methyllisine-silver nitrate AgNO_3 -sodium thiosulfate $\text{Na}_2\text{S}_2\text{O}_3$ molecular complexes

bond number	Hydrogen bridge length, Å	Frequency, ν , cm^{-1}	Frequency shift, $\Delta\nu$, cm^{-1}	Bond energy, $-\Delta H$, kcal/mole	Intensity I_{IR} , km/mole
Methyllisine and silver nitrate AgNO_3					
1	3.15	3462	82	1.90	49
1	3.16	3488	100	2.32	49
1	2.79	3273	252	4.37	1312
Methyllisine and sodium thiosulfate $\text{Na}_2\text{S}_2\text{O}_3$					
1	2.83	3316	64	1.46	227
1	3	3256	132	2.87	117
1	2.63	2782	743	8.01	3955
Methyllisine, silver nitrate AgNO_3 and sodium thiosulfate $\text{Na}_2\text{S}_2\text{O}_3$					
1	2.77	3221	304	4.88	1265
2	3.03	3161	227	4.10	442
Methyllisine, silver nitrate AgNO_3 (x2) and sodium thiosulfate $\text{Na}_2\text{S}_2\text{O}_3$ (x2)					
1	2.70	2937	588	7.02	1462
2	3.21	3247	297	4.80	172
3	2.94	3454	82	1.94	138

CONCLUSION

Based on the results of molecular modeling of various variants of complexation of methyllisine with silver nitrate AgNO_3 and sodium thiosulfate $\text{Na}_2\text{S}_2\text{O}_3$ salts and subsequent analysis of the parameters of the resulting bonds, the possibility of forming several medium-strength hydrogen bonds with energies from 2.75 to 8.01 kcal/mol during double or triple complexation and in a complex of 5 molecules (methyllisine, AgNO_3 x2, $\text{Na}_2\text{S}_2\text{O}_3$ x2) was established. In addition, it is necessary to note the special effect of the lysine methylation process, due to which the degree of its interaction in the flagellin composition increases significantly, which contributes to the formation of a stronger organic shell of synthesized nanoparticles. Thus, it can be concluded that methyllisine forms sufficiently stable molecular complexes with sodium thiosulfate and silver nitrate, which makes it possible to talk about its significant contribution to the formation of silver sulfide nanoparticles by biosynthesis using gram-positive bacteria *Bacillus subtilis* 168.

[1]. T.A.Voeikova, O.A. Zhuravliova, N.V. Bulushova, V.P. Veiko, T.T. Ismagulova, T.N. Lupanova, K.V. Shaitan, V.G. Debabov "The "protein corona" of silver-sulfide nanoparticles obtained using Gram-negative and – positive bacteria". Molecular Genetics, Microbiology and Virology, vol. 35(4), 2017, pp.204-211.