Seminar

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Institute for Plasma Research

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Title: Compositional Analysis of the Pyrotechnic materials using spectroscopic techniques

Speaker: Dr. Darpan Dubey
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Date: 9th May 2025 (Friday)

Time: 3.30 PM

Venue: Seminar Hall, IPR

Abstract: This talk primarily reports the detection and quantification of toxic constituents in firecrackers using LIBS coupled with PCA and FTIR. Spectral signatures of lethal elements along with other elements and electronic bands of Cyanide, AlO, BaO, and CaO are seen in their LIBS spectra which confirms the presence of inorganic and organic compound in the fireworks (Normal and Green firecrackers). The concentration of each constituent/element is determined using the CF-LIBS and PLSR method and results are compared with ICP-OES/AAS results. The concentration of Al is in adequate amount except S_4 (b). Li and Ba are present in all samples with maximum amount in S_4 (b) and S_3 respectively. Molecular stretching of SO_4-, C_4H_8-, CuCl-, CO_3-, and NO_3- are observed in the FTIR spectra of the samples. The combined results of LIBS and FTIR recommends the presence of $BaNO_3$, $LiCO_3$, $SrCO_3$, Al-chip, and charcoal in the firecrackers. To discriminate various firecrackers, PCA of the LIBS data is performed. The results show that S_3 and S_4 (b) are more harmful as they contain higher concentration the compounds of Al, Ba, Li, Sr i.e $BaNO_3$, $LiCO_3$, $SrCO_3$, ($Cu_3As_2O_3Cu(C_2H_3O_2)_2$). The results reflect that these normal firecrackers contain higher amounts of toxic elements like Al, Cr, Ba, P, Sr, Cu, Mg, and Fe. LIBS coupled with chemometric techniques are used to classify their categories based on their composition and behaviour. LIBS coupled with chemometric method is used to explain the crackling, sparkling and toxin effects of traditional firecrackers. The presence of spectral signa ture of electronic bands of diatomic molecules like AlO and BaO that directly indicate the corresponding elements (Al, Ba, etc.) are present in higher amounts in the crackers. The actual concentrations of the toxins are calculated to compare with the permissible limit in the crackers using calibration free LIBS, and results are validated with inductively cou pled plasma-optical emission spectroscopy. Both are in good agreement. Fourier transform infrared spectroscopy tech nique confirms the presence of functional groups (NO_3^-, SO_4^-, and charcoal) responsible for the emission of noise and fumes in the crackers. The UV–Visible (UV–Vis) tech nique is used to identify the compounds/molecules (AlO, FeO, KNO_3, charcoal, and CaO) that confirm the presence of a knocking agent. Principal component analysis is applied to discriminate the conventional

firecrackers into different groups/classes based on their amounts of constituents and behaviour. The hazardous constituents present in the residues of six type of normal and six type of green firecracker's samples. The residue of the normal firecracker's samples is containing the presence of spectral lines of toxic species like Al, Ba, Sr, Mg and Ti in the similar way as the fresh powder of normal crackers. The residues of the green firecracker's samples contain toxic elements like Al and Ba, and the intensities of these toxic elements are so high that theses samples also contain the electronic bands of the AlO and SrO. The UV-Visible spectra of residues of normal and green firecrackers samples contain the molecules of KNO_3, CaO, $Al2O_3$, and SrO in a similar way as the fresh powder of these firecrackers are contained. This reflects that the toxicity of the powder of firecracker's samples remains similar after the burning of these firecrackers' samples. Therefore, these toxic residues are mixed in the soil, where they burn and contaminate it. For the assessment of the contamination of the soil, the concentration of micronutrients like Fe, Cu, Mn, Zn, and P are calculated using the Atomic Absorption Spectroscopy (AAS) techniques and found to increase in concentration in all the contaminated soil comparative to blank soil. This reflects that the soil is contaminated. For the classification of the residues and soil contaminated with residues, the Principal Component Analysis (PCA) and Hierarchical clustering Analysis (HCA) is applied to the LIBS data-set. Along with this, the toxic molecules (like cancer causing or Asthma causing) are docked (using DFT and ADMET) with human protein and docking is successful which validate the adverse effect of this toxic molecules on human health.