The Analyst
AMC PAPER

Report by the Analytical Methods Committee
Evaluation of analytical instrumentation
Part XIII. Instrumentation for UV–visible–NIR spectrometry

Analytical Methods Committee†

The Royal Society of Chemistry, Burlington House, Piccadilly, London, UK W1V 0BN

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The Analytical Methods Committee has received and approved the following report from the Instrumental Criteria Sub-Committee.

Introduction

The following report was compiled by the above Sub-Committee of the AMC, which consisted of Professor S. Greenfield (Chairman), Dr M. Barnard, Dr C. Burgess, Professor S. J. Hill, Dr K. E. Jarvis, Dr M. Sargent and Mr D. C. M. Squirrell, with Mr C. A. Watson as Honorary Secretary. The initial input of the features for consideration was undertaken by a working party chaired by Dr C. Burgess with Dr D. G. Jones to whom the committee expresses its thanks.

The purchase of analytical instrumentation is an important function of many laboratory managers, who may be called upon to choose between a wide range of competing systems which are not always easily comparable. The objectives of the Instrumental Criteria Sub-Committee are to tabulate a number of features of analytical instruments which should be considered when making a comparison between various systems. As is explained below, it is then possible to score these features in a rational manner, which allows a scientific comparison to be made between instruments and as an aid to equipment qualification.

The overall object is to assist purchasers in obtaining the best instrument for their analytical requirements. It is de0ot8hopedthea

Column 3. The Sub-Committee has indicated the relative importance of each feature and expects users to decide on a weighting factor according to their own application.

Column 4. Here the Sub-Committee has given reasons for its opinion as to the importance of each feature.

Column 5. It is suggested that scores are given for each feature of each instrument and that these scores are modified by a weighting factor and sub-totals obtained. The addition of the sub-totals will give the final score for each instrument.

Notes on scoring

1. (PS) Proportional scoring. It will be assumed, unless otherwise stated, that the scoring features will be by proportion, *e.g.*, from worst/0 to best/100.

2. (WF) Weighting factor. This will depend on individual requirements. An indication of the Sub-Committee's opinion of the relative importance of each feature is indicated as follows: VI (very important); I (important), NVI (not very important). A scale is chosen for the weighting factor which allows the user to discriminate according to needs, *e.g.*, ×1 to ×3, or ×1 to ×10. The factor could amount to total exclusion of an instrument.

3. (ST) Sub-total. This is obtained by multiplying PS by WF.

Ultraviolet, visible and near-infrared spectrometry (UV–VIS–NIR) is a well established analytical technique with applications in many areas. An often bewildering range of instrumentation is available from a large number of different manufacturers. Systems range from simple filter based instruments for colorimetry to dual monochromator systems with variable extent, the selection process will inevitably be subjective, but if all the points have been considered, it should be an informed choice.

Definition and/or test procedures and

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score		
(*a*) Optical geometry	Score highest for the optical geometry most appropriate for the application, *i.e.*, single beam or double beam.	VI	Single beam instruments are often the lowest cost option and are generally used for single wavelength measurements. For spectral scanning, double beam instruments are preferred when using dispersive optics. Reverse confocal optics and interferometers are encountered only in specialised applications.	PS WF ST		
(*b*) Measurement mode	The majority of instruments operate in the absorbance/transmittance mode. Score additionally if concentration modes or specialist modes (*e.g.*, tristimulus values) are required.	NVI	Many simple instruments allow a conversion factor to be entered to convert absorbance values directly to a concentration. More sophisticated instruments can output absorbance data in a variety of colour data formats including tristimulus coordinates, CIE LAB units, *etc.*	PS WF ST		
4. *Sample compartment*						
(*a*) Size	Score maximum for the availability of adequate space for cuvette holders and, if appropriate, accessories.	I	Convenience of interchangeability of cuvettes and/or accessories increases productivity and reduces potential sources of error.	PS WF ST		
(*b*) Temperature stability	Score highest for sample compartments which are least sensitive to temperature changes during routine operation.	I(VI)	In the absence of thermostatic control, many solutions exhibit significant spectral changes with temperature. Spectrometers with sample compartments close to spectral sources and/or electronics are more likely to suffer heating effects.	PS WF ST		
(*c*) Accessibility	Score highest for spectrometers which allow ready access to accessory slots and service inlets to the sample compartment.	NVI	For spectrometers which require water thermostated cuvettes or sample changers, for example, ease of access is important for efficient operation.	PS WF ST		
(*d*) Gas purge	Score only if the presence of this feature is required.	I	For work below 200 nm, it becomes increasingly necessary to purge the optical path with dry particulate free argon to remove oxygen which absorbs significantly in this region.	PS WF ST		
5. *Sample presentation*						
(*a*) Cuvette						
(*i*) Design and size	Score highest for cuvette holders which allow positive and reproducible positioning. Score additionally for the ability to accommodate a range of cuvette sizes and types *e.g.*, flow through, microcell, if appropriate.	VI	It is essential to present the cuvette reproducibly centred and normal to the incident beam to minimise any optical effects due to non-parallelism of the cuvette faces and inter-reflection errors.	PS WF ST		
(*ii*) Thermostatic control	Score highest for systems with cuvette thermostating accessories. For kinetic and/or temperature jump applications, Peltier controllers are highly desirable.	VI	Many solutions exhibit significant spectral changes with temperature. Temperature control of the sample within ±1 °C is normal for multi-component deconvolution work. However, ±0.1 °C may be required for, *e.g.*, kinetic studies.	PS WF ST		
(*iii*) Autochanger	Score only if the application requires multiple cuvette operation.	VI	Some applications, *e.g.*, tablet dissolution or multi-sample kinetics, require programmable automatic cuvette changing.	PS WF ST		
(*b*) Skipper (flow cell) systems	Score for the presence of this accessory if required.	I(VI)	When a large number of samples are required to be measured, the use of a flow cell and peristaltic pump make the sample handling much easier and the quality of the data more consistent.	PS WF ST		
(*c*) Reflectance accessories	Score for the availability of diffuse or specular reflectance accessories and integrating spheres which enable solid and semi-solid samples to be measured. Score only if appropriate.	I(VI)	The vast majority of measurements are made in solution. However translucent and solid samples are increasingly being examined using transflectance or reflectance techniques.	PS WF ST		

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score
(*d*) Fibre optic probes	A variety of fibre optic probes for transmittance, transflectance and reflectance are available for remote measurement of liquid and solid samples. Score for the availability and suitability of each of these according to the application.	I(VI)	For many in-process control applications, the use of a probe allows measurement to be made rapidly and remotely from the spectrometer. Due consideration should be given to the optical performance of the fibre in the spectral region of interest.	PS WF ST
6. Wavelength selection devices				
	A range of wavelength selection devices are available in the UV–VIS–NIR spectral region. Some of the more technical aspects have been covered in Part IV of this series of papers.	VI		
(*a*) Filters	These are used in the simplest type of single beam colorimeters and photometers. Score highest for those with the largest number of filter options and smallest bandwidth.	I	A combination of interference and blocking filters can provide adequate monochromation for simple colorimetric measurements.	PS WF ST
(*b*) Single grating monochromators with fixed or variable slit	The majority of spectrophotometers are of this type. Score highest for those systems which have the slit widths required and additionally for scanning capability if required.	I	For spectral bandwidths of 2–10 nm, a single grating monochromator will provide adequate monochromation for qualitative scanning and quantitative single wavelength applications provided that the stray radiant energy requirements are not stringent. See below. Ð16 a double Ð[illegible] TD, InGaAiandwi13hro (STers and)Tj	PS WF ST
(*b*) Double monochromators	PS WF ob7 slit For the most exacting work particularly below 220 nm, the stray radiant energy performance is critical. Score highest for systems with the best stray radiant energy performance. Score additionally for the widest range of scanning speeds and spectral bandwidths.	I	Stray radiant energy causes deviations from the Beer–Lambert law. For consistent work above an absorbance of 2 the use of a double monochromator instrument is almost obligatory.	PS WF ST
(*d*) Polychromators	See Part III of this series of papers and Section 8(b) for details.Sectionfoubl0jvu /FT124stems wadv667age simples Foron -1oric measurementg			

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score
8. Spectral performance				
(*a*) Range	Score for the appropriate spectral range(s) needed, *e.g.*, UV 180–400 nm; visible 350–900 nm; NIR 750–2500 nm. Note that these boundaries are somewhat arbitrary and that some instruments will span the total range.	VI	The information content of the analytical signal is dependent upon the spectral region chosen.	PS WF ST
(*b*) Accuracy and reproducibility	Score for an accurate and reproducible wavelength scale. Standard materials such as rare earth oxides (solutions and glasses) and YAG crystals are available from national laboratories (*e.g.*, NPL and NIST) for calibration purposes. The wavelength accuracy may be checked using observed positions of atomic lines, *e.g.*, D_2 at 486 nm and 656 nm or other suitable line sources in the UV–visible region.			

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WF

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score
10. Instrument control and data collection				
(*a*) On-board computer	Score highly for a simple low cost effective routine instrument which has on-board software and is controlled from an integral keyboard. Score additionally for the facility to export data to an external computer (for further data manipulation if this is needed).	VI	Simplifies the operation and ideally should be able to provide simple method storage and limited data manipulation routines, *e.g.*, linear quantitation using standards.	PS WF ST
(*b*) Data output	For routine analyses score for an instrument that can output data to a printer/plotter or as an ASCII or industry standard file for external processing. A scanning instrument may output an analogue signal to a chart recorder or data logger.	I	A digital output is preferred so that if necessary further data processing may be easily performed.	PS WF ST
(*c*) External control of instrument parameters	For non-routine analyses or research, score highest for a comprehensive software package to control the spectrometer and collect the data.	VI	Ensures that the same analyses are always performed under identical preset conditions. This is vital if the system is in a regulated laboratory. Manufacturer supplied software will have to be validated. It is rarely cost effective to write one's own software.	PS WF ST
(*d*) Instrument performance diagnostics	Score maximum for an instrument which self checks on power up and has a simple validation routine programmed into the software.	VI	As more instruments are used in regulated laboratories, it is vital that the system performs diagnostic checks on power up. This information must be recorded.	PS WF ST
11. Data manipulation				
(*a*) Data collection software	Define the requirements before scoring these items. Most manufacturers offer software packages with routines for setting the instrument parameters and collecti9 sis 4.5 TDiald icitef howat the(softwarrunsat cad be vermay)Tj 0 -1.1256 TDm psoernald icims.akthectues that tor TDiae eees witt whic sis 4.at cad ay isam(sixpormanrd. Scoks ally for tay)Tj 0 -1.1256 TDavaid lacilitef oceidenrnah routinre.			

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score
(*b*) Data handling (*i*) Software to perform all arithmetic functions, *e.g.*, area, smoothing, derivatives, averaging, calculations on single points or spectra				