### KESHAV MAHAVIDYALAYA

Project Title: Design and development of a low cost computerized laser Raman spectrometer

indigenously for DU student laboratories

Project Code: KM-101



Set-up for Raman Spectrometer and the innovation project students team

### 1. Objective (150 words):

Raman spectroscopy, while continuing to gain importance in material science, chemical and biochemical research, remains an experimental technique not familiar to undergraduate students. The major hurdle of making Raman spectroscopy is the expensive equipments used in the spectroscopy analysis, thus placing the experiment beyond the budgetary scope of most undergraduate student's laboratory. The major objectives of the project are briefly outlined below.

- The present project introduces students to light scattering techniques and a low cost bench-top laser Raman spectrometer was designed and developed using the knowledge and ability of undergraduate students by integrating related technologies in optics, electronics and computer science. Further the setup was calibrated with standard samples. The possible uses of this instrument and its individual module would assist in undergraduate teaching laboratory
- Image processing techniques are used. Neighborhood averaging and smoothing by image averaging are done to remove additive noise and extract pure signal.

Simple ab initio quantum-chemical calculations on Raman vibrational spectra are been done which can provide detailed insight into molecular properties.

# 2.Final Findings (300 words):

A low cost Raman spectrometer is indigenously designed for undergraduate students (set up shown in page 1). The setup has a grating monochromator, photomultiplier-tube detector, and an intense monochromatic light source. The spectrometer uses a green laser pointer ( $\lambda$ =532 nm) to illuminate the sample via a microscope objective. Backscattered Raman radiation is collimated by the same objective, green-laser light is blocked by a filter, and the remaining Raman radiation focused into a glass fiber that is connected to a visible spectrometer with a grating monochromator and a linear diode array CCD detector. Signals are transferred via the USB connection to a computer where the signals are processed and displayed. During data acquisition of the spectrum with CCD, noise superimposes on the signal. Image processing is done to remove the additive noise to extract the pure signal. Most of the noise in the spectrum is recorded by the CCD array arises from different dark currents of the different pixels. The spectra for different liquids were recorded, which were superimposed by noise spectra (an example shown in Fig. 1).

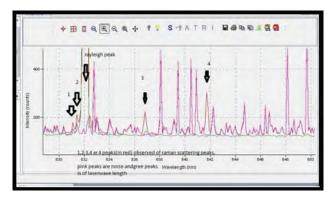


Fig1. Spectra of a sample superimposed by noise.

This systematic noise was reduced by subtracting a stored dark spectrum recorded with the laser switched off. Remaining statistical noise was minimized by increasing the integration time during exposure of the CCD array to achieve high signal levels and by accumulating and averaging several spectra thus using image processing techniques. A typical example is cited below:

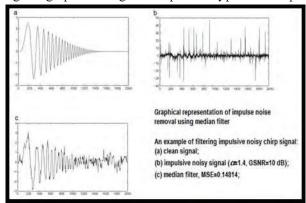


Fig 2: Graphical representation of impulse noise removal using median filter

Fundamental Raman bands were observed corresponding to known spectra of Benzene. For a benzene molecule, there are totally 20 vibrational modes and six of them have very large Raman scattering cross-sections. A dominant band of symmetric CC-ring vibration around 990 cm<sup>-1</sup> was observed.

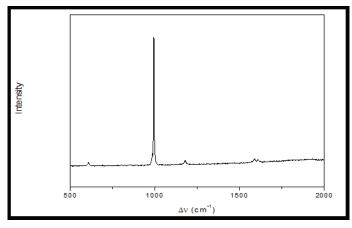
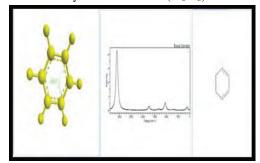


Fig 3: Raman Spectra of liquid Benzene.

In combination with theoretical calculations, spectroscopy can provide detailed insight into molecular properties. In the present project we have performed some simple ab initio quantum-chemical calculations on Raman vibrational spectra using quantum chemistry packages.

#### Raman analysis of benzene ( $C_6H_6$ )



# Raman analysis of CCl<sub>4</sub>

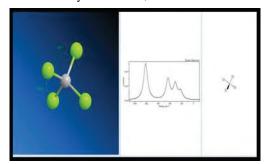


Figure 4: Raman spectra of benzene and carbon-tetrachloride using quantum chemistry software packages.

### 3. Learning for Students (200 words):

The present project work was a great learning experience for the students of both streams (physics & computer science). Students had a practical hands-on-experience and learned to design a low cost Raman spectrometer on their own. The project has triggered the creativity for innovative ideas amongst the students in setting up experiments in the science laboratories. They themselves had tried various setups and techniques to improve the Raman signals. This very process of learning has inculcated a research aptitude in these undergraduate students. The innovation project has motivated not only the students involved in the project but also has generated an interest among other undergraduate students towards research in science which is nowadays very feeble among the students.

Students had visited Chandigarh for presenting their paper in "1st IAPT National student symposium on Physics", held between 25-27th February 2013, organized by Indian association of physics teachers. Their work was appreciated by one and all and their paper may get published in a student's journal Prayas. During their visit to Chandigarh they had visited to various research labs including DRDO's lab TBRL (terminal ballistic research laboratory) situated in Ramgarh, 25 km from Chandigarh. Students has also participated and presented a paper in poster presentation in a national conference" Redefining Science Teaching: Future of Education", held between 7-9th March 2013 in South Campus, University and bagged a consolation prize for the same. Participating in conferences has given them an excellent platform for discussing their research work with eminent scientists and academicians which have given a new direction for the future work. Such opportunities are normally available for a PhD student but this innovation project has helped undergraduate students to avail the same.

### 4. Benefits to College (100 words):

The major benefits to the college due to the project are outlined below:

• Such a spectrometer is not available in the student laboratories anywhere in India, and shall greatly benefit in enhancing the curriculum by designing simple experiments for students in the Physics, Chemistry and Biology stream.

- The final setup is placed in the college, so students can perform Raman analysis of their samples.
- The individual modules used in the present setup can be used in the teaching laboratory in various undergraduate classes. Students are encouraged to design simple experiments that can be performed in college laboratories, which would further enhance the curriculum.

# 5. Benefits to Society (100 words):

In the project undergraduate students have indigenously designed a low cost Raman spectrometer. Raman spectroscopy experiment at the undergraduate level in India is neither explained in detail, nor is the experiment done due to the lack of an inexpensive Raman spectrometer. Such equipment is still not available from commercial sources in India, and need to be imported at a huge cost. Raman spectrometer designed in the present project resolves such issues and help an undergraduate student to learn indepth Raman analysis for which Sir C. V. Raman got a Nobel prize. This endeavor can be further extended with future students towards the development of miniaturized and portable Raman spectrometers for specific field use and for strategic applications of the Indian space research with further innovation in design and development.

### 6. Further Plans (100 words):

The cost of the present spectrometer can be further reduced by replacing the linear array of spectrometer with other options. The present setup would be improved as well as new setups would be designed so as to develop a commercial devise which would be useful for all DU colleges. The present setup is calibrated for liquid samples only so our future plans would also include the improvisation of the setup to analyze solid samples.