# ALESSANDRA SAVARESE

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# **EDUCATION**

<ul> <li>Master's Degree in Chemistry</li> </ul>	December 2022 - March 2025				
University of Pisa, Department of Chemistry and Industrial Chemistry Pisa, Italy					
- Curriculum in Physical Chemistry					
- Final grade: <b>110/110 cum laude</b>					
- Thesis title: "The Minimum Energy Principle Applie	d to the $C_3H_6O_2$ Isomer Family:				
Identification and Spectral Characterization of the Best	Candidates for Radioastronomical				
Detection"					
- Supervisors: Prof Filippo Lipparini (filippo lipparini@unir	oi it)				
Prof Cristina Puzzarini (cristina puzzarini@uu	nibo it)				
1101. Offstind 1 d22drini ( <u>Offstind-Pu22drini(@da</u>					
• Bachelor's Degree in Chemistry	September 2019 - December 2022				
University of Pisa, Department of Chemistry and Industrial C	hemistry Pisa, Italy				
- Final grade: 110/110 cum laude					
- Thesis title: "Characterization of 1D Coordination Poly.	mers by Means of Solid State NMR				
Spectroscopy"					
- Supervisor: Prof. Marco Geppi ( <u>marco.geppi@unipi.it</u> )					
<ul> <li>High School Diploma in Classical Studies</li> </ul>	September 2014 - July 2019				
Cornelio Tacito High School	Rome, Italy				
- Final grade: 100/100 cum laude					
Port Lincoln High School	Port Lincoln, Australia				
- Study Abroad Experience	July 2017 - December 2017				

# **RELEVANT COURSEWORK**

- Chemical-Physical Methods for Atmospheric Chemistry and Astrochemistry
- Advanced Spectroscopic Methods
- Biophysical Chemistry
- Theoretical Chemistry
- Quantum Chemistry and Molecular Modeling
- Statistical Thermodynamics
- Physical Chemistry II and Laboratory (Quantum Mechanics, Spectroscopy, Molecular Modeling)

- Photochemistry: Theory and Simulation Methods
- Photochemistry: Phenomenological Aspects
- Atmospheric Chemistry
- Errors and Data Analysis
- Complements of Mathematics for Chemists

# **RESEARCH EXPERIENCE**

# • POST-GRADUATE RESEARCH FELLOWSHIP: Computational study on polycyclic aromatic hydrocarbons (PAHs) growth

May 2025 - present Alma Mater Studiorum - University of Bologna, Department of Chemistry "Giacomo Ciamician"

Bologna, Italy

<u>Rotational and Computational Spectroscopy Laboratory</u> Supervisor: Prof. Cristina Puzzarini (<u>cristina.puzzarini@unibo.it</u>)

# • MASTER'S DEGREE RESEARCH INTERNSHIP: Computational and experimental rotational spectroscopy applied to astrochemistry

June 2024 - March 2025 Alma Mater Studiorum - University of Bologna, Department of Chemistry "Giacomo Ciamician"

Bologna, Italy

#### Rotational and Computational Spectroscopy Laboratory

Supervisor: Prof. Cristina Puzzarini (cristina.puzzarini@unibo.it)

- Employed a computation protocol based on the minimum energy principle to gauge the energetic stability of the members of the  $C_3H_6O_2$  isomer family, with the aim of identifying the best candidates for radioastronomical detection within the family. This energetic investigation was conducted by means of increasingly accurate calculations employing DFT and composite schemes rooted in Coupled-Cluster theory.

- Attempted to record the experimental rotational spectrum of 3-hydroxypropanal in the 80-120 GHz frequency range, with the aid of a simulated spectrum obtained through theoretically predicted spectroscopic parameters.

- Recorded and analyzed the experimental rotational spectrum of glycidol in the 65-120 GHz, 146-330 GHz, and 440-520 GHz frequency ranges, thus obtaining a new and improved set of spectroscopic parameters for its two most stable conformers.

## • MASTER'S DEGREE RESEARCH INTERNSHIP: Cholesky decomposition implementation of the perturbative triple excitations' correction to the Coupled-Cluster with single and double excitations energy

March 2024 - June 2024 University of Pisa, Department of Chemistry and Industrial Chemistry

#### <u>MoLECoLab</u>

#### Supervisor: Prof. Filippo Lipparini (filippo.lipparini@unipi.it)

- Implemented the perturbative triple excitations (T) correction to the Coupled-Cluster with single and double excitations (CCSD) energy, employing the Cholesky Decomposition of the twoelectron repulsion integrals (ERIs) matrix. This was done in a development version of the CFOUR suite of programs, employing the Fortran 90 programming language.

- Goals achieved through this preliminary implementation: removed the need for an initial transformation of the ERIs matrix from the atomic orbitals basis to the molecular orbitals basis, and decreased the memory storage requirements for the ERIs. This makes the present implementation more suitable for the description of medium-sized systems, with respect to the classical implementation.

## • BACHELOR'S DEGREE RESEARCH INTERNSHIP: Characterization of Hg(II)bispidine 1D Coordination Polymers by means of Solid State NMR Spectroscopy

September 2022 - December 2022

University of Pisa, Department of Chemistry and Industrial Chemistry Pisa, Italy SolStiCE

Supervisor: prof. Marco Geppi (<u>marco.geppi@unipi.it</u>)

- Exploited Solid State NMR (SSNMR) spectroscopy to study Hg(II)-bispidine 1D coordination polymers characterized by two different topologies (zig-zag, polycatenane) and by solvent molecules (chlorobenzene) trapped inside their structures.

- Recorded <sup>1</sup>H, <sup>13</sup>C and <sup>199</sup>Hg high-resolution SSNMR spectra of the aforementioned coordination polymers, and measured their T<sub>1</sub> and T<sub>2</sub> spin-relaxation times by means of temperature-controlled low-resolution SSNMR experiments.

- Analyzed the aforementioned spectra in order to characterize the Hg(II)-bispidine 1D coordination polymers in terms of their dynamics and mobility, with the final aim of understanding their adsorption and separation properties.

# **RESEARCH INTERESTS**

- Molecular spectroscopy: particularly rotational spectroscopy applied to the field of **astrochemistry**
- Implementation of new algorithms for computational chemistry
- Atmospheric chemistry, chemistry-climate connection

# SKILLS

- Languages
  - Italian (native language)

- English (Cambridge English C2 Proficiency Qualification, December 2018; IELTS: Overall Band Score 8.5, November 2024)

- German (rudimentary knowledge)

#### • Informatics Skills

- Programming languages: Fortran, Python
- Markup languages: LaTex
- Code parallelization: OpenMP
- Operating systems: Linux OS
- Computer Software: Microsoft Office Suite Word, Excel, PowerPoint, Outlook; iWork Pages, Numbers, Keynote
- Quantum Chemistry programs: CFOUR, Gaussian, CREST
- Chemistry software: PGOPHER, Pickett's SPFIT/SPCAT, LLWP, MestReNova, ChemSketch, ChemDraw, ChimeraX
- Bibliography Search Tools: Scifinder-n, Scopus, Google Scholar

#### • Lab Instrumentation and Techniques

- Usage of millimiter-wave frequency-modulation spectrometer
- Flash-vacuum pyrolysis
- Usage of high-resolution and low-resolution SSNMR spectrometers

# **CONFERENCE CONTRIBUTIONS**

#### • Poster presentations

- Melega L., Nottoli T., **Savarese A.**, Gauss J., Lipparini F., "*Implementation of Coupled Cluster* analytical gradients based on the Cholesky decomposition of ERIs", Chemistry for the Future International Conference, University of Pisa, July 3-5, 2024

- Della Latta E., Savarese A., Martini F., Calucci L., Cametti M., Geppi M., "Solid State NMR Study of Hg(II)-bispidine 1D Coordination Polymers", 3rd International School on Porous Materials, Lake Como School of Advanced Studies, June 19-23, 2023

# **MEMBERSHIPS**

• Mensa Italy - High I.Q. Society (November 2024 - present)

### REFERENCES

#### • Prof. Cristina Puzzarini

Full Professor

Master's thesis supervisor

Alma Mater Studiorum - University of Bologna, Department of Chemistry "Giacomo Ciamician",

Bologna, Italy Email: <u>cristina.puzzarini@unibo.it</u>

#### • Prof. Filippo Lipparini

Master's thesis supervisor

Associate Professor University of Pisa, Department of Chemistry and Industrial Chemistry, Pisa, Italy Email: <u>filippo.lipparini@unipi.it</u>

#### • Prof. Marco Geppi

Bachelor's thesis supervisor

Full Professor University of Pisa, Department of Chemistry and Industrial Chemistry, Pisa, Italy Email: <u>marco.geppi@unipi.it</u>

# ATTACHMENTS

- Cambridge English C2 Proficiency Qualification
- IELTS Test Report Form





# Cambridge English Level 3 Certificate in ESOL International (Proficiency)\*

This is to certify that

#### ALESSANDRA SAVARESE

has been awarded

Grade B

in the

# **Certificate of Proficiency in English**

213

Council of Europe Level C2

Overall	Score	
	C 3154	

Reading	224
Use of English	219
Writing	207
Listening	212
Speaking	203
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Christie Nuttall

Christine Nuttall Chief Executive

\* This level refers to the UK National Qualifications Framework

Date of Issue 23/01/2019 Certificate Number A7500845 Regulated by Ofqual Execution of the second second





#### **Test Report Form**

ACADEMIC

 NOTE
 Admission to undergraduate and post graduate courses should be based on the ACADEMIC Reading and Writing Modules.<br/>GENERAL TRAINING Reading and Writing Modules are not designed to test the full range of language skills required for academic purposes.<br/>It is recommended that the candidate's language ability as indicated in this Test Report Form be re-assessed after two years from the date of the test.<br/>To find out more about IELTS, IELTS band scores and the CEFR levels, please visit ielts.org/scores

 Centre Number
 IT010
 Date
 09/NOV/2024
 Candidate Number
 513009

#### **Candidate Details**

Family Name	SAVARESE					
First Name(s)	ALESSANDRA				00	
Candidate ID	CA09225HN				2.5	
Date of Birth	07/02/2001	Sex (M/	/F) F	Scheme Coc	le Private Candidate	
Country or Region of Origin						
Country of Nationality	ITALY					
First Language	ITALIAN					
Test Results						
Listening 9.0	Reading 9.0 W	<b>/riting</b> 7.5	Speaking	7.5 Over Score	all 8.5 CEFR C2	
Administrator (	Comments				Validation stamp	
				Recognising organisations m verify this score ielts.org/verif	ust at y	
	Date	11/11/2024	Te Fo	est Report orm Number	24IT513009SAVA010A	



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