PART IX. INSTRUMENTATION FOR THE SPECTRAL DISPERSION AND ISOLATION OF OPTICAL RADIATION

(IUPAC Recommendations 1995)

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1 INTRODUCTION

This document, Part IX, deals with nomenclature, symbols and their usage in the field of instrumentation for the dispersion and isolation of optical spectra in the wavelength region of 50 nm to 1 mm, as applied in analytical atomic and molecular emission, absorption and fluorescence spectroscopy.

In this document, most terms have been described and quantities expressed in units of radiation wavelengths. Definitions can be directly or easily converted into units of frequency or wavenumber, but where this is not the case, it is indicated in the text.

This document deals with nomenclature, symbols and their usage in the field of instrumentation for the dispersion and isolation of optical radiation in the wavelength region from 50 nm to 1 mm as applied in analytical atomic and molecular emission, absorption and fluorescence spectroscopy. The whole subject is divided into 10 chapters dealing with various aspects of dispersive and non-dispersive spectral apparatus including spectral filters and interferometers. Definitions are given for spectral instruments with and without detection and measuring facilities. The properties of optical components of dispersive and non-dispersive spectral instruments are defined in detail with emphasis on such fundamental figures of merit as spectral purity, resolution, resolving power, conductance of optical systems, characteristic wavelengths and polarization. Terms closely related to the optimum use of spectral instruments, e.g., optimal slit width and height, theoretical and practical effective spectral linewidth, line-to-background radiant power ration are given. Terms for various forms of mountings for spectral apparatus are included in the vocabulary.

2 SPECTRAL APPARATUS

An optical arrangement or an instrument which disperses *optical radiation* into a spectrum and/or isolates a specific *spectral band is* termed *spectral apparatus* or a *spectral instrument.* If the *entrance aperture,* which may be a slit, is sharply imaged in both dimensions, i.e., length and width in the same *focal plane*, it is called a *stigmatic arrangement* or when the focal planes are different in the two dimensions, *astigmatic.* When the radiation passes through the same optical components before and after being dispersed, the spectral system is *autocollimative.*

2.1 Dispersive Spectral Apparatus

Spectral separation or isolation of optical radiation may be achieved by using a *dispersive component* such as a *prism,* a *diffraction grating,* or a *multiple-beam interferometer.*

2.1.1 A *monochromator* enables a specific spectral band to be selected, e.g., by using two slits, i.e., an *entrance* and an *exit slit* (see Note [1]).

If two or more monochromators are specially constructed for simultaneous use the arrangement is termed *parallel monochromators* e.g. two parallel monochromators.

A *double monochromator* results when two single monochromators are arranged in series. The exit slit of the first becomes the entrance slit of the second either physically or by optical imaging, forming a common *middle slit.* Combinations of single monochromators may be repeated giving *multiple monochromators.* If, by an optical arrangement (e.g., reflection), the beam is passed twice through the same monochromator, the apparatus is called a *double-pass monochromator.*

A double monochromator, where the dispersion of the first is added to the second, is termed an *additive double monochromator* or, when the dispersions are subtracted, a *subtractive double monochromator.*

2.1.2 A *polychromator* results, when several spectral bands are isolated simultaneously, usually by a number of exit slits or some other arrangement.

2.2 Non-dispersive Spectral Apparatus

In such instruments isolation of a spectral band is achieved without wavelength dispersion by using *optical absorption, fluorescence, reflection* or *scattering* (see Note [2]). It is also achieved by the use of an *interference filter* based on multiple beam interference. These filters are examples of *spectral filters. A double-beam interferometer* may also be part of a non-dispersive spectral instrument.

3 SPECTRAL APPARATUS WITH DETECTION AND/OR MEASURING FACILITIES (see Note [2])

Dispersive or non-dispersive spectral instruments may be combined with one or more means for detecting and/or measuring the spectra. Most of the following refer to dispersive instruments.

3.1 A *spectroscope* enables visual observation and evaluation of optical spectra. It is usually confined to the visible spectral region.

3.2 A *spectrograph* is a combination of a spectral apparatus and a *camera.* This enables an image of a spectrum to be obtained. Spectra are recorded by a photographic emulsion or other means, e.g., two- dimensional electronic image sensors.

3.3 A *spectrometer is* the general term for describing a combination of spectral apparatus with one or more detectors to measure the intensity of one or more spectral bands (see Note [3]).

3.3.1 A *sequential spectrometer* enables the intensity of several spectral bands of radiation to be measured one after the other in time, i.e., sequentially.

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[1] The means whereby spectral band selection is achieved will be discussed in 8.

[2] See also Part 111, Sect.4.3.1. Some of these terms have been described in Part I and Part III.

[3] The words photometer, spectrophotometer, (also photometry, spectrophotometry) are sometimes used to describe some of those instruments and procedures related to them. These words should not be used in spectrochemical procedures because photometry relates to radiation evaluation according to visual effects (see Part I (Sect. 4.5).

3.3.2 A *simultaneous spectrometer* has more than one detector and enables the intensities of several spectral bands to be measured at the same time.

3.3.3 In a *multiplex spectrometer*, a single photodetector simultaneously receives signals from different spectral bands which are specifically encoded. In the case of *frequency multiplexing*, each spectral band is modulated at a specific frequency. Decoding is achieved by filtering out, by electronic means, the corresponding signals.

Frequency multiplexing may be realized e.g., with a *Michelson interferometer* (see 5.3) by changing the path difference between the two interfering beams at a uniform rate. Fourier transformation of the interferogram so obtained yields the spectrum. This method is called *Fourier Transform Spectrometry* (FTS).

3.3.4 A *filter spectrometer* has one or more spectral filters for isolating one or more spectral bands.

4 OPTICAL COMPONENTS OF DISPERSIVE SPECTRAL INSTRUMENTS

4.1 Entrance Collimator

An *entrance collimator* (see Fig. 1) is an optical arrangement for the production of a quasi-parallel beam of radiation of a required cross section. It consists of an objective lens or mirror, the cross section of which constitutes the *entrance aperture stop* and an *entrance field stop* at the front focal plane of the collimator. The entrance aperture stop may also form the limiting aperture stop, the *entrance pupil* of the whole apparatus.

The entrance field stop in most dispersive instruments is a *slit*. Both *curved slits* and *straight slits* are used. Distinguishing features are the *slit length* h (see Note [4]) and the slit *width* s (see Note [5]). Slits are either fixed or adjustable. They can be straight or curved depending on the optical design. An optical instrument may contain several real or virtual aperture and field stops. Those which determine the maximum throughput of radiant power are called the *limiting stops*.

Distinguishing features of the lenses or mirrors in the collimator systems are the *collimator focal length* f_{en} (see Note [6]) and the *relative aperture*. The relative aperture is defined in terms of the diameter D for circular entrance aperture stops and in terms of the effective diameter D_{eff}, where

$$D_{\text{eff}} = \left(\frac{4 B_{\text{en}} H_{\text{en}}}{p} \right)^{1/2}$$

for rectangular entrance aperture stops of width B_{en} and length H_{en}. The relative aperture k_{en} (see Note [7]), is then defined by the expression

$$k_{\text{en}} = \frac{f_{\text{en}}}{D}$$

for circular apertures and

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[4] The term slit height may be used when the slit is positioned vertically.
[5] The use of the word slit gap is discouraged.
[6] In this document the subscripts 'en' for entrance and 'ex' for exit will be used.
[7] The words f-number and optical speed are discouraged.

$$k_{en} = \frac{f_{en}}{D_{eff}}$$

for rectangular apertures.

The expressions for the following relative apertures

$$k_{B,en} = \frac{f_{en}}{B_{en}} \quad \text{and} \quad k_{H,en} = \frac{f_{en}}{H_{en}}$$

are also useful, e.g., for distinguishing diffraction properties in the plane of diffraction ("*B*") and perpendicular ("*H*") to it.

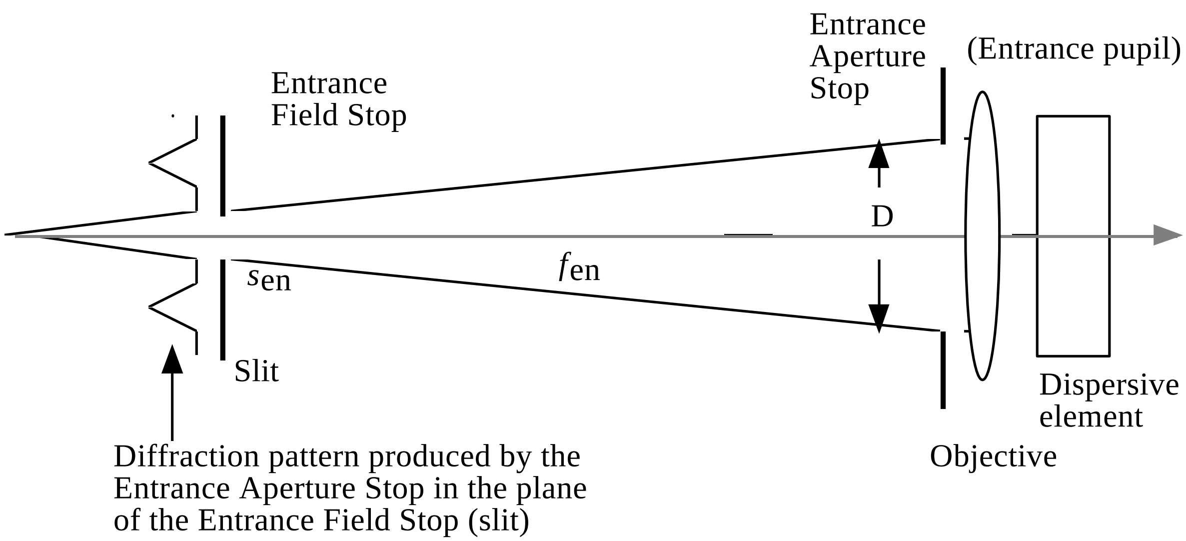

Fig. 1: For defining the optimal slit width in units of the virtual diffractiona pattern produced by the Entrance Aperture Stop in the plane of the Entrance Field Stop

4.2 Dispersive Elements

Distinctive characteristics of the dispersive element components are:

– the *total angle of deviation* Q (of the beam of radiation after refraction or diffraction);

– the *angular dispersion* $\mathrm{d}Q/\mathrm{d}l$ with respect to the wavelength l;

– the *theoretical resolving power*

$$R_0 = \frac{l}{d_0 l} \quad \text{(see 7.2.4);}$$

– the *upper* and *lower wavelength limits*, l_u and l_l between which the *transmission (or reflection) factor* exceeds a specified fraction of its maximum.

4.2.1 The characteristic quantities of prisms are:

– shape and type of the prism;

– the material from which it is made and its *refractive index* n which is a function of the wavelength l.

– the *material dispersion* $\mathrm{d}n/\mathrm{d}l$, which also changes with the wavelength;

– the *linear absorption coefficient* of the material;

– the *effective base length* b_{eff}, which is the path difference between the longest and the shortest possible parallel rays closest and farthest from the base, respectively;

– the *prism angle* a*;*

– the *prism height* parallel to the *refractive edge*

– the angle of minimum deviation Q_{min}.

The following terms are derived from these quantities:

– the theoretical resolving power

$$R_0 = b_{\mathrm{eff}} \frac{\mathrm{d}n}{\mathrm{d}\,l}$$

– the angular dispersion (in radians per wavelength)

$$\frac{\mathrm{d}Q}{\mathrm{d}\,l} = \frac{b_{\mathrm{eff}}}{B_W} \frac{\mathrm{d}n}{\mathrm{d}\,l}$$

where B_W is the width of the refracted *optical beam* in the plane of refraction.

4.2.2 Diffraction gratings may be transmission or reflection types. They are dispersive optical components with *grooves* (see Note [8]) or *lines* parallel to each other. *Ruled gratings* are mechanically produced by a *ruling engine* whereas *interferometric gratings* (see Note [9]) are made by interaction of an interference pattern with a photosensitive layer, e.g., a photographic emulsion. The grooves have a periodic structure in the direction of dispersion.

Replica gratings are duplications of the *master grating* (original grating). It is possible to repeat the process of the replication in several generations.

Characteristic quantities of gratings include:

– the *grating width* W of the grooved area (measured in a direction at right angles to the grooves, in the plane of the grating);

– the length of the grooved area (measured parallel to the grooves);

– the total *number of grooves* N_{r}. We have:

$$N_{\mathrm{r}} = n_{\mathrm{r}}\, W,$$

where n_{r} is the number of grooves per unit of length across W;

– the *grating constant* d which is the reciprocal of n_{r};

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[8] Grooves of mechanically ruled gratings are generally named *rulings*. With interferometric gratings, the recommended term is *lines*.

[9] The term 'holographic' grating is incorrect and should not be used.

– the *grating function* (formula) is the function relating the *angle of incidence* f_1 to the *angle of diffraction* f_2; i.e.:

$$\sin f_1 + \sin f_2 = m \frac{l}{d}$$

where m is the *order of diffraction;*

– the *efficiency of the grating* $h(l)$ *is* the ratio of the *diffracted* to the *incident spectral radiant power:*

$$h(l) = \frac{F_l\,(\mathrm{out})}{F_l\,(\mathrm{in})}$$

– the *usable free spectral range,* (without *order overlap):*

$$D l = \frac{l}{m}$$

– the *blaze* is the direction of optimum efficiency $h(l)$ of the grating;

– the *blaze angle g.* With *saw-tooth shaped grooves* g_B represents the angle between the *grating normal* and the normal of the groove surface.

– the *blaze wavelength* l_B is that wavelength or wavelength range at which blaze occurs. With plane gratings the blaze wavelengths are given for autocollimation;

From these quantities the following can be calculated:

– the theoretical resolving power:

$R_0 = m\,N_r$ (see 7.2.4);

– the angular dispersion (in radians per wavelength):

$$\frac{\mathrm{d}f_2}{\mathrm{d}l} = \frac{R_0}{B_W}$$

where B_W is the width of the diffracted optical beam in the plane of diffraction.

Plane gratings have lines on a flat surface. They consequently have no optical imaging properties.

Echelle gratings are *ruled plane gratings* having a comparably large grating constant *d* and at least one steep blaze angle g_W of the grooves. If used with this blaze angle as angle of incidence f_1 a high efficiency h at high orders of diffraction can be obtained yielding high angular dispersion $\mathrm{d}f_2/\mathrm{d}l$ and theoretical resolving power R_0 at the expense of the usable free spectral range Δl

Concave gratings have lines on a concave surface. The surface may be spherical, toroidal or elliptical. Concave gratings are generally used as objective components forming part of or acting fully as the collimator and/or camera of the instrument. Additional imaging characteristics may be achieved as a result of local displacement of the line or groove distance - as realized with some types of interferometric gratings.

4.2.3 The *Fabry-Perot interferometer* is an example of a multiple-beam interferometer which enables high resolution measurements to be made utilizing the interference of multiple beams of monochromatic radiation at very high orders, after reflection between two surfaces. A special case of such an interferometer is the *Fabry-Perot etalon interferometer* in which the thickness of a plane parallel plate of air or of another gas between the two surfaces remains unaltered. Another special case is the *etalon plate interferometer* basically consisting of a transparent solid plate with the reflective coating applied to the two surfaces.

Characteristic quantities are:

– the separation a between the (plane or concave) reflecting surfaces;

– the radius of curvature (with concave mirrors);

– the reflection factor r of the mirrors;

– the refractive index n of the medium between the reflecting surfaces which relates the wavelength l in the medium to that in vacuum by

$$l = \frac{l_{\mathrm{vac}}}{n} .$$

The following properties can be expressed in these quantities:

– the *order of interference:*

$$m = \frac{2a}{l} = \frac{2an}{l_{\mathrm{vac}}} ;$$

– the free spectral range

$$Dl = \frac{l}{m} ;$$

– the *finesse*

$$F = \frac{Dl}{dl} ;$$

where dl is the resolved wavelength distance (see definition in 7.2.1).

The following distinctions can be made: *theoretical finesse* or *reflectivity finesse*

$$F_0 = \frac{Dl}{d_0 l} = \frac{p\, r^{1/2}}{1 - r}$$

where $d_0 l$ is the theoretical resolution (see definition in 7.2.2);

– *surface defects finesse*

$$F_{\mathrm{d}} = \frac{Dl}{d_{\mathrm{d}} l} = \frac{p}{2}$$

where l/p denotes the maximum deviation of the plate surface from the ideal one usually measured at $l/ = 546.1$ nm;

– *scanning finesse*

$$F_{\mathrm{s}} = \frac{Dl}{d_{\mathrm{s}} l} = \frac{2p\, Dl}{W\, l}$$

where W is the solid angle subtended by a scanning aperture;

– *effective instrumental finesse* F_P is the result of a convolution of the previous forms of finesse;

– the theoretical resolving power (see 4.2)

$$R_0 = m F_0 = \frac{2a}{l} F_0 = \frac{2an}{l_{vac}} F_0 \; ;$$

– the angular dispersion df/dl, where f is the angle of diffraction (see 4.2.2).

4.3 The Exit Collimator

The *exit collimator* is an optical arrangement for the production of spectra as uniform adjacent images of the entrance slit. If the imaging optical system is supplemented by means for acceptance of a two-dimensional radiation detector in the focal plane, the whole system is then called a camera. Alternatively, the exit collimator may contain one or more exit slits. The objective optical system may consist of one or more lenses and mirrors. Quantities of importance are:

– the focal length f_{ex};

– the relative aperture k_{ex} (see 4.1);

– the usable length of the focal plane;

– the *inclination angle* Q_{ex} between the normal to the focal plane and the optical axis;

– the *linear dispersion* dx/dl in which x is the spatial coordinate in the direction of dispersion in the focal plane;

– *reciprocal linear dispersion* is the inverse of the linear dispersion.

5 OPTICAL COMPONENTS OF NON-DISPERSIVE SPECTRAL INSTRUMENTS

5.l Entrance Collimators

Entrance collimators for non-dispersive spectral instruments can be described in a similar way to those described in Sect. 4.1. Not all types of apparatus require collimators.

5.2 Optical Filters

An *optical filter* attenuates radiation either in its transmission or reflection. *Neutral filters* ideally attenuate all wavelengths of radiation uniformly over the optical spectral range while spectral filters have transmissive or reflective properties which are wavelength dependent.

In the case of spectral filters, *high-pass filters* attenuate radiation below certain *cut-off wavelengths*. The reverse holds for *low-pass filters*. *Band-pass filters* enable a limited spectral band to be selected. *Band-blocking filters* attenuate radiation within a specific band. Filters may be combined to achieve certain spectral characteristics (e.g., better resolution).

If the spectral characteristics of a spectral filter are independent of the direction or position of the beam of radiation, it is called a *homogeneous filter*, but if these characteristics are directionally or positionally dependent, it is called a *variable filter* (i.e., the central transmission wavelength changes with position or angle).

An *absorption filter* which reduces the intensities of certain portions of the spectrum may be e.g., a solution, glass, plastic or gelatin.

An interference filter which reflects or transmits radiation in certain spectral bands as a result of optical interference may consist of partly transmissive and partly reflective *dielectric layers* with fixed separations between them.

A *Christiansen filter* reduces the intensities at those wavelengths at which the refractive index of a transmission medium differs from the refractive index of immersed particles by scattering.

5.3 Double-beam Interferometer

An example of a double-beam interferometer is the Michelson interferometer. It makes use of the interference of two beams of radiation, split by means of a semitransparent dividing plate or *beam splitter.* The beams are recombined after reflection from two separate mirrors.

A correction plate is used to compensate for the optical path difference between the two beams introduced by the beam splitter.

The *Twyman interferometer* is a modification of the Michelson interferometer making use of an entrance collimator. Its characteristics are:

– the maximum shift a_{max} of the moveable mirror;

– the transmission factor, t, and the reflection factor, r, of the beam splitter;

– the effective beam diameter D_{eff}.

From these the theoretical resolving power R_0 follows

$$R_0 = \frac{2a_{\text{max}}}{l} .$$

6 PREDISPERSER AND POSTDISPERSER

A predisperser or *postdisperser* is a spectral arrangement for the additional spatial separation of radiation according to wavelength. It can be used for selecting or sorting orders in a grating or interferometric spectral instrument and/or for the reduction of stray radiation. The predispersion or postdispersion can occur in the same direction as the main dispersion or perpendicular to it. In the first case, it is an *order selector,* in the latter case an *order sorter.*

7 PROPERTIES OF SPECTRAL APPARATUS

7.1 Spectral Properties

Spectral purity depends on the ability of an instrument to isolate a wavelength region. It is characterized by the *full width at half maximum (FWHM)* $dl_{0.5}$ and the

full width at hundredth-maximum $dl_{0.01}$ of the spectral band.

The term *monochromatic radiation* is used only in an approximate and relative sense, depending on the particular context. In reality, strictly monochromatic radiation does not exist as it indicates radiation of infinitely narrow spectral bandwidth.

7.1.1 The instrumental profile

The *(spectral) instrumental profile* expressed by the *instrument function* describes the distortion of the registered spectrum as well as the spectral purity obtained with a spectral apparatus. Ideally, if the incident radiation were strictly monochromatic with wavelength l_r, the outgoing intensity should be zero if l_r differs from the wavelength l_i to which the spectral apparatus is set. In practice, however, the outgoing radiant power decays more or less smoothly when $|l_i - l_r|$ is increased. This decay is described by the instrument function $y(l_i - l_r)$, which is normalized by setting $y(0) = 1$. For a spectral absorption filter, for example, the instrumental profile can be related directly to the transmission factor as a function of wavelength. For a prism monochromator, for example, the instrumental profile is determined by dispersion, slit widths, diffraction effects and optical imperfections.

The width of the instrumental profile is a measure of the spectral purity. The *effective spectral width* may be defined by:

$$D l_{\mathrm{eff}} = \int_0^{\infty} y\left(l_i - l\right) \mathrm{d} l .$$

This width may be conceived as the width of an imaginary rectangular instrument profile that has the same area as the actual profile.

7.1.2 *Stray radiation is* that radiation reaching the detector and having wavelengths outside the spectral band defined by the $dl_{0.01}$ of its spectral instrument function. This stray radiation may be *heterochromatic* (consisting of many wavelengths). The ratio of the integrated total stray radiation to the selected radiation within the spectral band is called the *stray radiation factor.*

7.1.3 The *exit spectral slit width* is the product of the exit slit width s_{ex} and the reciprocal linear dispersion $\mathrm{d}l/\mathrm{d}x_{\mathrm{ex}}$, i.e.:

$$D l_{\mathrm{ex}} = s_{\mathrm{ex}} \frac{\mathrm{d} l}{\mathrm{d} x_{\mathrm{ex}}}$$

The *entrance spectral slit width is* the product of the entrance slit width s_{en} and the reciprocal linear dispersion as measured at the entrance slit, if the radiation passes through the instrument in the reverse direction:

$$D l_{\mathrm{en}} = s_{\mathrm{en}} \frac{\mathrm{d} l}{\mathrm{d} x_{\mathrm{en}}}$$

The *resultant spectral slit width* of a dispersive spectral instrument may be illustrated by the case of a monochromator. Here, the resultant spectral exit slit width Dl_s is the larger of the two slit widths viz. the entrance spectral slit width Dl_{en} and the exit spectral slit width Dl_{ex} (see Note [10]).

7.2 Characteristics of Resolution

7.2.1 The *resolved wavelength distance* is the minimum wavelength distance between two equally intense spectral lines which can be separated clearly, and whose FWHM in the radiation source are small compared with their wavelength distance. They are

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[10] In a subtractive double monochromator the resultant spectral slit width is the smaller of the spectral slit widths of the two single monochromators. In an additive double monochromator the resultant spectral slit width is the smallest of the three spectral slit widths including the intermediate slit.

considered *resolved lines*, when the intensity registered between the lines is $8/p^2$, i.e., 81% of the intensity of two maxima.

This is the modified or *second Rayleigh criterion* (see Note [11])

7.2.2 The *theoretical resolution* $d_0 l$ is the calculated wavelength distance between two equally intense lines where the resolution is limited only by diffraction in such a way that the centre of the *diffraction pattern* from one line coincides with the first minimum from the second (also described as the *first Rayleigh criterion* (see Notes [12,13]). In these cases it is assumed that the widths of the slits present are sufficiently small.

7.2.3 The *practical resolution* $d_0 l$ is the wavelength distance measured under practical conditions conforming to the criterion given in 7.2.2 (i.e., 81%).

Suitable emission line pairs are not always available so that the practical resolution may be obtained from the width of the instrumental profile measured at $4/p^2$ i.e., 40.5% of the maximum intensity. For this measurement, a line narrow with respect to the width of the instrumental profile can be used.

7.2.4 The *resolving power* is the ratio of (average) wavelength l to the resolution $d_0 l$ i.e.:

$$R = \frac{l}{d_0 l}$$ (see Note [14])

This relationship holds for both theoretical and practical resolving powers. The theoretical resolving power may be calculated from the instrument specifications according to the appropriate formulae (see Sects. 4.2.2 and 4.2.3).

The *practical resolving power* is calculated by using the practical resolution, but with the dimensions of the entrance and exit field stops (e.g., slit widths and lengths) of the collimators being specified.

7.2.5 The *optimal slit width* or *optimal slit length* (see Note [15]) in a dispersive instrument is equal to the distance between the main (central) maximum and the first minimum of the *virtual diffraction pattern* produced by the entrance aperture stop in the entrance field stop (see Fig. 1). For a rectangular aperture the expressions are:

$$s_0 = \frac{l\, f_{\mathrm{en}}}{B_{\mathrm{en}}} = l\, k_{B,\mathrm{en}};$$

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[11] If the lines do not have the same intensity, the same criterion may be applied approximately, when the recorded local minimum intensity is compared with the recorded maximum of the less intense line.

[12] Under these circumstances the resolved wavelength distance is the same as the half-intensity width of the spectral profile. For this reason, the same symbol $d_0 l$ is used to denote both concepts.

[13] Once the theoretical resolving power R_0 is known, $d_0 l$ may be derived from the definition of R_0, i.e., $R_0 = l / d_0 l$. The calculation of the theoretical resolution of an instrument follows from the theoretical resolving power according to the relation: $d_0 l = l / R_0$ or with dispersive instruments, $d_0 l = s_0(\mathrm{d} l / \mathrm{d}x)$, where s_0 is the optimal slit width used.

[14] Resolution as defined in Part I, 5.2.2 is the practical resolving power according to the present document. Resolving power as defined in Part I, 5.2.2 is the theoretical resolving power in the present document. The present definition is the recommended term.

[15] Optimal is used in terms of theoretical resolution and optical conductance.

$$h_0 = \frac{l\ f_{\text{en}}}{H_{\text{en}}} = l\ k_{H,\text{en}}\ .$$

For a circular aperture, the *optimal diameter* is:

$$s_0 = h_0 = 1.22\ l\ \frac{f_{\text{en}}}{D} = 1.22\ l\ k_{\text{en}}\ .$$

7.2.6 The *optimal entrance field stop* of a Fabry-Perot interferometer and of a Twyman interferometer is a circle of radius r which depends on the focal length of the entrance collimator and the theoretical resolving power:

$$r_0 = \frac{2 f_{\text{en}}}{R_0}\ .$$

From this it follows that the *optimal field angle* w_0 is obtainable from

$$\tan w_0 = \frac{r_0}{f_{\text{n}}}\ .$$

7.3 The Conductance of Radiation through Optical Systems

Radiation proceeds from the source to the detector through the optical system. With proper imaging, this process can be described using the *concept of optical conductance* (see Part I, Appendix B, Pure Appl. Chem. *30* (1992)).

7.3.1 In the simple case indicated in Fig. 2 the *geometrical conductance* G_0 the entrance collimator is defined as the product of the entrance slit area A_l and solid angle W subtended by the collimator lens measured from the centre of slit. Defining A_2 as the area of the entrance aperture stop, we have $W = A_2/a_{12}^2$ and

$$G_0 = \frac{A_1\ A_2}{a_{12}^2}$$

where a_{12} is the distance between A_l and A_2. This is an approximation of the correct expression

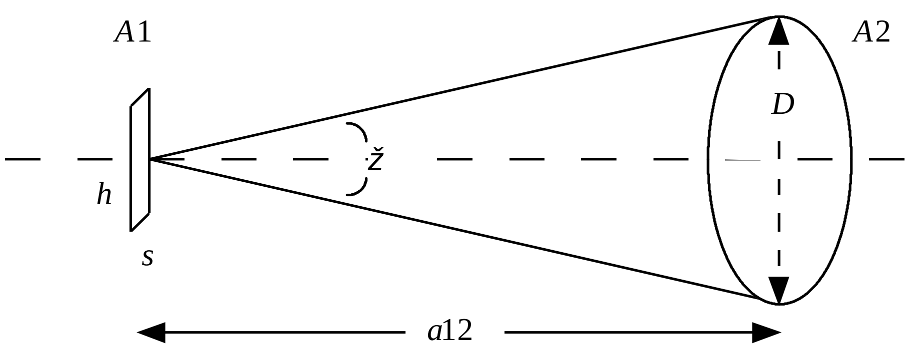

Fig. 2: Illustrating the Approximate Geometrical Conductance of a collimator in a spectral apparatus

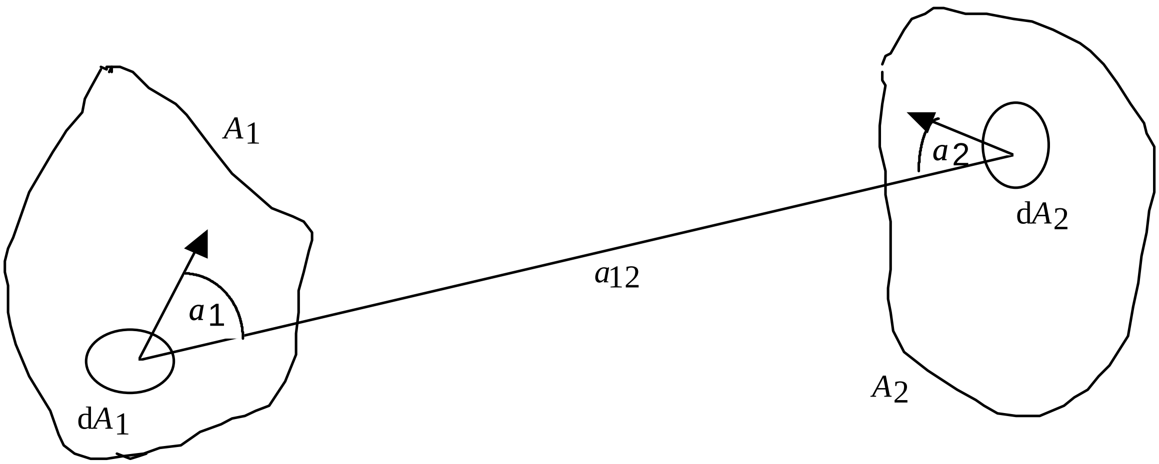

Fig. 3: General principal of Geometrical Conductance

$$G = \int_{A_1}\int_{A_2} \frac{\cos a_1 \cos a_2}{a_{12}^2}\, dA_1\, dA_2 \qquad \text{(see Fig. 3)}$$

where a_1 and a_2 represent the angles between the normals of the surface elements dA_l and dA_2 to their corresponding connecting straight lines. When the apertures A are small compared to the square of the distance a_{12} and perpendicular to the connecting line, the former equation is obtained. The geometrical conductance of a spectral apparatus with a rectangular slit and entrance aperture stop can be expressed by

$$G_0 = \frac{s_{en}\, h_{en}\, B_{en}\, H_{en}}{f_{en}^2} = \frac{l\, s_{en}^2\, h_{en}}{s_0\, h_0}.$$

7.3.2 The *optical conductance G* is the product of the geometrical conductance G_0 and the square of the refractive index of the medium between the planes of the apertures A_l and A_2:

$$G = G_0\, n^2.$$

7.3.3 The *effective optical conductance* G_{eff} is the product of the transmission factor, τ, and the optical conductance G:

$$G_{eff} = \tau\, G.$$

It determines the *radiant power, F,* conducted from a source having the *radiance L* through the instrument:

$$F = L\, G_{eff}$$ (see Note [16]).

7.3.4 The *spectral optical conductance of a monochromator*, G_λ, is the quotient of the optical conductance and the resultant spectral slit width:

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[16] When the various conductances depend on the wavelength, they can be written more precisely $G_0 = G_0(l)$, $G = G(l)$ and $G_{eff} = G_{eff}(l)$, respectively.

$$G_l = \frac{G}{D l_s}.$$

7.3.5 The *effective spectral optical conductance of a monochromator,* $G_{\lambda,\mathrm{eff}}$, is the product of the spectral optical conductance and its transmission factor:

$$G_{\lambda,\mathrm{eff}} = t\, G_{\lambda}.$$

The radiant power F_{U}, with the proper imaging of a *continuum source*, with a spectral radiance of L_{λ} is given by the relationship:

$$F_{l,\mathrm{U}} = L_l\, G_{l,\mathrm{eff}} \left(D l_s\right)^2 = L_l\, G_{\mathrm{eff}}\, D l.$$

The radiant power F_{L} with the proper imaging of a *spectral line source* with a total radiance:

$$L_0 = \int L_l \,\mathrm{d} l$$

is given by the relationship:

$$F_{\mathrm{L}} = L_0\, G_{l,\mathrm{eff}}\, D l_s\, F\left(l_L, l_{\mathrm{eff}}\right),$$

in which F denotes (in the plane of the exit slit) the convolution integral normalized to 1 of the instrument function y, and the *physical line profile function* of the *spectral line g(x),* also normalized to 1 by:

$$\int_{-\infty}^{+\infty} g(x)\,\mathrm{d}x = 1.$$

The complete expression for F is as follows:

$$F\left(l_L, d\, l_{\mathrm{eff}}\right) = \int_{-1/2\hat{s}_{\mathrm{ex}}}^{+1/2\hat{s}_{\mathrm{ex}}} \mathrm{d}x \int_{-\infty}^{+\infty} y\left(x' - x\right) g\left(x'\right) \mathrm{d}x' = 1$$

where

$$x = R_0 \frac{l - l_L}{l_L} \quad \text{and} \quad \hat{s}_{\mathrm{ex}} = \frac{s_{\mathrm{ex}}}{s_0}$$

are reduced dimensionless variables which are useful for matching different spectral apparatus.

7.4 Terms Relating to Wavelength of Radiation (see Note [17])

7.4.1 The *peak wavelength* l_{max} is that wavelength at which a filter or a monochromator setting has a maximum spectral transmission.

7.4.2 The *mean wavelength* l_{m} of a bandpass filter is the arithmetic average of those two wavelengths at which the transmission factor is half of the maximum.

7.4.3 The *weighted mean wavelength* $\bar{l}$ is the mean wavelength weighted by the instrument function, i.e.:

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[17] If wavenumber or frequency is used, different relationships apply.

$$\overline{l} = \int_{l_m - d l_{0.01}}^{l_m + d l_{0.01}} l_m(l)\mathrm{d}l \Bigg/ \int_{l_m - d l_{0.01}}^{l_m + d l_{0.01}} y(l)\mathrm{d}l \ .$$

7.4.4 The *median wavelength* l_{md} is that wavelength above and below which the instrument function contributes half the total signal:

$$\int_{-\infty}^{l_{md}} y(l)\mathrm{d}l = \int_{l_{md}}^{+\infty} y(l)\mathrm{d}l = \frac{1}{2}\int_{-\infty}^{+\infty} y(l)\mathrm{d}l \ .$$

7.5 Polarization

The *polarization state* of radiation is, as a rule, changed with its passage through an instrument as a result of reflection, refraction, double refraction, *dichroism* and diffraction.

To describe the polarizing properties, a 4 x 4 matrix (M) can be attributed to a spectral apparatus. The radiation entering the apparatus is described by a four-component vector $\mathbf{P}_1$, the *Stokes vector*. The state of polarization of the radiation leaving the apparatus can thus be given by another four-component vector $\vec{\mathbf{P}}_2$:

$$\vec{\mathbf{P}}_2 = (\mathbf{M})\vec{\mathbf{P}}_1$$

7.6 False Lines

Lines in the spectrum not emitted by the source are *false lines*. Depending on their origin they may be either *ghost* or *scatter lines*. They may occur in grating spectra (see Note [18]).

7.6.1 *Ghost lines*, symmetrically grouped on both sides of strong spectral lines and caused by a periodical error of a long period of the ruling engine are *Rowland ghosts*.

7.6.2 Ghost lines due to superposition of two unrelated periodical errors of different periods are *Lyman ghosts*.

7.6.3 Misplaced spectral lines situated very near the parent line and caused by slight non-periodic variations in spacing of the grating lines are called *satellites*. If the satellites are numerous, they are called near *scatter*.

7.6.4 Completely random variations of the groove spacing may be the cause of *far scatter*.

7.7 The *effective spectral FWHM* of a spectral line in the plane of the exit field stop is the convolution integral of the spectral distribution functions associated with the resultant spectral slit Δl_{en}, the theoretical resolution $d_0 l$, the FWHM of the spectral line $\Delta_{\mathrm{H}} l$, and a term $d_{\mathrm{z}} l$, due to optical imperfections. (Note [19])

8 TERMS RELATING TO CONDUCTANCE

8.1 The *line-to-background radiant power ratio is* given by the quotient $F_{\mathrm{L}}/F_{\mathrm{U}}$ with F_{U} (see 7.3.5):

$$F_U = L_{l,U} D l_{\mathrm{ex}} G_{\mathrm{eff}} \ .$$

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[18] Interferometric gratings do not show ghosts.

[19] The spectral resolution (see Section 7.2.3) may be estimated from the effective spectral FWHM.

8.2 The *irradiance E* is the radiant power divided by the irradiated area *S*:

$$E = \frac{F}{S}.$$

The *irradiance at the exit slit* is

$$E_{\mathrm{ex}} = \frac{F}{S_{\mathrm{ex}}} = \frac{F}{h_{\mathrm{ex}}\, s_{\mathrm{ex}}} = \frac{F}{h_{\mathrm{ex}}\, D l_{\mathrm{ex}}} \frac{\mathrm{d}l}{\mathrm{d}x}$$

8.3 The *radiant exposure H* is the irradiance integrated over the *measuring time.*

9 MOUNTINGS OF SPECTRAL APPARATUS

9.1 Prism Mountings

9.1.1 An autocollimation spectral apparatus with at least one reflecting (30°) prism as dispersive element and a lens or a mirror as objective element is *a Littrow prism mounting.*

9.1.2 If a separate mirror is used, it is a *Wadsworth prism mounting.*

9.1.3 A combination of prisms can be arranged to provide a *constant deviation mounting.*

9.1.4 Multiple prisms can be used in order to increase the deviation and provide a larger dispersion.

9.2 Concave Grating Mountings

9.2.1 A mounting with a concave mirror as imaging element of the entrance collimator and a concave grating acting at the same time as dispersive element and as imaging element (at normal angle of diffraction) of the exit collimator is called the *Wadsworth mounting* (Fig. 4). This mounting is used because of its stigmatic imaging properties .

9.2.2 A mounting in which entrance and exit collimators are fixed at an angle of about 70° and in which wavelength variation is effected by rotation of the grating is called the *Seya-Namioka mounting* (Fig. 5). It is mainly used in the vacuum UV region.

9.2.3 A normal incidence mounting, where for wavelength adjustment the grating is rotated and transported along the bisector of the angle subtended by the entrance and exit axis is called the *Robin mounting.*

9.2.4 *Flat-field mounting*

A mounting of a specifically corrected interferometric grating or *flat-field grating*, where for a considerable length of the spectrum a focal plane is obtained, is called a flat field mounting.

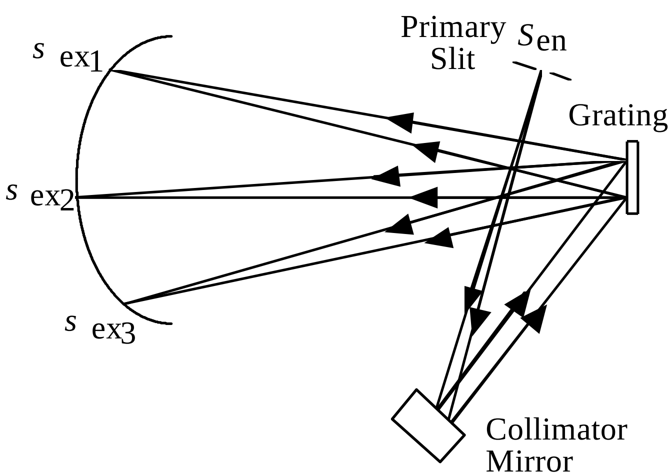

Fig. 4:-Wadsworth mounting

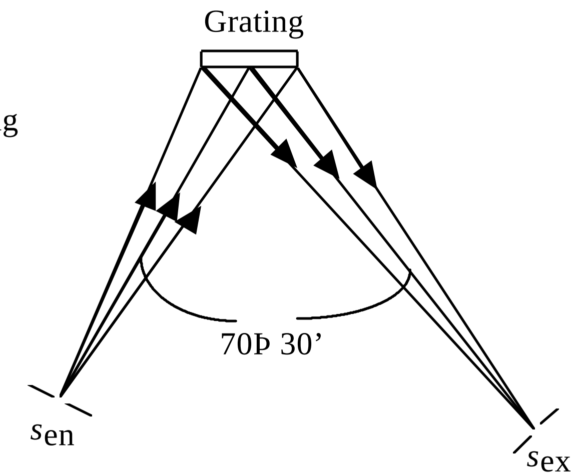

Fig. 5:-Seya-Namioka mounting

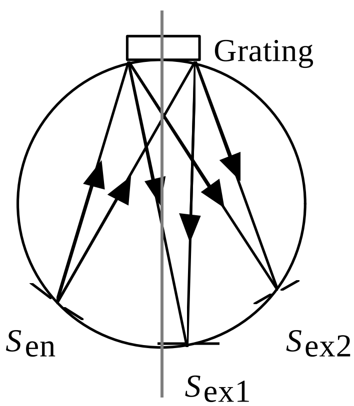

Fig. 6:-Paschen-Runge mounting

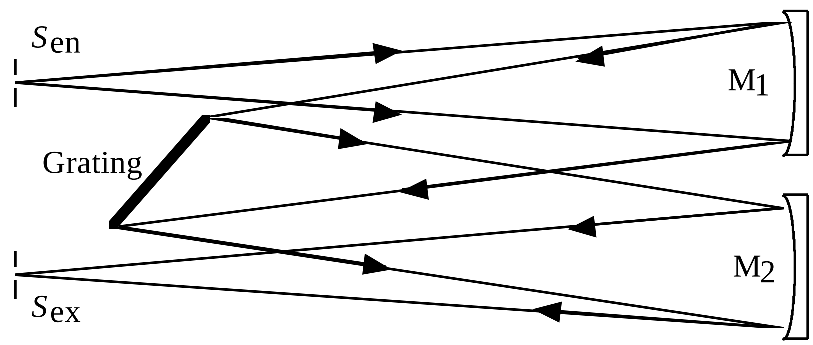

Fig. 7:-Czerny-Turner mounting

9.2.5 A *Rowland circle mounting* is one where a spherical concave grating with a radius of curvature R is mounted on the perimeter of a real or imaginary circle with a diameter equal to R. The lines of the grating are normal to the plane of the circle and the radius of the grating sphere passes through the centre of the circle. An entrance slit positioned on the Rowland circle produces a focused spectrum on the Rowland circle. The spectral lines are astigmatic.

9.2.6 A Rowland circle mounting, in which entrance slit and grating are fixed on the Rowland circle is termed the *Paschen-Runge mounting*. Photographic plates, film holders or exit slits are also attached to the circle. (Fig. 6).

9.2.7 A Rowland circle mounting near autocollimation is termed the *Eagle mounting*. It is suitable for e.g. vacuum instruments. If the entrance slit is located side by side with the camera or exit slit, it is called the *in-plane Eagle mounting*. If they are symmetrically placed above or below the plane of the Rowland circle, it is called the *off-plane Eagle mounting*.

9.2.8 *Grazing incidence mounting* is a Rowland circle mounting for the wavelength region below 100 nm, in which use is made of the high reflection near total reflection of the incident beam. Angles of incidence and diffraction are very large and of opposite sign.

9.3 Plane Grating Mountings

9.3.1 *A plane grating mounting* with one concave mirror acting as imaging element symmetrically for both the entrance and the exit collimator is an *Ebert mounting.* It is also called an *in-plane Ebert mounting.*

9.3.2 A similar mounting, but in which entrance and exit slits or the middle of the camera are displaced symmetrically in the direction of the grating grooves is called the *Fastie-Ebert mounting* or *off-plane Ebert mounting.*

9.3.3 A mounting similar to the in-plane Ebert mounting, but with separate mirrors for entrance and exit collimators is called the *Czerny- Turner mounting* (Fig. 7).

9.4 Echelle Grating Spectral Apparatus

An *Echelle grating spectral apparatus is* a plane grating spectrograph, monochromator or polychromator with an Echelle grating as dispersive element. Frequently, a pre- or post-disperser for order selection or order sorting is fully integrated. According to the chosen combination and its intended use, it is called an *Echelle spectrograph*, *Echelle spectrometer*, *Echelle monochromator* or *Echelle polychromator*.

10 SPECTRAL BAND SELECTION OF A MONOCHROMATOR OR A POLYCHROMATOR

The *spectral band selection* (or settings) may be obtained by moving the dispersive component (prisms or grating), by moving either the entrance slit or the exit slit in the focal plane, by rotating a *refractor plate* located for instance before the exit slit or by moving a collimating mirror.

11 LITERATURE

The following publications deal with aspects covered in this document:

IUPAC Manual of Symbols and Terminology for Physicochemical Quantities and Units, 2nd revision (Pure App. Chem., 51, 1-41 (1979).

IUPAC Quantities, Units and Symbols in Physical Chemistry, 2nd Edition (Blackwell Scientific Publications, Oxford, (1993)).

IUPAC Compendium of Analytical Nomenclature, Definitions, and Rules, 2nd Edition (Blackwell Scientific Publications, Oxford, (1987)).

Commission Internationale de l'Eclairage (CIE) International Lighting Vocabulary, Publ. No. 17, Paris.

DIN 5030-3 Spektrale Strahlungsmessung – Spektrale Aussonderung – Auswahlkriterien, DIN Deutsches Institut für Normung, Berlin.