

A training session report on
**Applications of XRD and FTIR in Science and
Technology**

Under STUTI program funded by DST



In association with
Indian Institute of Technology, Gandhinagar
(Project Management Unit)



Coordinated by

Dr. Ravi Katare

Department of Physics

Govt. Science College, Jabalpur, Madhya Pradesh India

1st to 7th November 2022

Acknowledgement

We convey gratitude for the encouragement and support received from multiple sources during the execution of this training since its beginning. First and foremost, we want to express our sincere appreciation to the IIT Gandhinagar (PMU) and Department of Science and Technology (DST) for entrusting us with this project. The workshop was coordinated by **Dr. Ravi Katare** and **Shikha Saxena** on the '*Applications of XRD and FTIR Techniques in Science and Technology*' on the instrument funded by the FIST program for **FTIR** (Sanction No.: SR/FIST/CS-I-020/2003) and for **XRD** (Sanction No.: SR/FST/College-079/2011). Our whole organizing team acknowledge the contributions of Resource persons & Participants in the implementation and the execution of the program to achieve the objectives of the workshop, particularly, **Dr.S.N.Acharya**, (NEMS, Chemistry Division, BARC, Mumbai), **Dr.Manik Roy**, (Chemistry Division, BARC, Mumbai), **Dr.Pankaj Sagdeo** (IIT Indore) **Dr.Uday Deshpandey**, (IIT Indore, M.P.), **Dr.Archana Sagdeo** (RRCAT Indore) **Dr. Naresh Kumar**, (MNNIT, Allahabad, U.P.), **Dr. P. D.Sahare**, (University of Delhi), **Dr.Shahid Anwar**, (CSIR, IMMT, Bhubnashwar, Odisha), **Mr. Bharat Phatak** (Lab India, Barodara, Gujrat), **Mr. Praveen Tirmali** (IR Technology), **Ms. Kavita Negi** (Ph.D. scholar) and **Mr. Om Prakesh** (Ph.D. scholar). We also acknowledge the contributions of laboratories staff without which these sessions could not have been possible. We also specially acknowledge the support of our College Principal **Dr. A. L.Mahobia**, **Dr.K.S.Dubey** (Prof. & Head, Department of Chemistry and all our colleagues of department of Physics and Chemistry.

Dr. Ravi Katare

Coordinator

Summary

The objective of this workshop was to popularize X-ray diffractometer (XRD) and Fourier Transfer Infrared (FTIR) techniques and the facility among students, faculty and scientists through a weeklong training workshop. The workshop was conducted at Government Science College, Jabalpur, M.P. from 01st to 07th Nov. 2022 and comprised of lectures and hands on training sessions. This initiative was funded by Department of Science & Technology under the program STUTI (Synergistic Training Program Utilizing the Scientific and Technological Infrastructure). This workshop was aimed to provide an insight into the basic principles and various techniques of crystallization of small molecules and atoms, functioning of X-Ray Diffractometer (XRD) instrument, crystal data analysis and interpretation, applications of XRD in material, pharmaceutical, biological sciences and Polymer Science. The workshop has also provided the basic knowledge about the principle, working and its applications of FTIR technique. The participants were introduced to the basic concepts of image generation, instrumentation, troubleshooting and the advanced modes of operation. The main focus of this workshop was to have *“A balance between theory and practical training on the equipment. Emphasis was on hands-on use of equipment for demonstration/ characterization by each participant and analysis of samples”* provided by participants.

Introduction

Government Science College, Jabalpur, M.P. conducted 7 - days long workshop on DST- FIST funded XRD and FTIR instrument in the campus. The participants from various backgrounds such as Post Graduate, B.Tech., Professors, and Ph.D. Fellows were invited (**Annex-1**). The resource persons from various prestigious institutes like BARC, UGC- DAE- CSR MNNIT, IIT Indore CSIR-IMMT and Delhi University were invited for the lecture and Hands on training (**Annex-2**). The following workshop's activities took place from 1st to 7th Nov. 2022 (**Annex-3**). This report provides a quick overview of both the lecture and technical sessions.

- Lecture Sessions:

Dr. Pankaj Sagdeo (Department of Physics, IIT Indore MP) gave an the overview on basic Crystallography and some of the essential principles and physics behind the operation during X-ray diffraction in significant detail, which made it easier for participants to understand the procedure while doing hands-on activities. **Dr.Archana Sagdeo** (Department of Physics, IIT Indore MP) discussed the data analysis and processing of X-Ray Diffraction pattern of various materials. She has nicely discussed the various pattern of X-ray diffraction and the applications of materials used in different field. **Mr.Bharat Phatak** (Lab India Vadodara, Gujrat) gave the detailed knowledge about FTIR Spectroscopy and importance of finger print region. He also delivered a lecture on Elucidation Functionality by IR spectrum and gave through knowledge about FTIR analysis. Mr. Phatak nicely gave hands on training on FTIR instrument and explained various applications of FTIR to determine the structure of molecules during IR absorption. **Dr.Gandhiji Griya** (Lab India Vadodara, Gujrat) explained the utility of OOPS Software connected with FTIR Instrument. **Dr. S.N.Acharya** (Department of Chemistry, NEMS, BARC, Mumbai) delivered a lecture on X-ray Diffraction & Generation. He explained the whole applicability of XRD instrument and discussed the powder, crystalline and amorphous materials for single crystal and polycrystalline material. With the help of mathematical formulas, He gave the analysis of X-Ray diffraction patterns and explained the role of points group and symmetries.

Dr. Mainak Roy (Department of Chemistry, NEMS, BARC, and Mumbai) has delivered a lecture on sample preparations and operation of FTIR Spectrophotometer and analysis of FTIR spectrum and explained the role of near and far IR region distribution for various types of bonds present in organic molecules. **Dr. Roy** explained the use of various above 1500 cm⁻¹ and fingerprint region. **Dr. Naresh Kumar** (Department of Physics, MNNIT, Allahabad, UP) delivered a lecture on crystal structure determination and sample analysis, he also gave hands on training on single crystal screening & data analysis. **Dr. P. D. Sahare** (Department of Physics, University of Delhi) delivered a lecture on crystalline X-ray radiation of powder diffractions in which he gave various ideas of analysis of materials which are being used for different fields. **Dr. Shahid Anwar** (CSIR, IMMT Bhubaneswar, Odisha) gave a lecture on applications of XRD in materials research. He explained the systematic manner of XRD technique used for the observation of materials used in research work.

- *Technical Session*

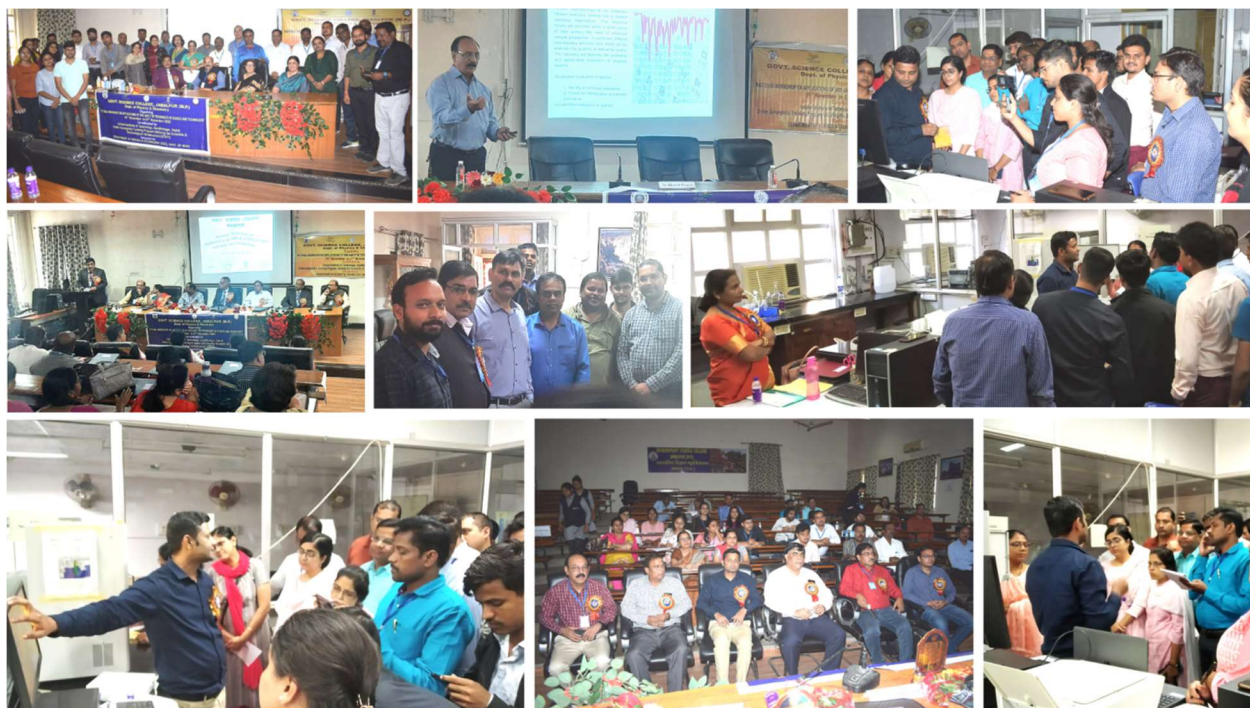
On the **second** day, **Mr. Bharat Phatak** (Lab India Vadodara, Gujrat) and **Dr. Mona Markam** started the training session by giving a general overview of analysis of sample on the latest ATR FTIR and Shimadzu 8400s. They have given the hands on training of the sample as well as its applications in the chemistry and pharmaceutical industries. On the **third** day, **Dr. S. N. Acharya** (Department of Chemistry, NEMS, BARC, Mumbai) has given the technique which allows the identification of structural changes in the molecular bonding and chemical shifts and to investigate the surface adsorption of functional groups on nano-particles. On the fourth day, all participants were granted access to the XRD setup in order to provide hands-on training by **Dr. Mainak Roy** and **Mr. Praveen Tirmali**. The participants were briefed about how to get the parameters for diffraction data collection. Also, they were taught about acquiring data from an unknown material. Fifth day's session included a similar activity of reviewing the specifics of data gathering methods from software, as monitored by **Dr. Naresh Kumar** and **Mr. Gandhiji Giriya**. The session included a discussion with participants on several fundamental principles and case studies, including crystal structure refinements, in-situ cryo-crystallization, and phase indexation. The sixth day was a concluding session in which **Dr. P. D. Sahare & Dr. Shahid Anwar** handled many participant questions on technical and software difficulties.

- Types of samples tested

During the technical session, all of the participants expressed their interest in learning from the workshop and characterized many samples with FTIR. **Mr. P. Maheshwar Reddy** analyzed some building materials based on biocomposite sample of the codes TPIPA, TPB1, TPB, FB, FB1, PILM3, PILM4. **Ms. Runjhun Dutta** analyzed semiconductor materials sample of the codes LFO, LFO+MWCNT, LW+MWCNT. **Mr. Ayush Dutta** analyzed semiconductor materials sample of the codes CZT, TZC. **Mr. Nishad** analyzed Nanoparticle sample of code ZrO. **Ms. Kavita Negi** analyzed Nanoparticle sample of code CdS, ZnS, aa, P+C, P+Z. and **Sonal Dhuria** analyzed Nanoparticle sample of code C-O, PS. In addition, the hands on training by **Dr. Praveen Tirmali** and analysis some of the sample by XRD (Rigaku). **Mr. P. Maheshwar Reddy** analyzed some samples of code TPIPA, TPB1, TPB, FB, FB1, PILM3, PILM4. **Mr. Ganesh Nishad** analyzed some samples of code ZrO. **Ms. Chandrani Samgaddar** analyzed Nanoparticle sample of code CdS, ZnS, aa, P+C, P+Z. and **Sadiya** analyzed Nanoparticle sample of code C-O, PS. In addition, the hands on training given by Dr.Praveen Tirmali and analysis some of the sample by XRD miniflex 600 (Rigaku) **Mr. P. Maheshwar Reddy** analyzed some sample of code TPIPA, TPB1, TPB, FB, FB1, PILM3, PILM4. **Mr. Ganesh Nishad** analyzed some samples of code ZrO. **Ms. Chandrani Samgaddar** analyzed Nanoparticle sample of code CdS, ZnS, aa, P+C, P+Z. and **Sadiya** analyzed Nanoparticle sample of code C-O, PS.

Outcomes of the Workshop

The STUTI workshop attracted participants from **26** different institutes (**Figure 1**). About **32** participants enrolled and attended the FTIR & XRD training sessions. The goal of this training event was to bring together participants from many disciplines and raise awareness of the institute's advanced facilities. Throughout the sessions, participants asked major questions regarding theoretical and practical aspects of FTIR & XRD instrumentations, techniques of developing good quality crystals, disorder treatments. Finally, the feedback from the participants was considered in the evaluation of the workshop (**Annex-4**). The majorities of the participants were pleased with the training session and suggested that more such workshops should be held in the future. Few participants suggested organizing such a workshop/ training sessions on more troubleshooting techniques of data collection.



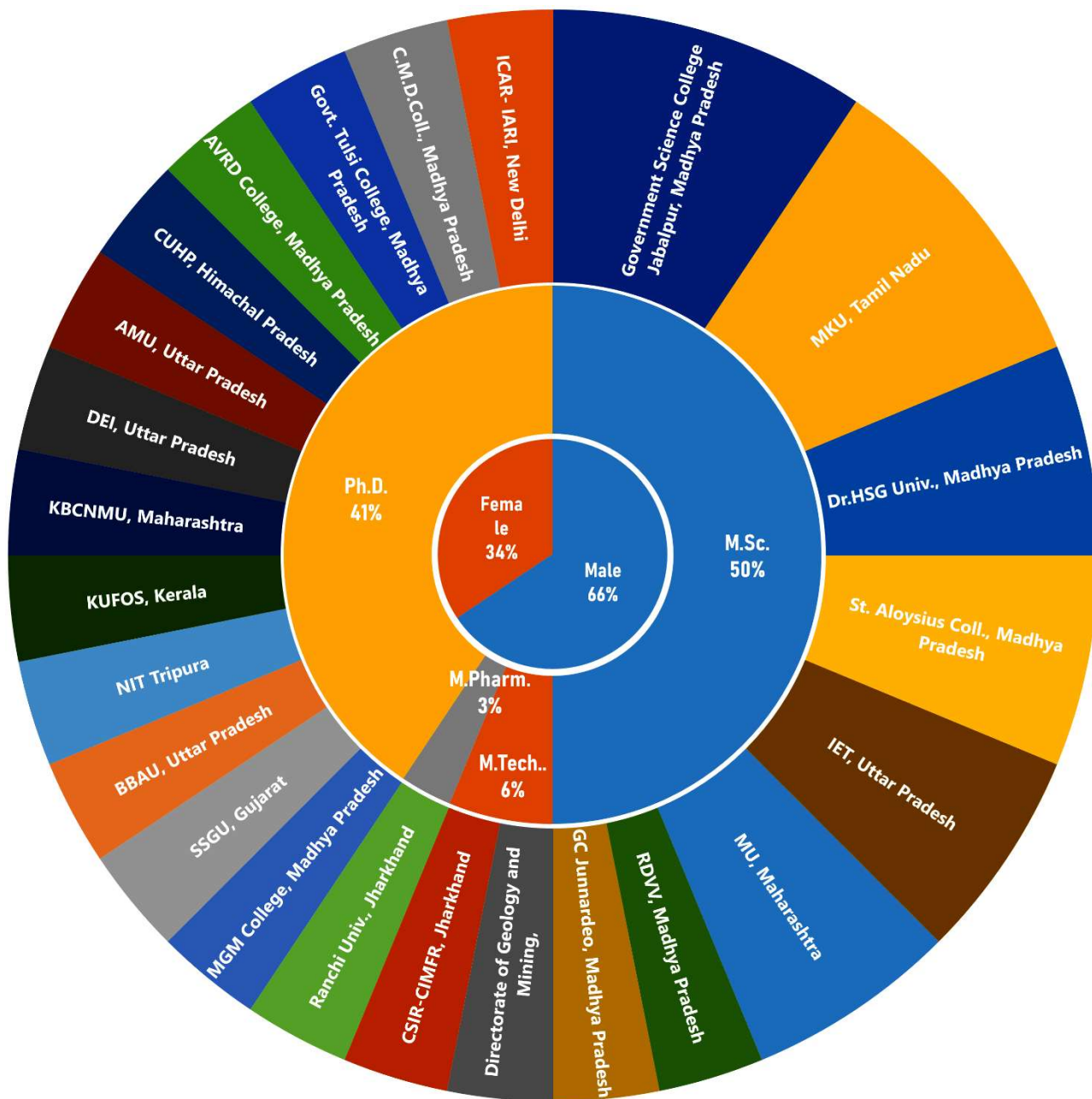


Figure 1. Participants registered workshop from different institutes

Annexure 1: Brochure for the program

Day-6 06.11.2022 Session I&II

- Crystalline X-Ray radiation of Power diffraction.
Speaker : Dr. P.D. Sahare, University of Delhi.
- Applications of XRD in material research.
Speaker : Dr. Shahid Anwar, CSIR, IMMT, Bhubnashwar, Odisha.
- Lab Session 1 Hands on Crystal screening and data collection/Assignment.
- Lab Session 2 Sample analysis of XRD/ Assignment.

Day-7 07.11.2022 Session I&II

- Local Tour.
- Valedictory Session.

Schedule

DAY-1	01.11.2022	DAY-4	04.11.2022
09:00	Registration	10:00	Session I
10:00	Inaugural Session	11:30	Tea Break
11:30	Tea Break	12:00	Session I (contd.)
12:00	Session I	01:30	Lunch
01:30	Lunch	02:30	Session II (Hands on)
02:30	Session II	03:30	Tea Break
03:30	Tea Break	04:00	Session II (Hands on)
04:00	Session II (contd.)		
DAY-2	02.11.2022	DAY-5	05.11.2022
10:00	Session I	10:00	Session I
11:30	Tea Break	11:30	Tea Break
12:00	Session I (contd.)	12:00	Session I (contd.)
01:30	Lunch	01:30	Lunch
02:30	Session II (Hands on)	02:30	Session II (Hands on)
03:30	Tea Break	03:30	Tea Break
04:00	Session II (Hands on)	04:00	Session II (Hands on)
DAY-3	03.11.2022	DAY-6	06.11.2022
10:00	Session I	10:00	Session I
11:30	Tea Break	11:30	Tea Break
12:00	Session I (contd.)	12:00	Session I (contd.)
01:30	Lunch	01:30	Lunch
02:30	Session II (Hands on)	02:30	Session II (Hands on)
03:30	Tea Break	03:30	Tea Break
04:00	Session II (Hands on)	04:00	Session II (Hands on)
		08.00	Networking Dinner
DAY-7	07.11.2022		
10.00	Site visit		
01.30	Lunch		
2.00	Valedictory Session.		

Registration & Contact Details

Participants must register and only selected candidates would be invited for the workshop.

For selected candidates TA, (Only Train/ Bus tickets), local travel, boarding and lodging will be borne by organisers.

Interested participants should register using the link: <https://forms.gle/yvawrg6tBqYQSHrR7>

Registration Deadline 10.10.2022

Short listed candidates will be intimated by email, latest by 15.10.2022

Eligibility criteria:

- Faculty/ Scientists/ Post-Doc Fellows/ Ph.D.
- Research Fellow minimum qualification: Post Graduate in Science.
- Not more than 3 participants from one institute.

For more information

Access:

Website-<http://sciencecollegejabalpur.org>

E-Mail: rkatare1960@gmail.com

shikhasaxena997@gmail.com

Mobile : 9425153690, 9425325697

Address:

GOVT. SCIENCE COLLEGE,

Pachpedi, South Civil Lines

Jabalpur M.P. 482001

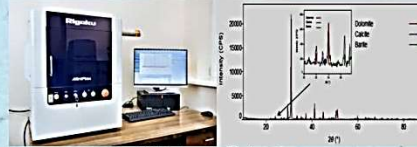
Acknowledgement



GOVT. SCIENCE COLLEGE Jabalpur (M.P.)

Organizing a workshop on
Applications of XRD and FTIR Techniques
in Science and Technology
01st Nov. - 07th Nov. 2022
Co-ordinated by Indian Institute of Technology,
Gandhinagar, Gujrat
Under Synergistic Training Program Utilizing the
Scientific & Technological Infrastructure (STUTI)
Sponsored by:
**Department of Science & Technology (DST)
Govt. of India**

X-Ray Diffractometer



Organizers:

Dr.A.L.Mahobia Principal
Dr. Ravi Katare Coordinator
Dr.Rajendra Kuraria Organizing Secretary

Dr.Shikha Saxena Convener
Dr.Arun Kakkar Co-convener
Dr.R.K.Shrivastava Jt Organizing Secretary

Annexure 2: List of registered participants for the workshop

Sr. No.	Candidate Name	Gender	Educational Qualification	Email address	University/Institute
1	Rohan Upadhyay	Male	M.Sc. (Nanoscience)	rohanupadhyay75@gmail.com	National Centre for Nanosciences and Nanotechnology University of Mumbai, Maharashtra
2	Suraj Shirke	Male	M.Sc. (Nanoscience)	surajshirke058@gmail.com	
3	Shreya Mandal	Female	Ph.D. (Biochem.)	shreyamandal1008@gmail.com	ICAR- Indian Agricultural Research Institute (IARI), Delhi
4	G.S.Argal	Male	Ph.D. (Chemistry)	drgsacy@gmail.com	Government C.M.D.College Maharajpur, Chhatarpur, Madhya Pradesh
5	Chandrani Samadder	Female	M.Sc. (Biotech)	chandranisamadder824@gmail.com	Madurai Kamaraj University, Tamil Nadu
6	Sauravi G.Choudhary	Female	M.Sc. (Biotech)	sauravi.bt@gmail.com	
7	S.M.Nawaz Akhtar	Male	M.Sc. (Biotech)	nawazbiotech11@gmail.com	
8	Sangita Basrani	Female	M.Sc. (Zoology)	sangitabasrani0@gmail.com	Government Tulsi College, Madhya Pradesh
9	Arunendra Kumar Patel	Male	Ph.D. (Physics)	patelarunendra@gmail.com	A.V.R.D.Government College, Madhya Pradesh
10	Jagdish Choudhary	Male	M.Sc. (Botany)	jagdishchoudhary1422000@gmail.com	Central University of Himachal Pradesh, Himachal Pradesh
11	Sadiya	Female	M.Sc. (Chem.)	sayyedsadiya1011@gmail.com	Aligarh Muslim University (AMU), Uttar Pradesh
12	Runjhun Dutta	Female	M.Sc. (Chem.)	runjhunduttaindia@gmail.com	Dayalbagh Educational Institute, Uttar Pradesh
13	Ayush Dutta	Male	M.Tech. (Mechanical)	2100520405002@ietlucknow.ac.in	Institute of Engineering and Technology Lucknow, Uttar Pradesh
14	Lokesh Kumar Dubey	Male	M.Tech. (Mechanical)	2100520405005@ietlucknow.ac.in	
15	Bhalerao Krishna D.	Male	M.Sc. (Chem.)	bhaleraokrishna573@gmail.com	Kavayitri Bahinabai Chaudhari North Maharashtra University, Maharashtra
16	Raja Priya R.	Female	M.Sc.(Biotechnology & Bioinformatics)	rajapriyar28@gmail.com	Kerala University of Fisheries and Ocean Studies, Kerala
17	P.Maheswar Reddy	Male	Ph.D. (Civil)	maheswarcivil.sch@nita.ac.in	National Institute of Technology Agartala, Tripura
18	Mritunjay Rai	Male	M.Sc. (Zoology)	mraibbau2020@gamil.com	Babasaheb Bhimrao Ambedkar University, Uttar Pradesh
19	Zabha Salman Ilyas	Male	M.Sc. (Physics)	salmanzabha1996@gmail.com	Shri Govind Guru University, Gujarat
20	Asra Kareemi	Female	Ph.D. (Chemistry)	asrakareemi2696@gmail.com	St. Aloysius College (Autonomous), Madhya Pradesh
21	Nitin Swamy	Male	Ph.D. (Biotech)	nitin.swamy21@gmail.com	
22	Bassa Satyanarayana	Male	Ph.D. (Chemistry)	satyanarayana.bassa@gmail.com	Government M.G.M. PG College Itarsi, Madhya Pradesh
23	Vikram Yadav	Male	M.Sc. (Geology)	vikramyadav1414@gmail.com	Ranchi University, Jharkhand
24	Akhilesh Agrawal	Male	Ph.D. (Geology)	akhileshgnio@gmail.com	Dr. Harisingh Gour University Sagar, Madhya Pradesh
25	Sunny Rathee	Male	M.Pharm (Pharmaceutical)	sunnyrathee11911@gmail.com	
26	Dependra Pratap Singh	Male	M.Sc. (Geology)	dps.geology@gmail.com	CSIR-Central Institute of Mine and Fuel Research Dhanbad, Jharkhand
27	Priyanka Agrawal	Female	Ph.D. (Chemistry)	22agrl.priya@gmail.com	Directorate of Geology and Mining, Regional office Jabalpur, Madhya Pradesh
28	Sujit Kumar Shende	Male	Ph.D. (Physics)	skshende500@gmail.com	Government College Junnardeo, Madhya Pradesh
29	Ganesh Prasad Nishad	Male	M.Sc. (Physics)	gp.nishad@gmail.com	Government Science College Jabalpur, Madhya Pradesh
30	Jyoti Shrivastava	Female	Ph.D.(Chem.)	jyotilokshri2017@gmail.com	
31	Suman Prabhakar	Female	Ph.D. (Chem.)	prabhakarsiman47@yahoo.com	
32	Mahendra Kumar Bhardwaj	Male	Ph.D.(Physics)	lachi8172@gmail.com	Rani Durgavati Viswavidhyalaya, Jabalpur, Madhya Pradesh

Annexure 3: Schedule date and activities during the workshop

Day-1 Session I&II

- Inauguration and welcome note.
- Introduction of the participants and Hosts.
- Overview of various DST sponsored program.
- Theory, Principle and Applications of IR spectroscopy.
(Speaker) Dr.Anjali Bajpai, Ex. Prof & Head Chemistry, Govt. Science College, Jabalpur
- Instrumentation of FTIR.
(Speaker) Dr.Uday Upadhyay, IIT Indore, M.P.

Day-2 Sessions I&II

- FTIR Spectroscopy and Importance of finger print region.
(Speaker) Mr. Bharat Phatak Lab India, Baroda
- Elucidation of functionality by IR spectrum. FTIR Analysis.
(Speaker) Mr. Bharat Phatak Lab India, Baroda.
Lab Session 1 IR spectrum Elucidation.
- Lab Session 2

Day-3 Sessions I&II

- Data Collection and processing.
(Speaker) Dr.Archana Sagdeo, RRCAT, Indore, M.P.
- Sample Preparation & operation of FTIR spectrophotometer.
(Speaker)Mr. Shashi Bhushan Sharma, IR Technology Service
- Lab Session 1 Analysis of simple/ complex molecules.
- Lab Session 2 Various sampling techniques in FTIR.

Day-4 Session I&II

- An overview on Basic Crystallography.
(Speaker) Dr. Pankaj Sagdeo Liti, IIT, Indore, M.P.
- Analysis of X- Ray Diffraction patterns.
(Speaker) Dr. Naresh Kumar, Head, MNNIT Allahabad, U.P.
- Lab Session 1 Sample preparations of XRD
- Lab Session 2 Typical spectrum patterns.

Day-5 Session I&II

- Various types of X-Ray generator and detector.
(Speaker) Dr.Archana Sagdeo, RRCAT, Indore, M.P.
- X-Ray Diffraction & Generation.
(Speaker) Dr.P.D.Sahare, Deptt. Of Physics & Astrophysics University of Delhi.
- Lab Session 1 Hands on single crystal screening & data analysis.
- Lab Session 2/ Assignment.

Day-6 Session I&II

- Analysis of X-Ray Diffraction pattern.
(Speaker) Dr.Mukesh Kumar Roy, IIITDM, Jabalpur
- Crystalline XRD & powder diffraction.
(Speaker) Dr.N.P.Lalla, Scientist at UGC-DAE, Indore, MP
- Lab Session 1 Hands on Crystal screening and data collection/ Assignment.
- Lab Session 2 Sample analysis of XRD/ Assignment.

Day-7 Session I&II

- Local Tour.
- Valedictory Function.

DAY -1 08.30 Registration 09.00 Inaugural Session 10.00 Session I 11.00 Tea Break 11.30 Session I 01.30 Lunch 02.30 Session II 04.00 Session II	DAY -2 10.00 Session I 11.00 Tea Break 11.30 Session I 12.30 Session I 01.30 Lunch 02.30 Session II (Hands on) 03.30 Session II (Hands on)	DAY -3 10.00 Session I 11.00 Tea Break 11.30 Session I 12.30 Session I 01.30 Lunch 02.30 Session II (Hands on) 03.30 Session II (Hands on)	
DAY -4 10.00 Session I 11.00 Tea Break 11.30 Session I 12.30 Session I 01.30 Lunch 2.30 Session II(Hands on) 3.30 Session II(Hands on)	DAY -5 10.00 Session I 11.00 Tea Break 11.30 Session I 12.30 Session I 01.30 Lunch 2.30 Session II(Hands on) 3.30 Session II(Hands on)	DAY -6 10.00 Session I 11.00 Tea Break 11.30 Session I 12.30 Session I 01.30 Lunch 2.30 Session II(Hands on) 3.30 Session II(Hands on)	DAY -7 10.00 Site visit 01.30 Lunch 2.00 Valedictory Function

Annexure 4: Feedback summary

Sr. No	Content	% Rating
1	Overall grading of the program with reference to relevance of course, module/ content etc.	98% Rated on or above 8 points
2	Overall grading of the facilities provided by the institute, i.e., Hostel, Mess, Classrooms, Transport/infrastructure etc.	99% Rated on or above 8 points
3	Overall grading of the faculty members conducting the training	97% Rated on or above 8 points
4	How do you rate the overall training methodology	98% Rated on or above 8 points
5	How far the field visit is relevant and related to your research study	99% Rated on or above 8 points
6	Usefulness of this training in your current role	98% Rated on or above 8 points
7	Usefulness of this training in future work/job you may handle	98% Rated on or above 8 points
8	How far have you benefitted from interaction with the fellow participants of the training	97% Rated on or above 8 points
9	How far the course material supplied relevant and related to the training curriculum	95% Rated on or above 8 points
10	Overall grading of the process of training	96% Rated on or above 8 points
11	Your recommendation to your peers/ colleagues for the training Program	98% Rated on or above 8 points