Development of a 6.65 m off-plane Eagle spectrometer for a high resolution vacuum ultraviolet beam-line at Indus-I synchrotron radiation source

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A 6.65 m vacuum ultraviolet (VUV) spectrometer has been designed and fabricated indigenously using concave grating (concave radius = 6.65 m) of frequency 4800 grooves/mm for carrying out spectroscopic research of atomic and molecular gases and vapours using synchrotron as a source of radiation. The wavelength range of the spectrometer is 700–2000 Å. The reciprocal linear dispersion of the instrument is about 0.3 Å/mm. The experimentally estimated value of the wavelength resolution is 0.01 Å. The spectrometer has been tested by recording spectral lines of wavelengths 1228.79 Å (nitrogen), 1243.18 Å (nitrogen), 1261.55 Å (carbon), 1288.42 Å (nitrogen), 1930.9 Å (carbon) under a vacuum of 10^{-5} torr by exciting residual gas molecules in a rotary pump evacuated discharge tube.

A 450 Mev synchrotron source Indus-1 is in operation at the Centre for Advance Technology (CAT), Indore. This synchrotron source emits electromagnetic radiation in the range of soft X-ray to near infrared region of the spectrum. Using this source, the Spectroscopy Division at BARC, Mumbai has been engaged in the development of high resolution vacuum ultraviolet (VUV) beam-line for carrying out photo absorption studies of atomic and molecular species in the wavelength region of 700–2000 Å. The high resolution beam-line consists of mirror boxes, a 6.65 m concave grating VUV spectrometer and an absorption cell. The article describes indigenous design, development and testing of a 6.65 m concave grating spectrometer for the wavelength region of 700–2000 Å.

Off-plane Eagle spectrometer

The optical design of the VUV spectrometer is based on the Eagle type[1–13] of mounting using concave grating as a dispersing element because of its compactness and a requirement of minimum volume of air to be evacuated from the chamber. Schematic optical arrangement (top view) of a 6.65 m concave grating spectrometer is shown in Figure 1. The spectrometer consists of the entrance slit, concave grating, exit slit and photo-multiplier tube (PMT) housed in an air leak-proof, sealed, hollow cylindrical pipe which can be easily evacuated to obtain a vacuum of 10^{-6} torr. The entrance slit and exit slit are placed at a distance of 6.65 m from the grating set in zero-order position. The separation between the entrance slit and the exit slit is such that the angle of 1.447395° is formed at the centre of the grating set in zero-order position. The synchrotron source is a fan-like beam of horizontal divergence of 60 mrad and vertical divergence of 6 mrad. Therefore, the focused beam of the synchrotron by a set of cylindrical mirrors is a horizontal line. Hence the entrance and exit slits are kept horizontal and the slits width is in the vertical plane. The dispersing plane of the grating must be vertical and therefore the ruling lines of the concave grating are to be kept horizontal.

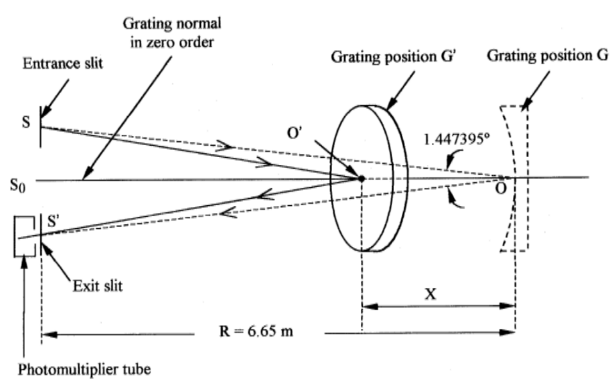

Figure 1. Plan view showing the principle of a concave grating used in off-plane Eagle mounting. Entrance and exit slit directions lie in the plane of the paper.

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The entrance and exit slits must be set parallel to the length of the ruling grooves of the grating. When the grating is placed at the position *G*, zero-order wavelength is focused on the central position of the Rowland circle. The other non-zero wavelengths are focused on the Rowland circle lying in the vertical plane. Thus the spectrum lies in the vertical plane. The optical arrangement of the entrance slit, concave grating, exit slit and the PMT assembly is chosen such that a spectrum can be recorded by moving the exit slit – PMT assembly along the vertical plane.

Calculations for grating rotation and grating displacement

For changing the wavelength region, it is necessary to rotate and translate the grating. The grating rotation and grating displacement are measured usually with reference to the zero wavelength position of the grating. For setting the grating position to obtain a central wavelength λ_0, the angle of diffraction β_0 for wavelength λ_0 is first obtained by the following grating equation:

$$\sin\alpha_0 + \sin\beta_0 = \frac{\lambda_0}{d}, \tag{1}$$

where α_0 is the angle of incidence.

Since $\beta_0 = \alpha_0$ for the central wavelength λ_0 in our optical configuration, the grating eq. (1) is written as

$$2\sin\alpha_0 = \frac{\lambda_0}{d}. \tag{2}$$

The grating is then rotated through the angle α_0 about the horizontal direction for obtaining the central wavelength λ_0 in the centre of the image plane as calculated by the following relation:

$$\alpha_0 = \sin^{-1}\left(\frac{\lambda_0}{2d}\right). \tag{3}$$

In order to obtain the well-focused wavelength λ_0 on the Rowland cylinder, the grating is moved towards the slit by a distance calculated from the following equation:

$$X = (1 - \cos\alpha_0)R, \tag{4}$$

where *R* is the radius of curvature of the concave grating.

The grating rotation and grating displacement for a central wavelength of $\lambda_0 = 2000$ Å are calculated to be 28.6854° and 81.62 cm respectively, for the grating of density 4800 grooves/mm from the eqs (3) and (4). Similarly, the grating rotation α_0 and grating displacement *X* are calculated for the wavelengths in the range of 700–2000 Å from eqs (3) and (4). Table 1 shows the grating rotation and grating displacement required for focusing the various wavelengths on the image plane of the spectrometer in the wavelength range of 700–2000 Å for a grating of groove density 4800 grooves/mm.

Design details of the spectrometer

Figure 2 shows the optical layout of the 6.65 m off-plane Eagle spectrometer. The spectrometer has been designed to obtain a resolution of 0.005 Å in the wavelength region of 700–2000 Å. To achieve this resolution we need a concave grating of the following specifications[12]:

Ruled area = 125 mm × 110 mm (groove length)
Blank size = 180 mm diameter × 30 mm thick
Rulings/mm = 4800
Concave radius of curvature = 6.65 m
Blaze wavelength = 1000 Å
Blaze angle = 13°52′

The reciprocal linear dispersion of the grating is calculated to be 0.3 Å/mm from the following equation:

$$\frac{d\lambda_0}{dl} = \frac{d\cos\alpha_0}{R} \times 10^4 \text{ Å/mm}, \tag{5}$$

where *R* is expressed in m and $1/d$ is the number of grooves per mm.

The other parameters of the instrument are as follows: The distance between the entrance slit and concave grating for zero wavelength setting is kept at 6.65 m. The distance between the entrance and exit slits is chosen to be 16.8 cm in the horizontal plane, which is perpendicular to the Rowland cylinder plane (i.e. vertical plane). The grating mount has been designed such that a maximum angle of rotation of the grating about the horizontal direction is 45° for

Table 1. Calculated grating rotation and displacement for various wavelength settings with respect to the zero-order wavelength setting for a grating of density 4800 grooves/mm

Wavelength λ (Å)	Rotation α_0 (degrees)	Displacement *X* (cm)
700	9.67155	9.451
900	12.47420	15.698
1100	15.30754	23.592
1228.79	17.15211	29.575
1243.18	17.35931	30.289
1261.55	17.62417	31.213
1288.42	18.01227	32.591
1300	18.17980	33.195
1500	21.10019	44.586
1700	24.07925	57.867
1900	27.12929	73.163
1930.9	27.60775	75.716
2000	28.68540	81.616

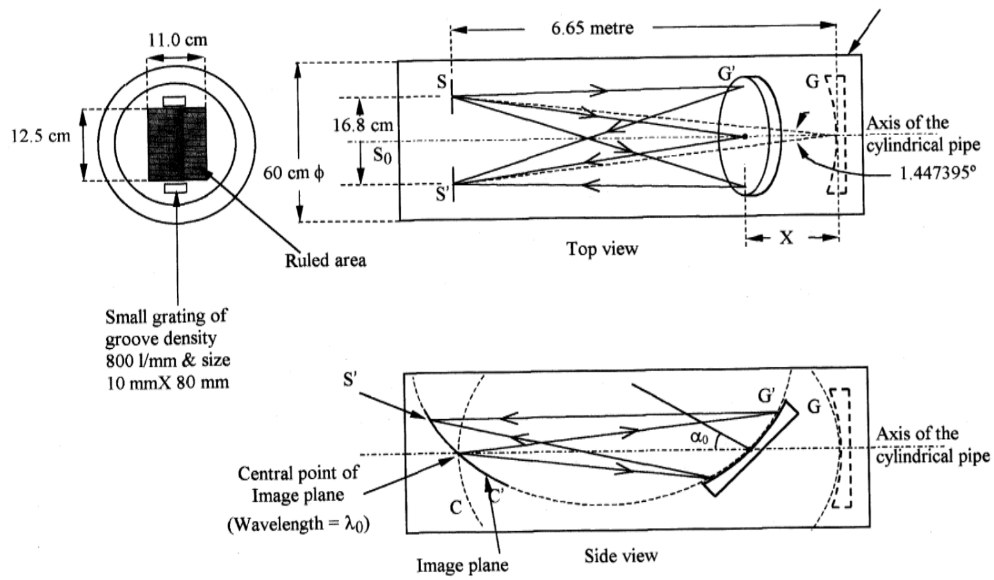

Figure 2. Optical layout and ray diagram of a 6.65 m off-plane Eagle spectrometer.

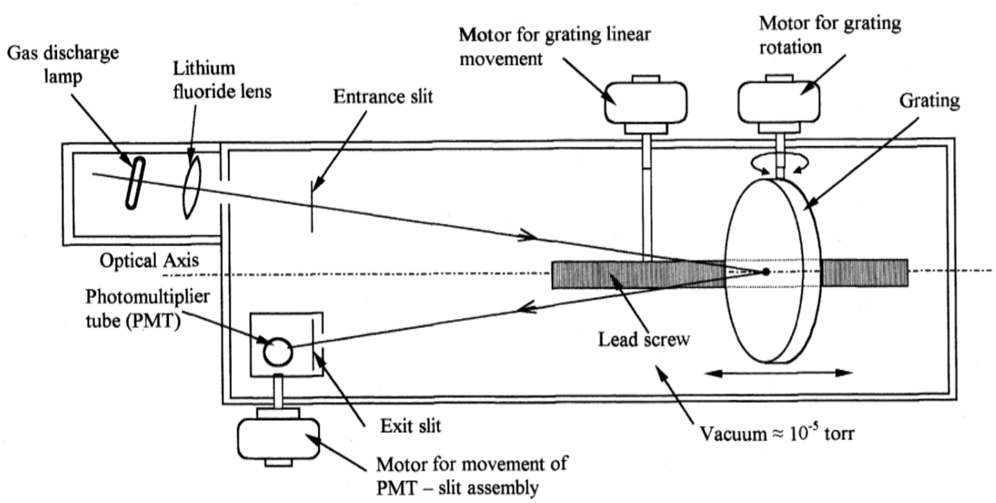

Figure 3. Schematic diagram showing complete assembly of the 6.65 m off-plane Eagle spectrometer.

setting various wavelength positions on the image plane. The linear drive assembly on which the grating moves has been designed such that the grating can be displaced linearly by a maximum distance of 84 cm for focusing the spectral lines of various wavelengths. The maximum displacement of the photo-multiplier tube coupled with the exit slit is 160 mm in the vertical direction giving a scanning range of bandwidth 48 Å.

There are three main motion drives needed for recording the spectrum in the spectrometer: (a) grating rotation (b) grating displacement, (c) photo-multiplier tube displacement. Figure 3 shows complete assembly of the 6.65 m off-plane Eagle-type concave grating spectrometer.

Electronic control system

Figure 4 shows a block diagram of the electronic control system and data acquisition system used in the spectrometer for grating rotation, grating displacement and PMT displacement. The electronic control system consists of three parts. Part 1 is an electronic control system for the linear displacement of the grating driven by a stepper motor. The linear displacement is controlled by a software program installed in the personal computer (PC). The minimum linear displacement is 22 μm for a step size of 0.03. Part 2 is an electronic control system for the rotation of the grating driven by a stepper motor. The angular rotation is

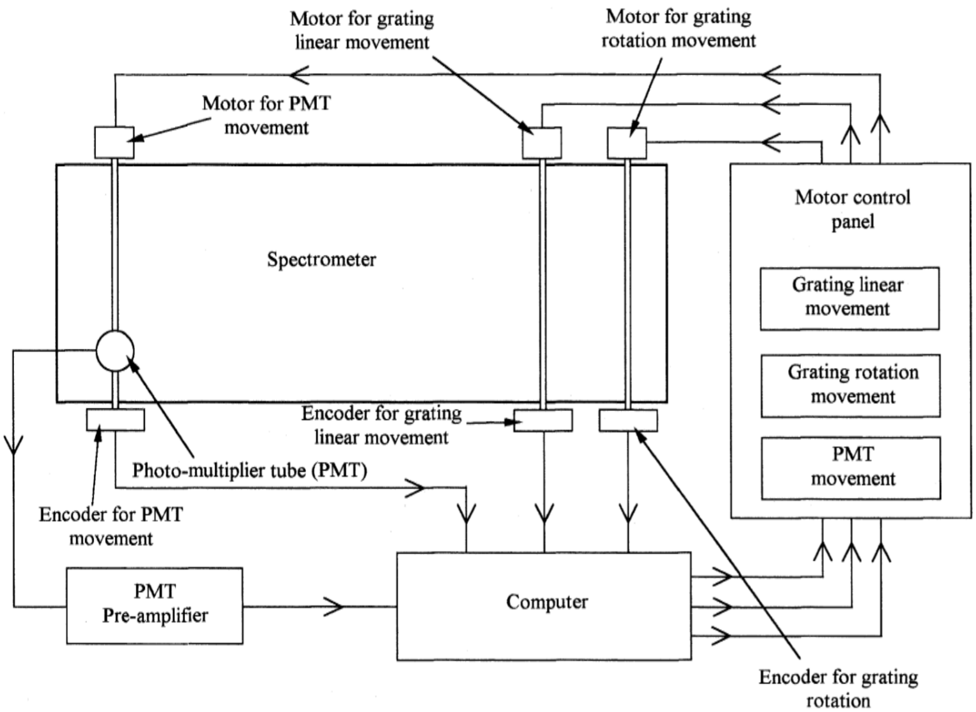

Figure 4. Block diagram of electronic control and data acquisition system.

controlled by a software program installed in the PC. The minimum angular rotation is 1.35 arc-min for a step size of 0.03. Part 3 is an electronic control system for movement of the PMT and exit slit assembly. The PMT and exit slit assembly is moved along a Rowland circle guide of radius of curvature 3.325 m by a stepper motor. The PMT movement is controlled by a software program installed in the PC. The minimum step in the PMT movement is 1.0 μm. The total PMT movement is 160 mm for scanning the spectrum.

Signal detection and data acquisition system

As mentioned earlier, the spectral radiation is detected by a PMT fixed behind the exit slit of the spectrometer. The exit slit and the PMT are mounted on a guide of radius of curvature 3.325 m. The PMT and exit slit assembly is driven by a stepper motor and the total movement of the assembly is 160 mm along the Rowland circle. Spectral bandwidth of 48 Å can be recorded by scanning the PMT in one span. The output of the PMT is fed to a pre-amplifier, which is coupled to the data acquisition system (DAS). The DAS consists of a precision multifunction analogue-to-digital converter system based on the NI-PCI-6013 card of National Instruments[14] mounted in the PC which records the output through a software program based on Visual Basic-6 graphic user interface platform. The radiation at the exit slit is thus converted to PMT current, which is amplified and converted to voltage and subsequently to a 16-bit digital signal. The intensity profile of a spectral line is recorded in the form of variation of digital signal with PMT displacement.

Precision optical alignment and focusing of the spectrum

The grating grooves must be set parallel to the horizontal direction in order to obtain vertical dispersion. In addition, the primary slit must be adjusted parallel to the grooves in order to achieve the best possible resolution. We have used a green He–Ne laser (λ = 5435 Å) for alignment of the grating grooves and slit length parallel to the horizontal direction. The diffraction angle for the green light of the He–Ne laser by the grating of high frequency (i.e. 4800 grooves/mm) is greater than 90°. Therefore the first-order diffracted laser spot cannot be seen on the image plane and cannot be used for aligning the grating lines parallel to the horizontal direction. Hence a grating of low frequency must be used for observing the diffracted laser spot on a screen placed on the image plane for aligning the grating lines parallel to the horizontal direction. For this purpose, the grating has a small strip of frequency 800 grooves/mm ruled on the lower and upper side of the main ruled area of 110 mm × 125 mm of the grating having a frequency 4800 grooves/

mm. This small strip of low frequency grating has its lines parallel to the lines of the grating of high frequency. The lines of the small grating can now be used for aligning the grating grooves parallel to the horizontal direction by means of a laser. The height of the laser beam and its direction are adjusted such that the laser beam passes through the centre of the entrance slit and falls on the pole of the small grating. Initially, the grating grooves are set parallel to the horizontal direction with an accuracy of about 1°. The grating surface is nearly set parallel to the vertical direction. The grating is then rotated about the vertical and horizontal axes such that the reflected spot is observed at the centre of the imaging plane. The grating is then rotated on the horizontal axis until the first-order diffracted laser spot is observed on the screen placed on the imaging plane. It is noticed that the laser spot may fall on any side of the centre of the imaging plane instead of the centre. The grating is then rotated about its centre within the mount to align the grooves parallel to the horizontal direction till the laser spot coincides with the centre of the imaging plane. The grating is then locked in this position. We can now check the alignment of the grooves by bringing back the zero-order wavelength in the centre of the imaging plane. The zero-order laser spot and the first-order laser spot must coincide with the centre of the imaging plane when the grating is rotated about the horizontal direction. The grating is then set for recording the zero-order spectrum of any light source. The He–Ne laser is replaced by a mercury discharge lamp. The mercury lamp is focused onto the entrance slit of the spectrometer by a lithium flouride lens of focal length 50 mm. The zero-order wavelength of the mercury lamp is observed on a ground glass plate placed in the imaging plane. The sharp focus of the zero-order spectral line is obtained by displacing the concave grating slightly on linear drive assembly. The position of the grating is noted down on the scale attached to the grating mount and this zero wavelength position serves as a reference point for measuring the displacement of the grating when it will be set for recording other wavelengths. For obtaining the green line of the mercury discharge spectrum ($\lambda = 5460.7$ Å) in the image plane, the grating is rotated through an angle of 12.616718° as calculated using eq. (3) by a stepper motor. The displacement of the grating is calculated to be 160.6 mm using eq. (4). The grating is then displaced by 160.6 mm using the stepper motor to obtain a well-focused spectral line on the image plane. In order to judge the sharpness of the image of the spectral line, the spectral line is recorded by moving the PMT and slit assembly. The grating is then rotated by an angle of 8.62144° for recording the wavelength ($\lambda = 2536.52$ Å) of mercury on the image plane. The grating is displaced by $X = 34.3$ mm to obtain the sharp focus of the 2536.52 Å line. The PMT and slit assembly is again moved to record the 2536.52 Å line. The recorded spectral line shows a well-focused line of wavelength 2536.52 Å, as shown in Figure 5. Similarly, we have recorded various wavelengths of mercury lines such as 4358.33, 4046.56, 4077.83, 3663.28, 3654.84, 3650.15, 3131.84, 3131.55 and 3125.67 Å by rotating and displacing the grating.

Calibration of the spectrometer

Vacuum of the order of 10^{-5} torr is obtained by evacuating the chamber with two turbo-molecular pumps, each having capacity of 500 lps, backed by rotary pumps for recording the spectrum in the VUV wavelength region. Various known spectral lines of nitrogen and carbon are obtained by exciting residual gas molecules in a rotary pump-evacuated discharge tube in the wavelength range from 1000 to 2000 Å and focused on the image plane by rotating and displacing the grating. The spectral line profiles have been recorded by moving the PMT – exit slit assembly along the Rowland cylinder. Figure 6 shows the intensity profiles of wavelengths 1228.89 (nitrogen), 1243.18 (nitrogen), 1261.55 (carbon), 1288.41 (nitrogen) and 1930.91 Å (carbon) recorded using the spectrometer. The intensity profiles of the spectral lines recorded are not symmetric as shown in Figure 6 *b–e*. The asymmetry of the spectral lines arises due to the presence of off-axis optical aberrations such as coma and astigmatism. This is the inherent property of a concave grating, which cannot be corrected in a single element spherical concave grating as in the present case. We have recorded the spectral lines emitted by an evacuated discharge source kept at a large distance, i.e. 300 mm from the entrance slit. We have also not used a focusing lens to collect light so as to fill the whole aperture of the concave grating. The illuminated area of the grating was sufficient for initial testing of the spectrometer in the VUV region. The line width of the spectral lines is large due to the use of large slit width (~ 1.5 mm) and smaller illuminated area of the grating. The spectral line width will be reduced considerably by the use of slit width of the order of 20 μm. The spectral lines will become sharper and more

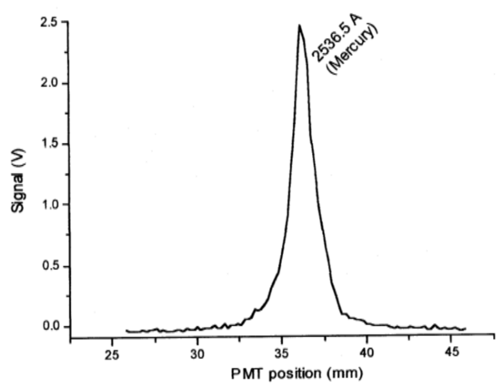

Figure 5. Mercury spectral line of wavelength 2536.5 Å recorded using the spectrometer. Intensity profile is obtained by moving the exit slit and PMT assembly along the Rowland circle. Wavelength is indicated on the peak of the spectral line.

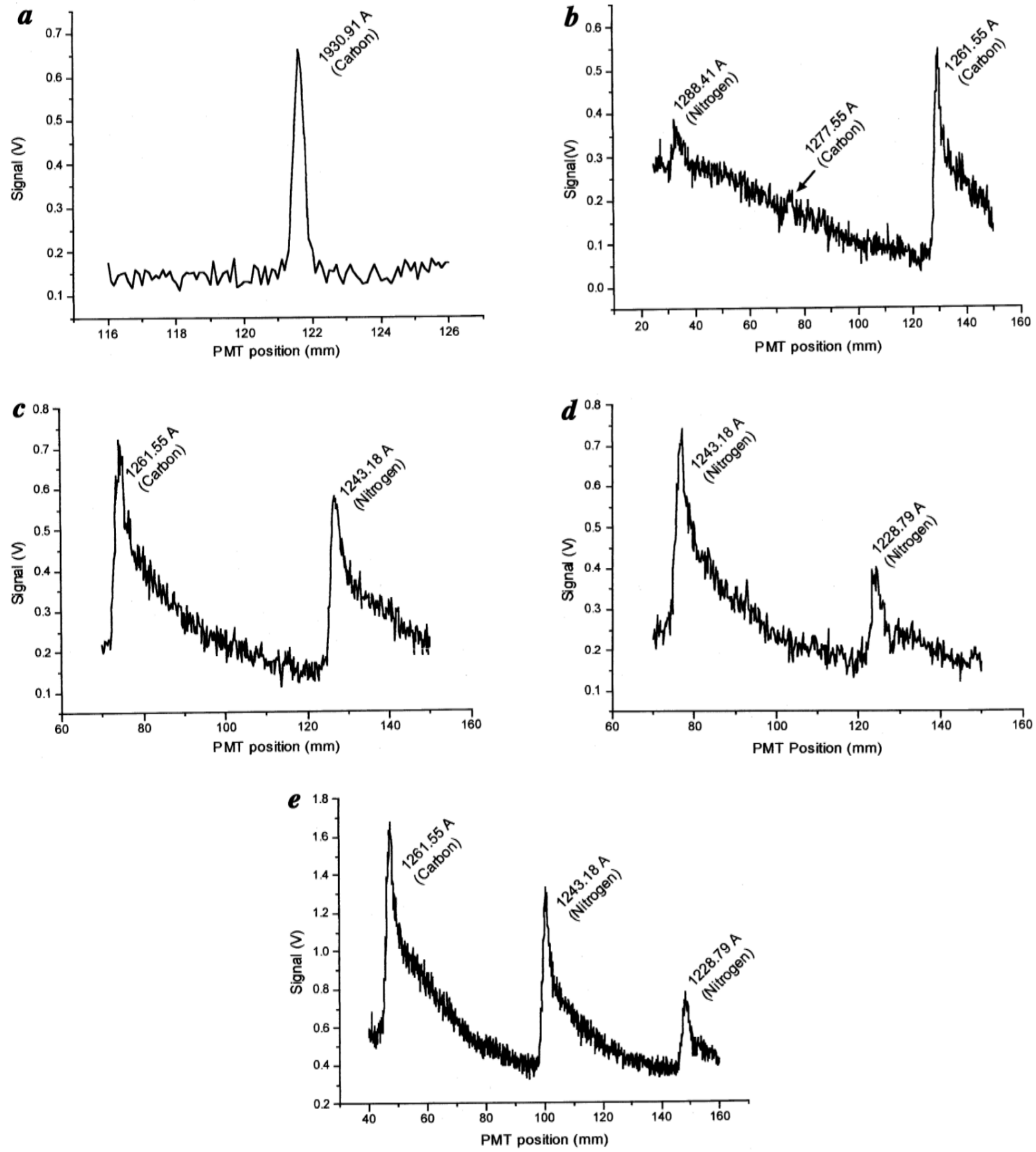

Figure 6. VUV line of carbon (***a***) nitrogen and carbon (***b***) carbon and nitrogen (***c***) nitrogen (***d***) and carbon and nitrogen (***e***) recorded using the spectrometer. Intensity profile is obtained by moving the exit slit and PMT assembly along the Rowland circle. Wavelength is indicated on the peak of the spectral line.

symmetrical in shape using the focused beam of the synchrotron source on the entrance slit, illuminating the whole area of the grating and reducing the slit width and slit length. Only under these conditions will the spectral resolution of the spectrometer be 0.01 Å. Several standard spectral lamps of known wavelengths are needed for determining the unknown wavelengths of the molecules or vapours under study in the wavelength region of 700–2000 Å. Figure 7 shows photographs of the spectrometer and its assemblies developed indigenously.

Wavelength reproducibility in the spectrometer

Wavelength reproducibility is dependent on the errors present in the assemblies of the various mechanical motions of the grating and the exit slit and PMT assembly. The reproducibility of the linear drive of the grating displacement is within 100 μm. This error does not have any effect on the focusing of the spectral lines on the exit slit. The reproducibility of the angular rotation of the grating is 2 arc sec. This error in the grating angle will produce a corre-

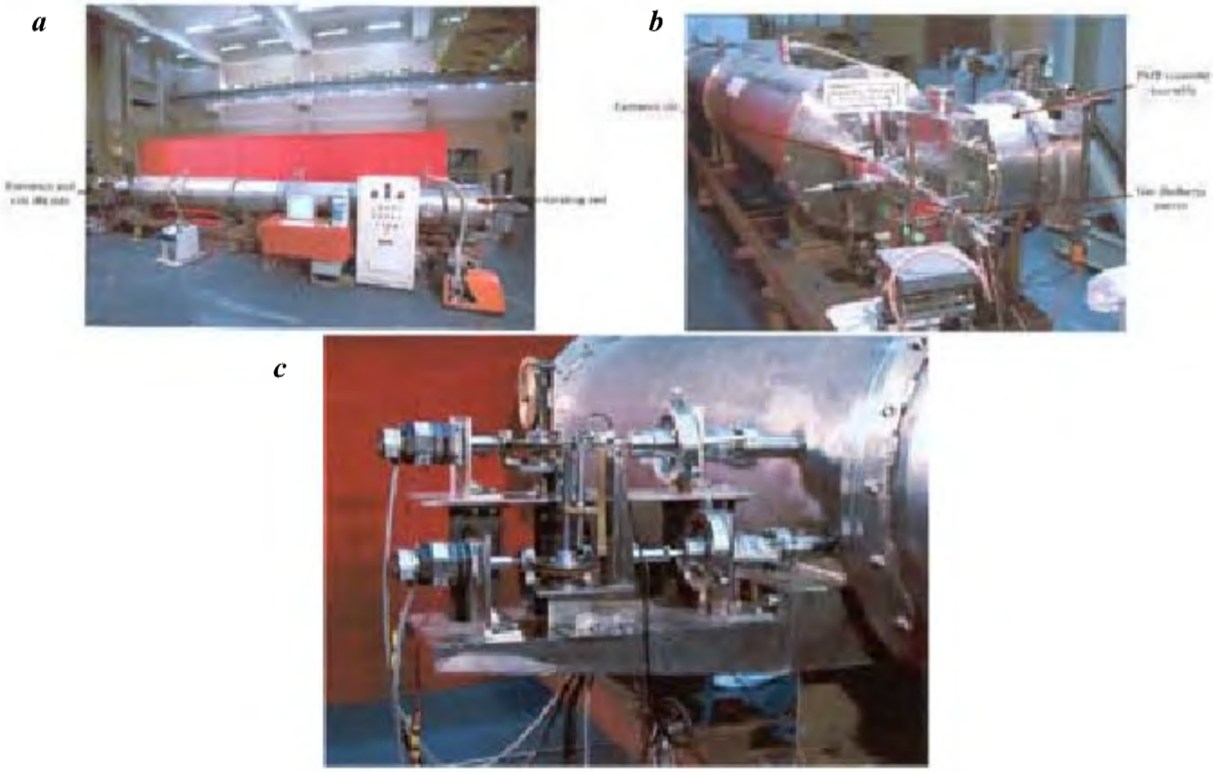

Figure 7. Photograph of off-plane Eagle vacuum ultraviolet spectrometer (***a***), view from the entrance slit side (***b***) and grating movement motor assembly (***c***).

sponding error of about 0.07 mm in the position of the spectral line on the image plane. Since the test spectrum is always recorded along with the spectrum of the known reference lines (i.e. calibration lines), the error in the grating angle will not have any effect on the wavelength measurement. Once the central wavelength is set, the error in the lead screw of the exit slit scanning mechanism will determine the wavelength reproducibility. The maximum lead screw error of the scanning mechanism is 8 μm for the whole range of movement of 160 mm. The maximum error in wavelength ($\Delta\lambda$) measurement is given by $\Delta\lambda$ = (Reciprocal linear dispersion) × (Lead screw error). Hence the error in the measured wavelength would be 0.0024 Å taking the reciprocal linear dispersion as 0.3 Å/mm.

Conclusion

A 6.65 m concave grating spectrometer has been fabricated indigenously using a concave grating of frequency 4800 grooves/mm for carrying out spectroscopic research of atomic and molecular gases in the wavelength region of 700–2000 Å. The reciprocal linear dispersion of the spectrometer is about 0.3 Å/mm. The experimentally estimated spectral resolution of the instrument is 0.01 Å. The spectrometer will be used for absorption studies of various molecules using synchrotron radiation (Indus-1) as a source of electromagnetic radiation at Centre for Advanced Technology, Indore.

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