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India's most important event on

**Vibrational Spectroscopy**

that links research with applications



Department of Science & Technology  
Ministry of Science & Technology  
Government of India



**VIII International Conference**

**on**

**Perspectives in Vibrational Spectroscopy**

**(8th ICOPVS-2020)**

**February 24 - 29, 2020**

**Organised by: JNCASR, Jakkur P. O., Bengaluru- 560 064, INDIA**



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## ICOPVS 2020

We are happy to invite and welcome you to the 8th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS) to be held at Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) in the garden city of Bengaluru, India during 24-29 February 2020. As a conference dedicated to recent advances in all areas of Vibrational spectroscopy, the International Conference on Perspectives in Vibrational Spectroscopy is an opportunity to share, discuss and exchange latest scientific knowledge, innovative ideas and up to date research developments in Vibrational spectroscopy.

## About ICOPVS

ICOPVS has come up as the most important international conference on Vibrational/Raman Spectroscopy, held biennially in India as a vibrant academic platform of Internationally renowned research professionals and inspired students. Founded and initiated at CCS Meerut University, by a community of committed, passionate International and Indian Vibrational Spectroscopy professionals led by Professor Wolfgang Kiefer (Germany) and Professor Vinod Rastogi (India) in 2006, ICOPVS has become an attractive avenue of Vibrational Spectroscopists around the world.

The 8<sup>th</sup> ICOPVS-2020, is setting the stage for the decade long visionary global scientific mission for Vibrational and Raman spectroscopy research excellence, and is being hosted at JNCASR, Bengaluru, India's prestigious centre for advanced research founded by Professor C N R Rao.

The scientific sessions of ICOPVS consist of plenary talks, invited talks, contributed talks, and poster presentations. Awards are made to outstanding presentations/fellows, two awards for young scientists and a number of poster prizes.

ICOPVS 2020 aims to provide the best opportunity to connect with researchers, application scientists and instrumentation developers actively involved in Vibrational Spectroscopy research and implementation, leading to unique opportunities to build relationships and valuable partnerships.

ICOPVS is expected to showcase the galaxy of outstanding researchers, application applied scientists, medical professionals, engineers, instrumentation developers and grad students, connected to Vibrational / Raman Spectroscopy from universities, research institutes, government agencies, and industry.

## HISTORY

Vibrational Spectroscopy consisting of Raman and Infrared spectroscopy, has become a very vibrant research and technology area, as it allows an easy interpretation and highly sensitive structural identification of trace amounts of chemicals based on their unique Vibrational characteristics (fingerprints). The novel applications of Raman spectroscopy and recent technology developments in Vibrational spectroscopy, have resulted in advanced newer technologies and devices with potential for much more innovative science and technology applications.

India has made significant scientific contribution to Vibrational Spectroscopy during the past 90 years with the discovery of Raman Effect by Sir C V Raman in 1928 and the remarkable contributions of Professor C N R Rao in the fields of Infrared spectroscopy and Chemistry of vibrational spectroscopy during the past six decades.

The coming decade (2020-2030) is very significant for the scientific world and India, as we are getting ready for well directed research excellence with new Vibrational and Raman spectroscopic innovations as the world moves forward towards 100 years of Raman Spectroscopy in 2030.



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**8<sup>th</sup> ICOPVS - 2020** will be held in beautiful portal of Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur P.O., Bengaluru - 560064, INDIA, during February 24-29, 2020, with Prof Chandrabhas Narayana as conference Chair. On behalf of Organising Committee of ICOPVS-2020, we feel pleasure in inviting you to participate actively in this exciting conference.

**icopvs20@gmail.com**

Patron : **C N R Rao** (JNCASR, Bangalore, India)

Hony Chairman : **W Kiefer** (Germany) | Hony Vice Chairman : **Pingheng Tan** (China)

Conference Chair: **Chandrabhas Narayana** (India)

Co-chair : **Umesh V Waghmare** (India), **A Sundaresan** (India)

### REGISTRATION FEE:

Faculty/Scientists	Rs. 4,500/-
Research Students/Post Docs	Rs. 3,000/-*
Foreign participants	US \$ 450
Foreign students/Post Docs	US \$ 250
Participant from Industries	Rs. 7,500/-

*(Registration Fee doesn't include Accommodation)*

\* Research students early bird registration includes accommodation

**For Members of Indian Spectroscopy Society there will be a discount of Rs. 500/- before August 6, 2019.**

They can submit their Registration through Indian Spectroscopy Society.

**Abstract:** One Full Page (A4 size), may be submitted on icopvs20@gmail.com

### ACCOMMODATION FEE:

Hotel Attide	Rs. 4000/- (Single), Rs. 4500/- (Double)
White Castle	Rs. 4000/- (Single), Rs. 4500/- (Double)
I-House	Rs. 1400/-
Jawahar Guest House	Rs. 1120/-
Centenary Guest House	Rs. 1500/- and 1200/-
New Visiting Student's Hostel	- 350/- (for students)

### Confirmed Speakers

- |                                |                                     |                                  |
|--------------------------------|-------------------------------------|----------------------------------|
| 1. Wolfgang Kiefer (Germany)   | 17. R S Stenner (USA)               | 33. Ralf Ludwig (Germany)        |
| 2. Ajay Sood (India)           | 18. Pedro Venezuela (Brazil)        | 34. Michael Springborg (Germany) |
| 3. S. Umapathy (India)         | 19. Wei Xie (China)                 | 35. Johannes Kiefer (Germany)    |
| 4. Hiro-o Hamaguchi (Japan)    | 20. Mustafa Culha (Turkey)          | 36. Torsten Frosch (Germany)     |
| 5. Janina Kneipp (Germany)     | 21. Young Mee Jung (Korea)          | 37. T Yamamoto (Japan)           |
| 6. Koichi Iwata (Japan)        | 22. L Nafie (USA)                   | 38. Alain Polian (France)        |
| 7. J Popp (Germany)            | 23. Oliver Pages (France)           | 39. Sevim Akyuz (Turkey)         |
| 8. Giulietta Smulevich (Italy) | 24. Mariangela Di Donato (Italy)    | 40. S Prabhu (India)             |
| 9. Abhay Shukla (France)       | 25. Yang Yang (China)               | 41. Alka Ingale (India)          |
| 10. Kendall Cathrine (UK)      | 26. Dennis K Hore (Canada)          | 42. Biman Bagchi (India)         |
| 11. Ingo Fischer (Germany)     | 27. Gerwin Puppels (Netherlands)    | 43. Sandip Dhara (India)         |
| 12. H Barr (UK)                | 28. Katarzyna Maria MARZEC (Poland) | 44. Samrat Mukhopadhyay (India)  |
| 13. Hartwig Schulz (Germany)   | 29. Tobias Brixner (Wurzburg)       | 45. Venugopal Rao Soma (India)   |
| 14. M A Palafox (Spain)        | 30. Kamilla MALEK (Poland)          | 46. Goutam Dev Mukherjee (India) |
| 15. Pinheng Tan (China)        | 31. Andrea Lapini (Italy)           | 47. Anushree Roy (India)         |
| 16. Jae Hyeon Ko (Korea)       | 32. Katarzyna Majzner (Poland)      | 48. Poonam Tandon (India)        |
|                                |                                     | 49. Surajit Saha (India)         |

### IMPORTANT DATES

Release of Brochure	: 18 July 2019
Early Bird Registration deadline	: 6 August 2019
Abstract (One A4 size page) submission deadline	: 31 August 2019
Abstract acceptance notification	: 31 October 2019
Regular Registration deadline	: 31 December 2019

*Note: The acceptance of Abstracts will be sent only after proper review process by a committee*



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## AWARDS / PRIZES:

\* Dayawati Rastogi Lecture Award (Male) : Rs. 21,000/- (Aprox US \$: 300 + Citation)

\* Dayawati Rastogi Lecture Award (Female) : Rs. 21,000/- (Aprox US \$: 300 + Citation)

First Dayawati Rastogi lecture Award was jointly given to Prof Pingheng Tan (China) and Prof Manik Pradhan (India) and the Second Dayawati Rastogi Award was given to Prof S Schlücker (Essen, Germany).

**Prizes: There are 6 Prizes each for Rs. 2000/- + Citation**

(3 for Oral Presentation and 3 for Poster Presentation)

### Contact

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### Sample Abstract

**FTIR and FT-Raman spectra of the biomolecule 5-Fluorocytosine. Effect of the fluorine atom in the interaction with human proteins (Molecular Docking) and in the microhelix DNA:RNA**

**W Kiefer<sup>1</sup> and V K Rastogi<sup>2</sup>**

<sup>1</sup>Institute for Physical and Theoretical Chemistry, University of Würzburg, Germany, and  
<sup>2</sup>Eisingen Laboratory for Applied Raman Spectroscopy, Eisingen, Germany

<sup>3</sup>Indian Spectroscopy Society, KC 68/1, Old Kavinagar, Ghaziabad-201 002, India

The properties of purine and pyrimidine bases are determined by their hydrogen and  $\pi$ -bonding systems [1]. Past crystallographic studies [2] have indicated that halogen substituents affect solid state base stacking patterns, and have suggested that stacking interactions involving the halogen substituents may contribute to the unusual physical and biological properties of nucleic acids which contain halogenated pyrimidines [3]. A survey of large number of synthetic pyrimidines having interesting biological properties reveals that in such compounds, the position of importance is C-5 and C-6 [4]. 5-Fluorocytosine (5-FC) (Fig 1) and its nucleoside exhibit anti-tumor (anti-leukemia), anti-fungal and anti-viral activities [5]. Its experimental and theoretical IR spectra including tautomerism have been carried out.



Fig. 1. Structure of 5-FC.

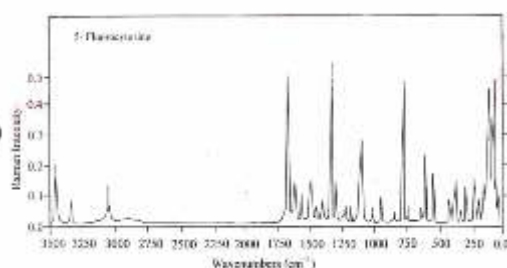


Fig. 2. Raman spectrum of 5-FC in KBr pellets.

The FT-Raman and FT-IR spectra of 5-FC were recorded (Fig 2) and accurately assigned in the solid state using the B3LYP method together with the LSE scaling procedure and the solid state simulation of the crystal unit cell through a tetramer form. With the 6-31G(d,p) basis set was used the LSE:

$$n_{\text{scal}} = 34.6 + 0.9447 \cdot n_{\text{cal}}$$

### Summary and conclusion

(i) The harmonic wavenumbers of 5-FC in the isolated state and in tetramer forms were calculated at the B3LYP level. . In the isolated state, the scaled vibrational wavenumber appear reasonable when they are compared with IR experimental data in Ar matrix. (ii) In the solid state the scaled wavenumbers of the simulated tetramer form also appear in accordance with the experimental IR and Raman data. The studies indicated that the biomolecule 5-FC in solid state exists mainly/only in the amino-oxo form. (iii) Many common features were found between the spectra of 5-FC and those of cytosine. The assignments proposed, in most cases, agree well with those reported earlier, although some bands were now better identified, and the use of an accurate scaling equation procedure remarkably reduces the error in the calculated wavenumbers. Thus, the assignment of most of the fundamentals provided in this work is believed to be unambiguous. (iv) The molecular docking analysis confirms that the 5-FC molecule may play an important role as a promising inhibitor against breast cancer. (v) A decrease in the stability of the base pairs appears when the fluorine atom is introduced, leading to a remarkable increment in the rise  $D_z$  parameter of the microhelix and a slight increment in its diameter  $d$ .

### References

1. Fallen Lawrence III, *Acta Cryst*, B29(1973)2549-2556.
2. Sternglanz H, Freeman G R, Bugge Charles, *Acta Cryst*, B31(1975)1393-1395.
3. Chandra R, Chawla S C, Singh A, Gupta S L, *Asian J Phys*, 2(1993)109-112.
4. Palafox M A, Rastogi V K, Singh S P, *Spectrochim Acta*, A188(1918)418-423.
5. Palafox M A, Rastogi V K, Kumar S, Joe I H, *Spectrochim Acta*, A111(1913)104-122.



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