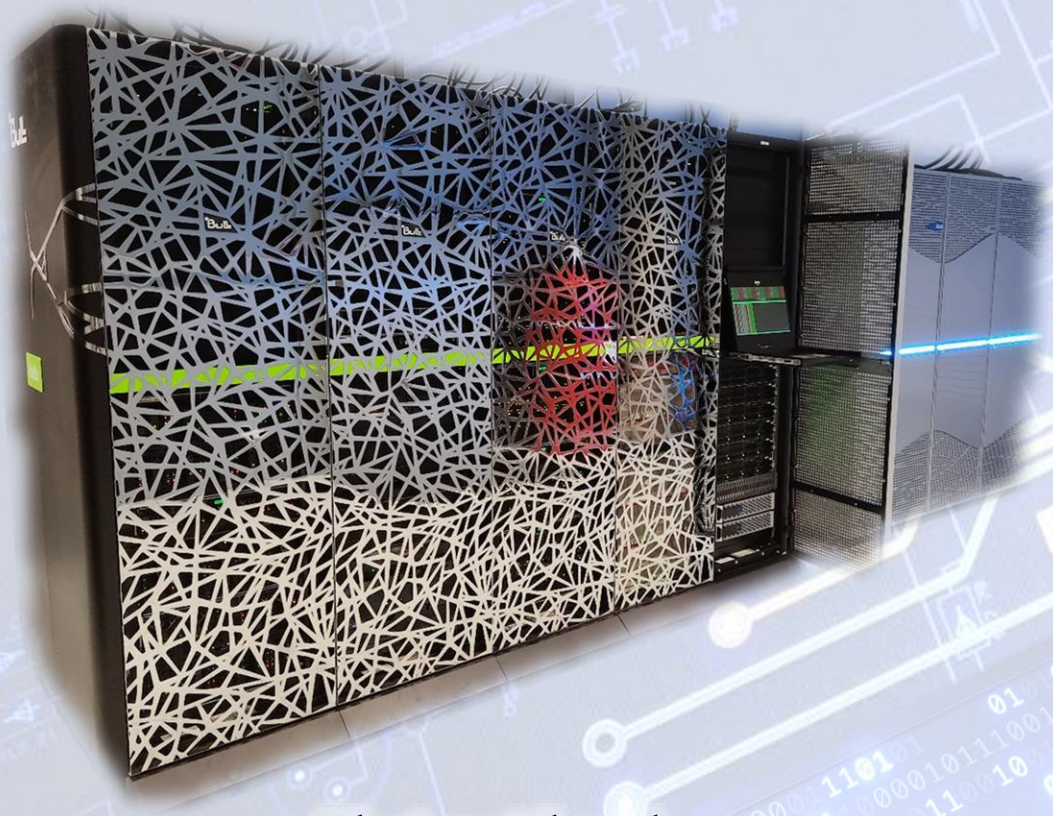
3RD EUROCC VILNIUS WORKSHOP ON USING HPC



Abstract book

https://doi.org/10.5281/zenodo.14748386

January 20–21, 2025

Vilnius, Lithuania

Workshop organizers

Local organizing committee

Mindaugas Mačernis
Laura Baliulytė
Jonas Franukevičius

Scientific committee

Mindaugas Mačernis
Jevgenij Chmeliov
Andrius Gelžinis

Funding

Co-funded by the European Union

EuroHPC Joint Undertaking

Funded by the European Union. This work has received funding from the European High Performance Computing Joint Undertaking (JU) and Germany, Bulgaria, Austria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Greece, Hungary, Ireland, Italy, Lithuania, Latvia, Poland, Portugal, Romania, Slovenia, Spain, Sweden, France, Netherlands, Belgium, Luxembourg, Slovakia, Norway, Türkiye, Republic of North Macedonia, Iceland, Montenegro, Serbia under grant agreement No 101101903.

Bendrai finansuoja Europos Sąjunga

Projektas bendrai finansuojamas 2021–2027 metų ES fondų investicijų programos (sutartis Nr. 10-051-P-0001).

EuroCC2-EuroCC4SEE
Project Organiser

Vilniaus universitetas 1579 Universitas Vilnensis

Project Implementers

Vilniaus universitetas 1579 Universitas Vilnensis — Fizikos fakultetas

Vilniaus universitetas 1579 Universitas Vilnensis — Matematikos ir informatikos fakultetas

ktu kauno technologijos universitetas 1922

VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

Importance of Anharmonic Calculations for the Assignment of the Vibrational Bands of Butyric Acid

Jogile Macyte, Klaudija Pukalskaite, Valdas Sablinskas

Institute of Chemical Physics, Vilnius University, Sauletekio av. 3, Vilnius, LT- 10257, *Lithuania*

E-mail: jogile.macyte@ff.vu.lt

Butyric acid, or butanoic acid, is a short-chain saturated carboxylic acid [1]. Carboxylic acids are organic compounds that include one or more carboxyl groups, and their chemical and biochemical properties strongly depend on the length of the carbon chain, molecular structure, and presence of additional functional groups [2]. The main objective of this work is to perform conformational analysis of butyric acid using high-level quantum chemical calculations and low-temperature matrix isolation infrared absorption spectroscopy. The results are presented in Fig. 1.

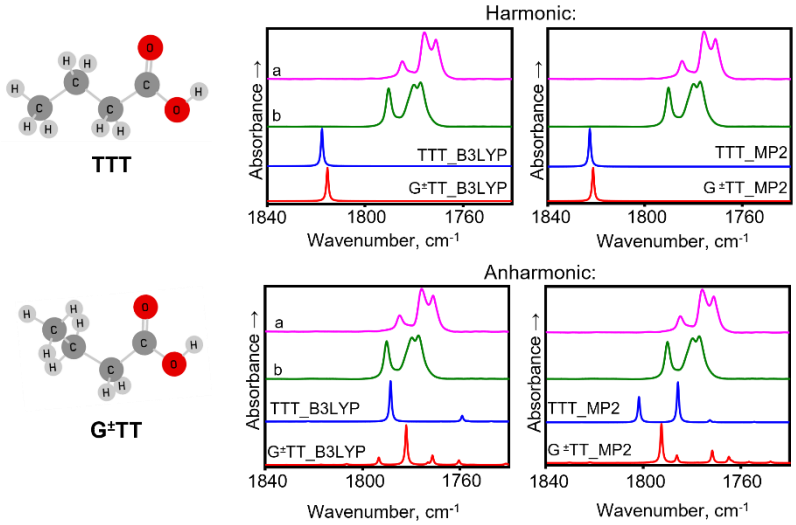


Fig. 1. Infrared absorption spectra of butyric acid: (a) experimental spectrum in argon matrix, (b) experimental spectrum in neon matrix together with theoretically in harmonic and anharmonic approximations calculated spectra of the TTT and G±TT conformers

Geometry optimization and calculations of the fundamental vibrations for three staggered conformers of butyric acid were carried out using Density Functional Theory (DFT) with the B3LYP functional and Møller-Plesset perturbation theory (MP2) approaches. In both cases, the same cc-pVTZ basis set was employed, and the vibrational frequencies were calculated using both harmonic and anharmonic methods. Our study shows that three stable conformers of butyric acid molecules are trapped in argon and neon matrices. It was found that anharmonic calculations are extremely useful for identifying Fermi resonance experimental spectral bands.These calculations allow for a more accurate assignment of spectral bands in the C=O stretch vibration region, with the origin and behavior of these bands upon matrix annealing correctly identified only after employing anharmonic calculations at the MP2 level.

REFERENCES

[1] I. Goldberg and J. S. Rokem, Organic and Fatty Acid Production, Microbial, Encyclopedia of Microbiology, 3rd ed., Elsevier Science, Amsterdam (2009), p. 421–442.

[2] S.-T. Yang (ed.), Bioprocessing for Value-Added Products from Renewable Resources: New Technologies and Applications, 1st ed., Elsevier Science, Amsterdam (2007), Chapter 16.