

CURRICULUM VITAE

Name: Pujarini Banerjee

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Academic Background:

- **B. Sc.** in Chemistry (Honours) (2005–2008), Presidency College, Kolkata, West Bengal, India.
- **M. Sc (Integrated PhD)** in Chemistry: (2008–2010) Indian Association for the Cultivation of Science, Kolkata, West Bengal, India.
- **Ph. D** (2010-2016) in Molecular Spectroscopy, at Department of Physical Chemistry, Indian Association for the Cultivation of Science, Kolkata, West Bengal, India
- **Research Associate** (2017-2018) at Department of Physical Chemistry, Indian Association for the Cultivation of Science, Kolkata, West Bengal, India

Awards:

- Awarded post-BSc Integrated PhD fellowship in July 2008 at the Indian Association for the Cultivation of Science, Kolkata, West Bengal
- Qualified for CSIR-UGC NET(LS) in December 2009.
- Qualified in GATE, 2010
- Member, Royal Society of Chemistry, 2017

Research interests:

My research interests involve the IR spectroscopic elucidation of structures and conformations of atmospherically and biologically important molecules, and various non-covalent interactions involving such molecules. Also, understanding of the physical origin of infrared spectral shifts in binary non-covalently bonded complexes is an aim of the research. Molecular complexes are synthesized in solution at ambient conditions, or in cryogenic environment. Additionally, molecular structures are investigated in gas phase at high resolution. The results are supported and interpreted by state-of-art quantum chemical calculations.

List of publications:

- 1) CH...O Interaction Lowers Hydrogen Transfer Barrier to Keto–Enol Tautomerization of β -Cyclohexanedione: Combined Infrared Spectroscopic and Electronic Structure

Calculation Study, Biman Bandyopadhyay, Prasenjit Pandey, Pujarini Banerjee, Amit K. Samanta and Tapas Chakraborty J Phys. Chem A **2012**, 116, 3836-3845.

- 2) Why does ethane prefer staggered conformation? Pujarini Banerjee and Tapas Chakraborty Education in Chemical Science and Technology (Published by Indian Chemical Society) **2013**, 1, 19-25.
- 3) Correlation of ν_{OH} Spectral Shifts of Phenol–Benzene O–H $\cdots\pi$ Hydrogen-Bonded Complexes with Donor's Acidity: A Combined Matrix Isolation, Infrared Spectroscopy, and Quantum Chemistry Study, Pujarini Banerjee and Tapas Chakraborty J Phys. Chem A **2014**, 118, 7074-7084.
- 4) On the Origin of Donor O–H Bond Weakening in Phenol-Water Complexes, Pujarini Banerjee, Deb Pratim Mukhopadhyay, Tapas Chakraborty, J. Chem. Phys. **2015**, 143, 204306-1-9
- 5) Gas-Phase Molecular Spectroscopy in the Past Five Decades: Bearings of the Advancements in Light Source Technologies, Pujarini Banerjee; Tapas Chakraborty, Proceedings of the National Academy of Sciences, India **2015**, 85, 501.
- 6) Matrix Isolation Infrared Spectroscopy of an O–H $\cdots\pi$ Hydrogen-Bonded Complex between Formic Acid and Benzene, Pujarini Banerjee, Indrani Bhattacharya and Tapas Chakraborty, J Phys. Chem A **2016**, 120, 3731-3739.
- 7) Matrix Isolation Infrared Spectra of O–H $\cdots\pi$ Hydrogen Bonded Complexes of Acetic Acid and Trifluoroacetic acid with Benzene, Pujarini Banerjee, Indrani Bhattacharya and Tapas Chakraborty, J. Chem. Sci. **2016**, 128, 1549-1555.
- 8) Cooperative effect on phenolic ν_{OH} frequencies in 1:1 hydrogen bonded complexes of o-fluorophenols with water: A matrix isolation infrared spectroscopic study, Pujarini Banerjee, Indrani Bhattacharya and Tapas Chakraborty, Spectrochim. Acta Mol. Biomol. Spectrosc. **2017**, 181, 116-121.
- 9) Antagonistic Interplay between an Intermolecular CH \cdots O and an Intramolecular OH \cdots O Hydrogen Bond in a 1:1 Complex between 1,2-cyclohexanedione and Chloroform: A Combined Matrix Isolation Infrared and Quantum Chemistry Study, Amit Kumar Samanta, Pujarini Banerjee, Biman Bandyopadhyay, Prasenjit Pandey and Tapas Chakraborty, J. Phys. Chem. A **2017**, 121, 6012–6020.
- 10) Weak hydrogen bonds: insights from vibrational spectroscopic studies, Pujarini Banerjee and Tapas Chakraborty, Int. Rev. Phys. Chem **2018**, 37, 83–123.
- 11) Stereo-preference of camphor for H-bonding with phenol, methanol and chloroform: A combined matrix isolation IR spectroscopic and quantum chemical investigation, Pujarini

Banerjee, Prasenjit Pandey and Biman Bandyopadhyay, *Spectrochim. Acta Mol. Biomol. Spectrosc.* **2019**, 209, 186-195.

- 12) Modulations of $\nu_{\text{O-H}}$ and $\nu_{\text{C=O}}$ Stretching Frequencies of Difluoroacetic Acid with Internal Rotation of CHF_2 Rotor: A Combined Vapor Phase and Matrix Isolation Infrared Spectroscopy Study, Indrani Bhattacharya, Pujarini Banerjee, Jayshree Sadhukhan, and Tapas Chakraborty, *J. Phys. Chem. A* 2019, 123, 13, 2771–277
- 13) $\text{CH}\cdots\text{O}$ H-bond mediated tautomerization of 2-methyl-1,3-cyclohexanedione: A combined IR spectroscopic and theoretical study, Pujarini Banerjee^a, Prasenjit Pandey^b, Biman Bandyopadhyay, *Spectrochim. Acta Mol. Biomol. Spectrosc.* 2021, 253, 119550 (2021).
- 14) Direct matrix isolation IR spectroscopic evidence of halogen bonding from a comparative study of complexes of CBr_4 and CCl_4 with acetone and formic acid, Pujarini Banerjee, Indrani Bhattacharya, *Spectrochim. Acta Mol. Biomol. Spectrosc.* 2021, 250, 119355
- 15) Confinement effects on C–H and C–F stretching vibrational frequencies of difluoromethane in cold inert gas matrixes: a combined infrared spectroscopy and electronic structure theory study, Pujarini Banerjee, Tapas Chakraborty, *European Physical Journal D*, 2021, **75**, 131.
- 16) Separation of $^{71,72}\text{As}$ from alpha-particle induced reaction on gallium oxide target using naturally occurring alkaloid caffeine, Sayantani Mitra, Nabanita Naskar, Puja Samanta, Pujarini Banerjee, Susanta Lahiri*, Kalpita Ghosh and Punarbasu Chaudhuri, *Radiochimica Acta*, 2023, 111, 691.
- 17) Separation of ^{90}Nb from bulk yttrium target using two food derived alkaloids, Sayantani Mitra, Nabanita Naskar, Puja Samanta, Pujarini Banerjee, Susanta Lahiri*, and Punarbasu Chaudhuri, *J Radioanal Nucl Chem.* 2024, 333, 1393
- 18) From ‘halogen’ to ‘tetrel’ bonds: matrix isolation IR spectroscopic and quantum mechanical studies of the effect of central atom substitution in donor tetrahalogens on binary complex formation with formic acid, Indrani Bhattacharya and Pujarini Banerjee, *Phys. Chem. Chem. Phys.*, 2024, 26, 21538

Details of major national/international events attended:

- 1) **Name of event:** 70th International Symposium on Molecular Spectroscopy, 2015
Date: 22-26 June 2015
Venue: University of Illinois at Urbana-Champaign, US

Title of talks: (i) Matrix isolation infrared spectroscopy of a series of 1:1 phenol-water complexes
(ii) Matrix isolation IR spectroscopy and quantum chemistry study of 1:1 π -hydrogen bonded complexes of benzene with a series of fluorophenols
(iii) Matrix isolation IR spectroscopy of 1:1 complexes of Acetic and Trihaloacetic acids with water and benzene.

2) **Name of event:** 4th International Conference on Physical and Theoretical Chemistry

Date: 18-19 Sept, 2017

Venue: Dublin, Ireland

Title of talk: Matrix isolation infrared spectroscopy and structures of weak (O-H $\cdots\pi$) and strongly bound (O-H \cdots O) binary hydrogen bonded complexes

3) **Name of event:** Conference on Electronic Structure, Spectroscopy and Dynamics

Date: Feb 22-25, 2018

Venue: Indian Association for the Cultivation of Science, Kolkata, West Bengal, India

Title of talk: Matrix isolation IR spectroscopy of strong (O-H \cdots O) and weakly bound (O-H $\cdots\pi$) binary H-bonded complexes: Origin of donor $\nu_{\text{O-H}}$ shift

4) **Name of event :** 6th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS), 2016

Date: 5-8 November, 2016

Venue: University of Lucknow, India

Title of talk: Matrix Isolation Infrared Spectroscopy of Phenol-Water complexes

5) **Name of event:** 11th Discussion Meeting on Spectroscopy and Dynamics of Molecules and Clusters 2014

Date: 20-23 February, 2014

Venue: The Hans Coco Palms, Puri, Odisha, India

Title of poster: $\nu_{\text{O-H}}$ Spectral shifts of phenol-benzene O-H $\cdots\pi$ hydrogen bonded complexes correlate with donor's acidity (pK_a): Matrix isolation IR spectroscopy and quantum chemistry study

6) **Name of event:** 12th Discussion Meeting on Spectroscopy and Dynamics of Molecules and Clusters 2015

Date: 19-22 February, 2015

Venue: The Naini Retreat, Nainital, Uttarakhand, India

Title of poster: Matrix Isolation Infrared Spectra of 1:1 Complexes of Water with a series of Fluorophenols

7) **Name of event:** Application of Radiotracers and Energetic Beams in Sciences

Date: January 31st to February 5th, 2023

Venue: Sidho Kanho Birsha University, Purulia, India

Title of poster: Prediction of Nature-resourced chemicals-metal conjugates by theoretical computational study