

## CURRICULUM VITAE

**Name:** Pujarini Banerjee

**E-mail:** pujarini.banerjee87@gmail.com



### 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

### Research interests:

My research interests involve the understanding of the physical origin of infrared spectral shifts in binary hydrogen bonded complexes from interpretation of experimentally obtained high resolution IR spectroscopic data. The molecules of interest are primarily small organic molecules of atmospheric or biological relevance. The binary complexes are generally synthesized in matrices of inert gases at very low temperatures of ~8K. This involves working with high vacuum equipment under cryogenic conditions. The results are supported by state-of-art quantum chemical calculations performed primarily with the Gaussian and Gamess program packages.

### List of publications:

- 1) CH...O Interaction Lowers Hydrogen Transfer Barrier to Keto–Enol Tautomerization of  $\beta$ -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  $\nu_{\text{OH}}$  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  $\nu_{\text{O–H}}$  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  $\text{CHF}_2$  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**, DOI: 10.1021/acs.jpca.8b12528

#### Details of major national/international events attended:

- 1) Name of event:** *70<sup>th</sup> 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  $\pi$ -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:** *4<sup>th</sup> 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 ( $\text{O-H}\cdots\pi$ ) and strongly bound ( $\text{O-H}\cdots\text{O}$ ) 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 ( $\text{O-H}\cdots\text{O}$ ) and weakly bound ( $\text{O-H}\cdots\pi$ ) 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 ( $\text{p}K_{\text{a}}$ ): 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