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GENERAL PAPER

Analytical Methods Committee

Evaluation of analytical instrumentation. Part XIX CHNS elemental analysers

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Abstract The reports of this series tabulate a number of features of analytical instruments that should be considered when making comparison between various systems. Scoring these features in a rational manner allows a scientific comparison to be made between instruments as an aid to selection. This is the XIXth report of the series and deals with CHNS elemental analysers.

Keywords CHNS analysers · Instrumentation · Overview · Evaluation

Introduction

The following report was compiled by the above Sub-Committee of the AMC, which consisted of Professor S Greenfield (Chairman), Mr. D J H Edwards, Dr M Barnard, Dr C Burgess, Professor S J Hill, Dr K E Jarvis, Dr G Lord, Dr M West, Dr M Sargent, Dr P J Potts, Dr J Price with Dr E J Newman as Secretary. Dr J A Price to whom the committee express their thanks undertook the initial input of the features for consideration and the reasons for their consideration.

The purchase of analytical instrumentation is an important function of many laboratory managers, who may be called upon to choose between a wide variety 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 that 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 over-all object is to assist purchasers in obtaining the best instrument for their analytical requirements. It is hoped that this evaluation will, to some extent, also help manufacturers to supply the instrument best suited to their customer's needs. It is perhaps pertinent to note that a number of teachers have found the reports of use as teaching aids.

No attempt has been made to lay down a specification. In fact, the Committee considers that it would be invidious to do so, rather it has tried to encourage the purchasers to make up their own minds as to the importance of the various features of the equipment that are on offer by the manufacturers.

The XIXth report of the Sub-Committee deals with the application of CHNS elemental analysers.

Notes on the use of this document

Column 1	The features of interest.
Column 2	What the feature is and how it can be evaluated.
Column 3	The Sub-Committee has indicated the relative importance of each feature and expects the 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 the 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 of features will be by proportion, e.g., Worst/0 to Best/100.
2. (WF) Weighting factor. This will depend on individual requirements. All features mentioned in the tables have some importance. If, in Sub-Committee's opinion, some features are considered to be of greater importance they are marked I. Those features of greatest importance

are marked as VI (very important). A scale should be 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 the total exclusion of the instrument.

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

With these requirements in mind, the user should then evaluate the instruments available on the market while bearing in mind the guidelines and any financial limitations. In many instances it will quickly become clear that a number of different instruments could be satisfactory and non-instrumental criteria may then be important. However, in some specialised cases only one or two instruments will have the ability or necessary features to carry out the required analyses.

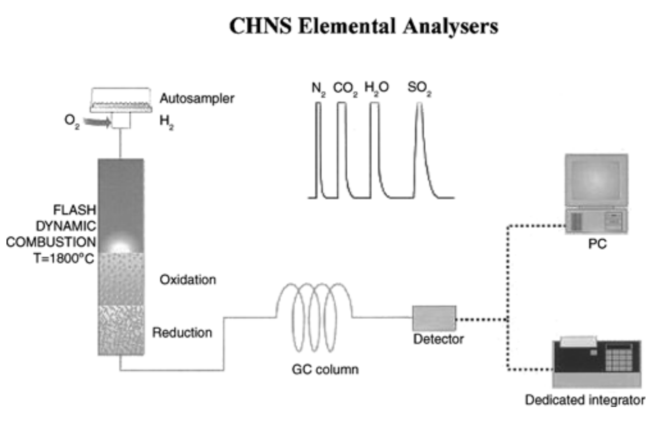
The guidelines are intended to be used as a checklist of features to be considered, mostly of the instrument itself, but some also of its service requirements and of the relationship of the user with the manufacturer. Their relative importance will depend on the installation requirements of the instrument as well as the uses to which it will be put. Therefore, to some extent, the selection process will inevitably be subjective, but if all the points have been considered, it should be an informed choice.

The Committee consider that instrumentation for CHNS analysis is safe in normal use, but care should be taken in handling toxic chemicals and high temperatures.

Finally, as many laboratories are now working to established quality standards, some consideration should be given to third party certification of the manufacturer to standards such as ISO 9001:2000. Such certification should extend to the service organisation.

An overview of CHNS elemental analysers

In considering the use of elemental analysers to perform CHN and S analysis, it was decided that the remit should be restricted to only combustion systems as other techniques, particularly for sulphur analysis (ICP, XRF etc), are also available.



Basis of instrumentation

In its simplest form, simultaneous CHNS analysis requires high temperature combustion (ca 1000 °C furnace temperature) in an oxygen-rich environment. This combustion can be carried out under both static conditions i.e. introduction of a set volume of oxygen or dynamic conditions i.e. A constant flow of oxygen for a set period. Both types of technologies have or are being used by instrument manufacturers in elemental analysers at the present time. Often, catalysts are also added to the combustion tube in order to aid conversion.

Other elemental combinations can also be carried out using these elemental analysers: carbon alone; nitrogen alone; sulfur alone; CN; CHN; CNS depending on the configuration of detectors and catalyst/absorbants used (see below). Traditionally, CHN analysis has been the most popular option of elemental analysis and all manufacturers in this microanalytical field offer this configuration.

In the combustion process, carbon is converted to carbon dioxide, hydrogen to water; nitrogen to nitrogen gas/oxides of nitrogen and sulfur to sulfur dioxide/trioxide. It must also be remembered that if other elements are present such as chlorine, they will also be converted to the appropriate combustion product, such as hydrogen chloride. A variety of absorbents are used to remove these additional combustion products as well as some of the principal elements e.g. sulfur if these latter entities do not require determination.

Once formed, the combustion products are swept out of the combustion chamber by inert carrier gas such as helium and passed over heated high purity copper. This copper can be situated at the base of the combustion chamber or in a separate furnace (ca 600 °C). The function of this copper is to remove residual oxygen not consumed in the combustion and to convert any oxides of nitrogen-to-nitrogen gas. The gases are then passed through the absorbent traps in order to leave carbon dioxide, water, nitrogen and sulfur dioxide.

Detection of the gases can be carried out in a variety of ways including (i) GC separation followed by quantification using thermal conductivity (ii) partial separation by GC ('frontal' chromatography) followed by thermal conductivity detection (CHN but not S) (iii) use of a series of separate infra-red cells and thermal conductivity for detection of each gas.

Quantification of the elements requires calibration of the instrument each time it is used. There are several ways in which this is achieved but, in principle, requires the determination of response factors (referred to as K factors) for each element using high purity 'microanalytical standard' compounds e.g. acetanilide, benzoic acid, etc.

In most instruments, there is some flexibility for changing the configuration of the absorbents; catalysts etc so that it can be run in a number of modes e.g. CHN, CHNS, CNS, N only as mentioned above.

Apparatus

As can be seen, there are a number of different formats which have been applied to combustion elemental analysers depending on the elements of interest; sample size; concentration range etc. Each of these different formats has its own advantages and disadvantages. The choice of analyser for particular applications will depend on a number of factors which are tabulated in the instrument evaluation form given below.

(i) 'Blank' contributions When considering the accuracy of measurement, one of the important factors is an assessment of the blank contribution from the gases, the capsules used for sample containment and the instrument system.

In the case of the gases, the purity of the carrier gas (e.g. helium) and the oxygen are very important, the latter where a level of 99.9995% is advisable. Together with use of suitable GC gas traps to remove traces of organics, water etc, this minimises the contribution of nitrogen etc to the blank. Another important consideration is to reduce the length of piping from the cylinders to the instrument to a minimum and to avoid any jointing. This situation also allows effective flushing of the line when cylinders are changed.

The second contribution to the blank values is from the capsules used to entrain the samples, normally tin capsules for solids or viscous liquids and aluminium for mobile liquids. In both cases, the capsules are washed with toluene and acetone before final drying in an oven. Using this procedure, the contribution to carbon dioxide and water values are minimised because any traces of oils or organics arising from the manufacture of the capsules are removed.

The third contribution arises from any leaks in the system resulting from failure of seals; O-rings etc. This will be seen as an increased contribution to the nitrogen blank. Since combustion and reduction tubes need to be replaced regularly, most instruments have facilities to allow automatic leak tests to be carried out on the different sections of the analyser.

As part of the calibration process, a series of blank capsules are run in order to determine the overall blank contribution from the three factors mentioned above. It is important that the blanks are as low as possible and consistent.

(ii) Sample types One of the main reasons for the different types of elemental analysers is that they have applicability to an extremely wide range of both liquid and solid product types. Liquids can include aqueous solutions, organic solvents, chemicals, petroleum products, etc. Solids or viscous liquids include inorganic chemicals, catalysts, and deposits as well as organic chemicals. The variations in sample matrix, the elements present and their levels means that a number of considerations have to be borne in mind.

Initially, thought has to be given to obtaining as homogeneous a sample as possible. In the case of clear liquids, this is relatively straightforward but for solids this can prove problematical. With regard to the choice and operation of the instrument, it must always be borne in mind that it is a combustion technique and thus certain limits are set by the fact that excess oxygen must be present at the end of the combustion to ensure complete conversion.

If consideration is given to CHN analysis where obtaining a homogeneous sample can prove difficult e.g. food analysis, a decision has to be taken on the weight required in order to provide a representative test portion. The larger the test portions and the higher the organic content, the more oxygen will be needed to carry out the combustion successfully. This in turn means that larger capacity copper filled reduction tubes are needed to remove the excess oxygen and provide capacity for a reasonable number of combustions before replenishment. Thus, for this particular type of application, a macro-CHN analyser would be required for gram-sized samples rather than a micro–type analyser designed for milligram quantities.

For solids, wherever possible the samples are ground to a fine powder before weighing into tin capsules. In cases where the samples are wet, oily or heterogeneous, judgement has to be made as to the best way to handle them. For most systems, the working weight range is 1–4 mg for purely organic compounds. As mentioned above, the limit is governed by the amount of oxygen available for the combustion. For the majority of sample types, a single 'flash' combustion is sufficient using one dosage of oxygen. However, for slow burning material such as coals and cokes, multiple additions of oxygen are required for complete combustion. In this case, the copper usage will be significantly increased. The ultimate analysis under this category of compounds would be silicon carbide which requires significant oxygen addition.

Another important consideration is the amount of ash that is formed during the combustion and its removal. The ash will be produced both through the use of the tin capsules and any inorganic residues present. Instruments have been manufactured with either vertical or horizontal furnace arrangements. In the case of vertical systems, ceramic crucibles are added to the combustion tubes to accommodate the ash. This allows autosampler operation of the instrument but can cause potential back-pressure problems if the ash is not removed regularly. The presence of ash during analysis has also led to some debate as to its potential to interfere with subsequent combustions. In the case of the horizontal systems, the ash is removed after each combustion but this arrangement is very difficult to automate. Thus, the vertical arrangements are the more popular of the two configurations.

For liquid samples, sample introduction can be via very small weighed aluminium capsules that are sealed in a special crimper or by direct injection via a microlitre syringe. The latter arrangement can be automated but is not as accurate as the weighing method due to temperature fluctuations in the laboratory and very small changes in the dispensing volumes.

(iii) Modes of operation As mentioned above, the sample masses that can be successfully accommodated in particular instruments are governed by the amount of oxygen avail-

able and the organic content present. In addition, attempts have been made to improve limits of detection (LOD) etc by different modes of detection.

In the first approach, the combustion gases, after removal of excess oxygen and non-CHNS products, are fully separated on a GC column into nitrogen, carbon dioxide, water and sulfur dioxide. If the column deteriorates or is overloaded, the nitrogen and carbon dioxide peaks overlap resulting in incorrect data. Nowadays, the instrument is connected to a computer so that this problem is easily detected. If only trace nitrogen is being measured (<0.02 percent m/m) in CHN mode, it is possible for the peak to be 'missed' by the computer if appropriate analytical conditions are not used.

In the second approach, the sample weight can be increased because only partial separation is required using a GC column. This is referred to as 'frontal' chromatography. In this case, all the CHN combustion products are collected in a gas-mixing chamber (impeller driven) and pressurised to 2 atmospheres (note: sulfur cannot be measured simultaneously in this mode of separation). At a set time interval, these gases flow through the GC column and continue to flow throughout the period of the analysis (approx. 4 minutes). This results in an accumulative stepwise trace which allows automated measurement of plateau heights for the three gases.

In the third approach, no separation step is included. This requires a more complicated detection system in that individual infra-red cells are used to quantify separately the carbon dioxide water and sulfur dioxide content with a thermal conductivity cell for nitrogen detection. This approach has the advantage that it allows separate measurement but is more complicated to use and more expensive in the first place.

Other approaches have also been used such as the separate adsorption of the gases followed by release and quantification in turn.

(iv) Calibration procedures Though there are different configurations of instrument, the calibration procedures are very similar in each case. Use is made of a number of certified reference materials for primary calibration e.g. acetanilide, benzoic acid, etc, which can be purchased from a number of suppliers. Acetanilide has traditionally been the compound of choice for CHN analysis as it can be produced with high purity.

In the case of instruments using GC separation, it is normal to run two or three 'bypass' acetanilide samples to condition the system before running three or four empty capsules to achieve 'blank' values. (The need for conditioning runs is primarily to stabilise the trace water content on the GC column.) Next, several weighed acetanilide samples are used as calibrants to give response factors for each element. With thermal detectors, there is inherent linearity across the entire concentration range. In the case of infra-red detectors, the response is pre-linearised at the factory. Once the instrument is calibrated, a secondary reference compound is analysed to check that the calibration is correct. It is advisable that controls are run throughout the day to monitor any drift.

Competitive techniques

Since the determination of such parameters as carbon contents or hydrogen contents of organic compounds have been basic measurements for many years, a number of complementary combustion technologies has also grown up around elemental analysers. Thus, though the 'CHNS' type of elemental analyser can be considered the workhorse, complementary techniques are also available for either specialised applications or trace analysis. In the case of a requirement for carbon analysis in aqueous solutions, a TC (total carbon)/TOC (total organic carbon) analyser should be considered. This can determine purgeable and non-purgeable organic carbon as well as total carbon and carbonate. In the case of trace nitrogen analysis, a combustion-and-chemiluminescence system could be preferable (LOD less than 1 mg/kg). For sulfur analysis, a number of techniques may merit consideration including energy dispersive and wave-length dispersive X-ray fluorescence (EDXRF/WDXRF), combustion/UV fluorescence detection, combustion/ microcoulometry, inductively coupled plasma emission spectrometry (ICP-AES), and electron capture detection and Fourier transform mass spectrometry.

For specialised applications, for example trace analysis or individual isotope concentrations; interfacing to mass spectrometric detectors is often possible.

Elemental analysis is normally carried out in combination with other techniques such as chromatography to provide underpinning fundamental data.

Instrumental criteria sub-committee instrument evaluation form

Type of Instrument: Elemental Analyser (CHNS)						
Manufacturer						
Model No:						
Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score		
A. non-instrumental criteria *selection of manufacturer*						
(a) Previous instruments	Laboratories in possession of other CHNS systems should score highest for the manufacturer with the best past record based on the following sub-features:					
(i) Innovation	Company's record for developing instruments with innovative features	I	The manufacturer should be alert to developments in technology	PS WF ST		
(ii) Reliability record	Company's record for instrument reliability. Score additionally if the manufacturing operation is accredited to a recognised Quality System e.g. ISO 9002	I	Indicates history of sound design and manufacturing concepts	PS WF ST		
(iii) Up-grading compatibility	Availability and ease of software and hardware upgrades and compatibility with earlier versions	I	Allows extension of instrument capabilities whilst ensuring the ability to reprocess old data files or methods. This is particularly important for laboratories that are accredited or regulated	PS WF ST		
(iv) Similarity of layout and design to instruments existing in laboratory	Consideration should be given to manufacturers of CHNS equipment who manufacture the other forms of elemental analysis instruments. For routine purposes this may be important. However, this may be less important for research applications	I	Similarity of layout means that operators can draw on in-house expertise, resulting in reduced training costs and time. It can also maximise the use of spares and fittings. Suites of elemental analysis equipment from a single manufacture imply similar computer software, reducing training and duplication of computer equipment	PS WF ST		
(v) Confidence in supplier	Confidence gained from past experience	I	Good working relationship already in place	PS WF ST		
(b) Servicing	Score according to manufacturers claims and past record, judged by the sub-features (i)-(vi) below:					
(i) Service contract	Availability of suitable service contracts from the supplier, agent or third party contractor	VI	Suggests long commitment to user. Often ensures preferential service and can guarantee a specific response time to call-outs	PS WF ST		
(ii) Calibration	A certificate of calibration, including traceability of calibrants should be issued at any service	VI	The calibration department, on or off site, should be accredited as a calibration laboratory operating to ISO 17025	PS WF ST		
(iii) Availability and delivery of spares	Range of stock carried by, or quickly available to, the manufacturer/agent/contractor	I	Rapid delivery of spares reduces downtime	PS WF ST		
(iv) Call-out time	The time for an engineer to reach the laboratory following a call	I	Keeps laboratory in operation by reducing down time (see also *(i)* and *(iii)*)	PS WF ST		
(v) Effectiveness of service engineers	The ability of the service engineers as judged from previous experience and reports of others, including the carrying of adequate spares. Training records of service engineers should be available on request	I	Ability to repair on-site avoids return visit or removal of equipment to supplier and reduces service time, costs and downtime	PS WF ST		
(vi) Cost of call-out and spares	It *may* be inappropriate to score this feature if downtime is not critical	I	The proximity of service centre may be a factor in travel costs	PS WF ST		
(c) Technical support	As in (b) score in consideration of the quality of sub-features (i)-(vi) below		Rapidly available technical help reduces the number of call-outs. Spares costs may be significant			
(i) Applications department	The advice and training available from the manufacturer's applications department	I	Guidance on optimum use of instrument suggests manufacturer's awareness of applications	PS WF ST		
(ii) Technical information	The range and quality of technical information including the operating manual. Also availability of updates and routine provision for existing users	I	This guides operators in the effective use of the instrument and with application problems	PS WF ST		
(iii) Telephone assistance	Willingness of the manufacturer to give effective advice on problems over the telephone. This can normally only be evaluated by reference to existing users	I	Rapidly available technical help reduces the number of call-outs and enhances productivity	PS WF ST		
(iv) Training	This includes initial training when setting up the instrumentation and follow-up courses for more advanced users	VI	A comprehensive training scheme will ensure that operators and instrumentation are working effectively	PS WF ST		
(v) Pre - installation	Full specification of site and services requirements	I	Providing the essential services and fittings required before installation will save time	PS WF ST		
(vi) User group	Newsletters, meetings, etc. organised by manufacturer or third party	I	Other users are often the best source of advice on problems, solutions and applications	PS WF ST		
B. Instrumental criteria						
1. General features Facilities required for:	Score according to convenience, taking into account the proposed location for the instrument					

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score		
(i) Location of connections and controls on instrument	Score according to convenient access taking into account the proposed location of the instrument	I	Depending on bench positioning and layout, these may limit accessibility for servicing and installation, particularly at rear of instrument	PS WF ST		
(ii) Power requirements	Many systems require multiple power inputs. Score maximum for instruments with the minimum of separate power leads		Excessive numbers of power cables when combined with other services create hazards and make servicing more difficult	PS WF ST		
(iii) Power failure effects	Score highest for systems that allow recovery from power failure with minimal data/control loss	VI	Down time is increased if power failure necessitates manual resetting of instrument control parameters. Data loss may be critical particularly in laboratories working in a regulatory environment. Power failures can damage furnace elements	PS WF ST		
(iv) Size of equipment	Score according to convenience of installation, taking into account the proposed location of the instrument and the instrument 'foot print'	I	Dimensions may be critical if space is limited	PS WF ST		
(v) Gases	High purity helium and very high purity oxygen (99.9995%) are required for operation. Score highest for the system that uses the least amount of oxygen in any particular application	VI	CHNS analysis can be carried out under either 'static' or 'dynamic' combustion conditions. In the first case, a set amount of oxygen is added via a gas loop; in the second, oxygen is added continuously. Very high purity oxygen is expensive to purchase. There should be provision for monitoring and controlling gas flow rates, ideally using mass flow controllers	PS WF ST		
(vi) Automatic weight entry	Score highest for instruments that allow for this feature	I	In general, transcription errors area major source of quality problems. Automatic weight entry minimises this occurrence	PS WF ST		
2. Instrument Features						
(a) Ease of replacement of combustion tube	Score taking into account the ease of replacement in terms of safety, downtime etc	I	Elemental analysers require regular replacement of combustion tubes, either because of depletion of catalysts or changes to the element suite being monitored e.g. change from CHN to CNS. Normally, the furnace is reduced in temperature prior to removal of tubes but they are still taken out 'hot'	PS WF ST		
(b) Replacement of reduction tube (if fitted)	Score in relation to the ease of replacement	VI	Reduction tubes (containing copper granules or wire) are also replaced on a regular basis. The frequency of replacement depends on the amount of oxygen used in the combustion but is typically of the order of 200-300 runs. Similar comments as those given for The replacement of the combustion Tube applies. In this case, it is particularly important to reseal the system quickly. The ingress of air will cause conversion of copper to copper oxide	PS WF ST		
(c) Removal of sample crucibles	Score in relation to the ease of removal	I	For systems using a vertical furnace arrangement, ceramic crucibles are added to the top of the combustion tube to collect the ash from the samples and tin/aluminium capsules. Opening of the system at operating temperature will introduce air, which in turn will reduce the life of the reduction tube. Thus the time taken for crucible replacement should be minimised	PS WF ST		
(d) Removal of GC column (if fitted)	Score in relation to the ease of removal	I	For systems that use GC separation, replacement of the column is required on an occasional basis e.g. if peak resolution is lost. The GC column is housed in a heated oven, often in the central part of the instrument making access difficult	PS WF ST		
(e) Repacking combustion tubes	Score in relation to the ease of repacking tubes	VI	The chemicals used as combustion aids, absorbents, etc. vary in type and quantity depending on the application. The combustion tubes need to be repacked on a regular basis due to the depletion of the activity of these chemicals	PS WF ST		
(f) Maintenance of detectors	Score highest for the instrument configuration which gives easiest access to the detectors	I	Normally, thermal conductivity and/or infra-red detectors are used for detection and quantification of gases. Periodic maintenance is required since thermal conductivity detectors can be subject to long term drift and infra-red detectors are prone to contamination if combustion conditions are not optimised	PS WF ST		
(g) Limits of quantification (LOQ)	Score highest for the lowest limits of quantification (LOQ)	I	The limits of quantification (LOQ) for the relevant elements will depend on a number of factors including configuration; sample size etc. as well as detector sensitivity	PS WF ST		
(h) Drift	Score highest for the instrument which gives the least amount of drift. Score additionally for low gas pressure alarm	VI	During normal operation, small changes in drift can be compensated for within the relevant software. However, excessive drift is normally caused by reduction in helium gas pressure and thus a low gas pressure alarm is a useful feature	PS WF ST		
(i) Assessment of precision	Score highest for the best precision data obtained from the analysis of certified reference materials and/or pure materials representative of the sample matrices	I	Precision is influenced by instrumental factors as well as weighing ability of the analyst	PS WF ST		

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score		
3. Instrument Configuration	The choice of interfacing, autosamplers, balances and output to e.g. LIMS systems		Important depending on the use of the equipment			
(a) Unattended operation	Score highest for instruments which have multiple sample holders	I	Since elemental analysers are often used as high throughput instruments, autosampler options extend the flexibility of the instrument by allowing unattended operation. Both autosampler carousel systems (solids) and vial injectors (liquids) are available	PS WF ST		
4. Instrument Control and Data Collection						
(a) Control of instrument	Score highest for a comprehensive software package to control the instrument and collect the data automatically	VI	This is vital if the system is in a regulated laboratory. In the regulated/accredited environment, manufacturer supplied software operating within the instrument will have to be validated	PS WF ST		
(b)Data output	For routine analyses score for an instrument that can output data (raw and/or processed) to an appropriate industry standard file for external processing and exporting	I	A digital output is preferred so that if necessary further data processing may be easily performed	PS WF ST		
(a) Instrument performance diagnostics	Score highest for an instrument which self-checks on power- up and has a validation routine programmed into the software	VI	In laboratories operating to regulatory requirements, it is vital that the system performs diagnostic checks on power up. This information must be recorded	PS WF ST		
(b) Audit trail	Score for the presence of this feature within the control software only if required	I	Some regulatory authorities require that all electronic data records be accompanied with an uneditable audit trail to show which operations were performed by whom and when for reasons of data security and integrity	PS WF ST		
5. Hardware and Output Requirements						
(a) Computer	Score for compatibility with either existing or company selected computer	I	There may be a company requirement for uniformity. Speed and ability to upgrade are important	PS WF ST		
(b) Data storage and archiving	Score for the possibility to store data on suitable archive media for future retrieval and use	VI	This is very important, as is the provision of metadata. Date and acquisition parameters must also be archived	PS WF ST		
(c) Data output from simple instruments	Score for the ability to output either digital or analogue data		It is beneficial if the system can be coupled to a standard printer to produce a hard copy of data output	PS WF ST		
(d) Ability to be networked	Score only if this feature is required		In some laboratories data will need to be transferred to a server directly from the instrument and/or a PC	PS WF ST		
6. Data processing						
(a) Data acquisition	Define the requirements before scoring these items. Most manufacturers offer software packages with routines for collecting the data. Make sure that the features offered are fully evaluated. The ease with which the data can be acquired is of prime importance Score as listed below only for the availability of essential routines		Data collection software options are essential for data integrity and must include all of the required routines. Software packages from the manufacturer are expensive, but the effort it will take to write and validate one's own software would prove to be extremely time-consuming and therefore more expensive			
(i) Storage of data files	Score maximum for a system where all relevant data collection parameters are stored with the raw data files	I	Essential in many laboratories for regulatory requirements e.g. GLP, GMP and all regulated industries. There is a need to ensure that raw data files can be reprocessed at a later time to demonstrate validity of original results	PS WF ST		
(ii) Data capture and collation software	Score maximum for the most comprehensive routine available to control all data capture and collation activities to ensure data integrity. Deviations must be flagged by the software and a comprehensive "error logging" routine is highly desirable	I	Essential for many regulatory requirements e.g. GLP, GMP and all regulated industries	PS WF ST		
(b) Data handling						
(i) Software to perform relevant calculations	Software is written by the manufacturer to convert the raw data to elemental composition values based on response factors; sample sizes etc	I	The software enables routines to transform raw data without having to use third party software. This is particularly important for regulatory requirements e.g. GLP, GMP and all regulated industries	PS WF ST		
(ii) Specific application routines and the ability to customise them	Score maximum if this feature is present and appropriate	I	This facility enables routines to be made so that less experienced staff can perform the analysis under optimum conditions routinely	PS WF ST		
(iii) Routines for checking qualification software	Score maximum for supplied software which allows for ease of verification of the basic operational control and tracking calibration of the system	VI	Essential in laboratories that need to meet regulatory requirements e.g. GLP, GMP etc	PS WF ST		
				Sum of sub-totals		
7. Value for money (Points per currency unit)	Sum of the previous sub-totals divided by the purchase price of the instrument. Subject to proportional scoring and weighting factors, including ST in grand total	I	'Simple' instruments are often good value for money, whereas those with unnecessary refinements are often more costly	PS WF ST		
				Grand Total		

Other reports

The Analytical Methods Committee has published the following reports in the series:

Part I	Atomic absorption spectrophotometers, primarily for use with flames (1984) Anal Proc 21:45. Revised in (1998) Analyst 123:1407
Part II	Atomic absorption spectrometers, primarily for use with electrothermal atomizers (1985) Anal Proc 22: 128. Revised in (1998) Analyst 123:1415
Part III	Polychromators for use in emission spectrometry with ICP sources (1986) Anal Proc 23:109
Part IV	Monochromators for use in emission spectrometry with ICP sources (1987) Anal Proc 24:3
Part V	Inductively coupled plasma sources for use in emission spectrometry (1987) Anal Proc 24:266
Part VI	Wavelength dispersive X-ray spectrometers (1990) Anal Proc 27:324
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Part XVI	Evaluation of general user NMR spectrometers (2006) Accred Qual Assur 11:130–137
Part XVII	Instrumentation for inductively coupled emission spectrometers (2005) Accred Qual Assur 10:155–159
Part XVIII	Instrumentation for differential scanning calorimetry (2005) Accred Qual Assur 10:160–163
Part XIX	CHNS elemental analysers (2006) Accred Qual Assur, DOI 10.1007/s00769-006-0185-x
Part XX	Instrumentation for energy dispersive X-ray fluorescence spectrometry (2006) Accred Qual Assur, DOI 10.1007/s00769-006-0187-8
Part XXI	NIR instrumentation for process control (2006) Accred Qual Assur 11:236–237
Part XXII	Instrumentation for liquid chromatography/mass spectrometry (2006) Accred Qual Assur DOI 10.1007/s00769-006-0188-7

References

1. ASTM D5291 Instrumental determination of carbon; hydrogen and nitrogen in petroleum products and lubricants, test method for.