Report by the Analytical Methods Committee

Evaluation of Analytical Instrumentation. Part VIII Instrumentation for Gas–Liquid Chromatography

Analytical Methods Committee
The Royal Society of Chemistry, Burlington House, Piccadilly, London W1V 0BN

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

Introduction

This report was compiled by the above Sub-Committee of the AMC which consisted of Professor S. Greenfield (Chairman), Professor E. Bishop, Dr. P. J. Potts, Mr. D. C. M. Squirrell, and Mr. P. Warren, with Mr. C. A. Watson as Honorary Secretary. The initial input of the features for consideration and the reasons for their consideration was undertaken by a working party Chaired by Dr. R. M. Smith with Mr. M. Humphrey and Dr. K. D. Bartle, to whom the committee express their thanks.

The purchase of analytical instrumentation is an important function of many laboratory managers, who may be called upon to choose between a 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 which should be considered when making a comparison between various systems. As explained below, it is possible to score these features in a rational manner, which allows a scientific comparison to be made between instruments.

The overall-all object is to assist purchasers in obtaining the best instrument for their analytical requirements. It is hoped that, to a degree, it will also help manufacturers to supply the instrument best suited to their customers' 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 is on offer by the manufacturers.

The eighth report of the Sub-Committee deals with Instrumentation for Gas–Liquid Chromatography.

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 needs.
Column 4. Here the Sub-Committee has given reasons for its opinion as to the importance of each feature.
Column 5 onwards. 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 of 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. An indication of the Sub-Committee's opinion of the relative importance of each feature will be indicated by the abbreviations VI (very important), I (important) and NVI (not very important). A scale is then 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.

Gas chromatography is a well established analytical technique with applications in many areas. An often bewildering range of instrumentation is available from well over a dozen different manufacturers. Systems range from simple instruments, with a single column and detector, to complex multi-channel systems with autosamplers and microcomputer-based controllers for continuous operation and sophisticated mass spectrometric or FT–infrared spectroscopic detectors.

Selection of a suitable instrument for purchase is, therefore, not an easy task and the purpose of these notes is to provide some guidance to areas which should be considered so that the choice is based on a full consideration of the available options. However, the performance of any gas-chromatographic method depends primarily on the separation conditions and thus on the nature of the column material, stationary phase and carrier gas and whether a packed or open-tubular column is used. The type of detector will also influence the sensitivity and selectivity of the assay. A number of alternative instruments may thus be suitable.

The first task in the selection of an instrument is to examine the range of analyses that it will be expected to perform. Care should be taken not to specify these requirements too closely as uses change with time. The analytical scientist should also not try to envisage every potential application or the selection criteria may become too detailed. The choice of the column and detector type are outside the scope of these guidance notes but any specific requirements should be noted, such as special detectors, injectors or accessories.

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 specialized cases only one or two instruments will have the ability or necessary features to carry out the assay.

The guidelines are intended to be used as a check list 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.

In addition, because a separation depends so much on the column and operating conditions, it may sometimes be difficult to assess the actual operating performance of a particular feature from the manufacturer's specifications. Few standard tests have been developed for gas chromatography columns and for some applications it may be necessary to evaluate the performance of the column using the instrument under consideration. Gas chromatographs are often sold as complete units, so that compromises between features may have to be accepted, but it will still be important to distinguish between critical features and those which are optional.

The Committee consider that, in general, gas-chromatography equipment is safe in normal use, but care should be taken to allow sufficient cooling time when changing columns and detectors and taking suitable precautions when handling inflammable gases such as hydrogen. If hydrogen is used as a carrier gas it is recommended that a suitable leak detector should be fitted in the oven.

Finally, as many laboratories are now working to quality standards such as GLP/NAMAS/ISO9000, some consideration should be given to third party recognition of the manufacturer to standards such as BS5750 and ISO 9000. Such accreditation should extend to the service organization, which is particularly important when working to NAMAS or GLP criteria.

INSTRUMENTAL CRITERIA SUB-COMMITTEE INSTRUMENT EVALUATION FORM

Type of Instrument: Gas chromatograph

Manufacturer:								
Model No:								
Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
NON-INSTRUMENTAL CRITERIA *Selection of manufacturer* (*a*) Previous instruments	Laboratories in possession of other gas chromatographs should score highest for the manufacturer with the best past record based on the following sub-features:	I						
(*i*) Innovation	Company's record for developing instruments with innovative features.		The manufacturer should be alert to developments in technology and chromatography.	PS WF ST				
(*ii*) Reliability record	Company's record for instrument reliability.		Indicates history of sound design/manufacturing concepts.	PS WF ST				
(*iii*) Up-grading compatibility. Interchangeability of column and detectors	The ease with which columns, injectors, pneumatic modules and detectors can be changed between different instruments.		Shapes of packed columns often differ. Common column fitting methods allow columns to be transferred between instruments, giving greater flexibility. Open tubular columns are usually interchangeable. If detectors have the same base and electrical connections as existing instruments, the user can interchange detectors between instruments. Also common spares and components such as amplifiers can be interchanged.	PS WF ST				
(*iv*) Similarity of layout and design to instruments existing in laboratory			Similarity of layout means that operators can draw on in-house expertise, resulting in reduced training costs and time. It can also maximize the use of spares and fittings.	PS WF ST				
(*v*) Confidence in supplier	Confidence gained from past personal experience.		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*)–(*iv*) below:	VI						
(*i*) Service contract	The availability of a suitable service contract from the manufacturer or agent.		Suggests long commitment to user. Often ensures preferential service and can guarantee a specific response time to call-outs.	PS WF ST				
(*ii*) Availability and delivery of spares	Range of stock carried by the manufacturer and delivery time.		Rapid delivery of spares reduces downtime.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
(*iii*) Call-out time	The time for an engineer to reach the laboratory following a call.		Keeps laboratory in operation by reducing down time [see also (*i*)].	PS WF ST				
(*iv*) Effective-ness of service en-gineer	The ability of the service engineer as judged from previous experience and reports of others, including the carrying of adequate spares.		Ability to repair on-site avoids return visit or removal of equipment to supplier and so reduces service time, costs and downtime.	PS WF ST				
(*v*) Cost of call-out and spares	It *may* be inappropriate to score this feature.		The proximity of service centre may be a factor in tra-vel costs.	PS WF ST				
(*c*) Technical Support	As in (*b*) score in consideration of sub-features (*i*)–(*iii*) below.	VI for new user						
(*i*) From Appli-cations Depart-ment	The advice and training available from the manufacturer's applications department.		This helps in-house staff with new application problems.	PS WF ST				
(*ii*) Technical literature	The range and quality of technical literature including the operating manual.		Guidance on optimum use of instrument suggests manufacturer's awareness of applications.	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.		Rapidly available technical help reduces the number of call-outs.	PS WF ST				
INSTRUMENTAL CRITERIA								
1. General features								
(*a*) Facilities re-quired for:								
(*i*) Location of connections and controls on instrument	Score according to convenience, taking into account the proposed location for 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*) Snap-on coded fit-tings on gas lines	Score for provision of snap on fittings and clarity of coding.	I	Coded supplies should be more secure and reduce risk of incorrect connections.	PS WF ST				
(*iii*) Power and heat dissi-pation	The ability to remove heat particularly during oven cooling cycles. Score highest for instrument most suited to proposed location.	I	Needed because the oven generates considerable heat during operation. Air conditioning or ventilation may be needed. Depending on the design of the oven exhaust vent an area of bench may need to be left free for heat dissipation.	PS WF ST				
(*iv*) Dimen-sions	Score according to compatibility of dimensions (width and depth) to space available.	I	Availability of suitable bench space. This may be important in some circumstances.	PS WF ST				
2. *Carrier and detector gas supplies*								
(*a*) Flow control	Score maximum for a flow control system which gives the most precise and reproducible gas flows. This may be tested using a bubble flow meter.	VI	Control is needed to give a constant gas flow, upon which precision and reproducibility are dependent.	PS WF ST				
(*i*) Flow con-trollers	Score maximum for the provision of the most precise mass-flow controllers. Score additionally if the controller is computer compatible.	VI	Used for packed and wide-bore open tubular columns.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
(*ii*) Pressure controllers	Score maximum for the provision of the most precise pressure controllers.	VI	Used with open-tubular columns. For either gas control system, digital control is generally more precise and reproducible than manual control. This is particularly desirable if the settings will be changed frequently.	PS WF ST				
(*iii*) Controlled temperature	Score additionally if the flow controllers are contained within a controlled temperature environment.	I	A controlled temperature environment can increase the stability of the system.	PS WF ST				
(*b*) Carrier gas supply								
(*i*) Ability to use hydrogen or helium	Score according to availability of sub-features (*i*), (*ii*) and (*iii*) if capillary columns are to be used.	I	Needed for capillary columns as they give higher efficiency and faster separations than nitrogen.	PS WF ST				
(*ii*) Carrier leak detector		VI	Needed if hydrogen is used as carrier gas to avoid build-up of gas in oven in the case of a leak.	PS WF ST				
(*iii*) 'Make up gas'		VI	Needed to maintain a suitable gas flow through the detector when capillary columns are used.	PS WF ST				
(*c*) Connections								
(*i*) Gas supply lines	Score according to availability and ease of fitting of non-permeable gas lines.	I	Nylon lines are porous to air and should not be used with an electron capture detector as air causes a high background. They are also not recommended for the nitrogen–phosphorus detector (NPD). Nylon can age if exposed to sunlight. Metal tubing is more robust.	PS WF ST				
(*ii*) Gas purifiers	Score according to availability, stated efficiency, and ease of fitting of on-line traps, such as activated carbon or molecular sieves, into gas supply lines.	VI	Removal of oxygen and water from carrier gas is essential for ECD detectors and desirable for some sensitive stationary phases or for operation at high sensitivity. Oil may also need to be removed from air lines if a compressor is used.	PS WF ST				
3. *Injection ports*								
(*a*) General								
(*i*) Ease of cleaning	Score according to ease by which units can be dismantled and reassembled for cleaning.	I	The need to remove involatile residues.	PS WF ST				
(*ii*) Replaceable liners	Score for provision of replaceable liners for injection ports.	VI	Replacement of liners removes involatile residues and reduces contamination.	PS WF ST				
(*iii*) Septum replacement	Score according to ease of removal and replacement of septa.	VI	Frequent changes of septa are necessary for satisfactory operation.	PS WF ST				
(*iv*) Septum purge	Score additionally for provision of bleed of carrier gas from just below septum.	I	Removes volatiles arising from degradation of the septum and reduces background peaks. Particularly needed for temperature programmed separation on open-tubular columns.	PS WF ST				
(*b*) Heaters								
(*i*) Injector heater control	Score highest for most stable control of temperature of injector heater unit.	I	Injector temperature can affect volatilization and sample stability on injection.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
(*ii*) Programmable cooling/heating of injection zone	If capillary or open tubular columns are to be used, score for availability of a programmable unit for heating/cooling the injection zone.	I	Can be used in split/splitless injection (particularly important for capillary chromatography) to focus sample and in on-column injection to raise rapidly the temperature after start of run.	PS WF ST				
(*iii*) Independent temperature control	Score additionally for provision of a separate oven for the sample injection ports.	I	Temperature of the injection ports should not be altered by programming of column ovens if repeatable subsequent injections are to be obtained.	PS WF ST				
(*v*) Heater temperature range	Score maximum for widest range normally provided.	I	Normal applications need up to 350 °C. Some high temperature applications may need up to 450 °C.	PS WF ST				
(*c*) Types of injection port								
(*i*) Capillary or open-tubular column injectors	For capillary (open tubular) columns score for provision of both split/splitless and on-column injection facilities. Score additionally according to ease of changing ports and provision of manual or automatic operation.	VI	Choice enables wider range of analytes to be examined. *Split*—Mainly used for samples with limited volatility range. Wide ranging samples may suffer some discrimination. Need ability to set split ratio for quantitative results. *On-column*—Needed for thermally sensitive samples and to avoid discrimination effects in wide boiling range samples.	PS WF ST				
(*ii*) Gas sampling valves	Fixed volume loops which can be switched into the carrier gas line. Score according to availability and ease of connection.	I (depending on application)	Needed for gaseous samples as syringe injections can give poor quantification.	PS WF ST				
4. *Column ovens*								
(*a*) Oven design	General preference should be for a size of oven which will accommodate two columns with adequate access. Score accordingly.	I	Usually only one column is used for open-tubular separations but with packed columns two columns are often used to provide column bleed compensation.Only one column is needed if electronic background compensation is available. Sufficient space is required to enable work in oven to install and replace columns.	PS WF ST				
(*b*) Oven temperature								
(*i*) Hysteresis	Score maximum for smallest temperature lag during heating and cooling cycles.	I	Slow response can limit programming and cooling rates and prolong re-equilibration time.	PS WF ST				
(*ii*) Maximum temperature	Most ovens operate satisfactorily up to 350 °C. If higher temperatures required score additionally if oven will operate up to 450 °C.	VI	Some high temperature separations using special columns may need up to 450 °C.	PS WF ST				
(*iii*) Thermal fuse/electronic cut-out	Score for provision of thermal fuse or electronic cut-out to turn off oven heater in case of controller failure.	VI	Safety device to protect columns (and injector) from excessive heating.	PS WF ST				
(*iv*) Near-ambient operation	Most ovens operate satisfactorily down to 10 °C above ambient. For the examination of volatile samples score additionally for satisfactory control at near ambient temperature.	I	Enables repeatable analysis of volatile samples. Some ovens have minimum usable temperatures for reproducible control.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
(*v*) Sub-ambient capability	If required, score additionally for availability of an add-on cooling system.	I	Needed for some gas samples and for highly volatile samples.	PS WF ST				
(*vi*) Temperature gradients across oven	Score maximum for minimum temperature gradients within oven.	I	Gradients due to poor air mixing in the oven can produce poor peak shapes with open-tubular columns because of their low thermal mass. Packed columns are less sensitive to the effects of thermal gradients.	PS WF ST				
(*c*) Oven programmers								
(*i*) Temperature/gradient settings	Score highly for provision of digital control rather than analogue control for temperature gradient settings.	I	Digital controlled programmes are easier to reproduce.	PS WF ST				
(*ii*) Number of steps available	Score according to the numbers of separate delay periods and temperature ramps that can be programmed.	I (for complex samples)	The more steps available, the greater the flexibility. Desirable for complex samples, particularly to flush off involatiles. Most samples will only need a limited number of steps in the programme.	PS WF ST				
(*iii*) Heating rate	Score most for the highest maximum ramp rate that the oven can follow.	I	High rates are needed for cold on-column injections or with short columns. Also needed when chromatograph is linked to autosampler to co-ordinate injection with temperature programme and data collection.	PS WF ST				
(*iv*) External control programme	If an external computer or data system is likely to be used, score for ability to control oven temperature by these means.	VI	A computer can also vary conditions to match mixed samples in autosampler.	PS WF ST				
(*v*) Reproducibility of programmed temperature	Score highly for good reproducibility in temperature control on resetting programme.	VI	Programme reproducibility is more important than accuracy. Needed to ensure consistency of results.	PS WF ST				
(*d*) Column installation								
(Column materials and stationary phases are outside the scope of this evaluation.)								
(*i*) Column fittings	Score according to ease of changing columns.	I	Self evident.	PS WF ST				
(*ii*) Interchangeability between open tubular and packed columns	Score for the ability to interchange between open-tubular, packed and wide-bore columns. When narrow open-tubular columns are to be used, score additionally for minimum dead volume in detector.	I	Gives maximum flexibility in use of system, bearing in mind that most instruments are dedicated to one mode. Presence of large dead volumes in detectors degrades separation efficiency and may cause discrimination effects.	PS WF ST				
(*iii*) Ability to use wide-bore columns	If the application may call for the use of wide-bore columns, score additionally for the provision of this feature.	NVI	In some applications, wide-bore columns may produce better separations than packed columns.	PS WF ST				
5. *Detectors*								
(*a*) Detector types	In most instances detector selection is circumscribed by the analytical method. Detector selectivity may be needed to distinguish between analyte and matrix.							
(*b*) Availability	If appropriate, score maximum for highest number of detectors which can be fitted on standard instrument.	I	Enables a wide range of applications; increases versatility.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
(*c*) General detector and amplifier features								
(*i*) Linearity of response	Score maximum for widest linear dynamic range.	VI	Wide linear dynamic range facilitates an extended calibration range for quantitative studies. For ECDs this is usually greater in constant current mode than constant pulse rate mode.	PS WF ST				
(*ii*) Sensitivity	For the major analytes of interest, score maximum for the best signal to noise ratio.	VI	High signal to noise ratio permits increased sensitivity and enables smaller quantities of analytes to be detected.	PS WF ST				
(*iii*) Dead volume	Score maximum for lowest dead volume of detector cell and connections.	VI	To minimize band broadening when used with capillary columns. Make-up may be needed to reduce effective volume.	PS WF ST				
(*iv*) Amplifier response time	Score maximum for the amplifier with the shortest time constant.	VI	Peaks from capillary columns will be broadened or merged if response is not rapid. This is less important for packed columns.	PS WF ST				
(*v*) Autoranging amplifier	These automatically switch gain according to signal, avoiding saturation of the data system. Modern instruments and data systems are normally compatible so it may be inappropriate to score this item.	I	Excessive amplifier output can saturate A–D converter in some systems.	PS WF ST				
(*vi*) Dual detector channels	Score for provision to compare output signals from different columns if temperature programming is envisaged.	I	Useful to compensate for changing background signals during temperature programming.	PS WF ST				
(*d*) Katharometer (hot wire) detector	Score maximum for the detector with the lowest internal dead volume.		Maximum performance will be found for detectors with the lowest 'dead volume'. This is particularly important for use with capillary columns.	PS WF ST				
(*e*) Flame ionisation detector								
(*i*) Ease of cleaning		VI	Access and disassembly needed for routine maintenance.	PS WF ST				
(*ii*) Ease of lighting	Score maximum for a design which best satisfies sub-features (*i*)–(*iii*).		Electronic ignition reduces danger of contamination.	PS WF ST				
(*iii*) Internal dead volume			Needs to be minimal to avoid band spreading from capillary columns at low carrier gas flows. Can be reduced by passing open-tubular column through jet to base of flame. This also reduces decomposition on metal surfaces of detector.	PS WF ST				
(*f*) Electron capture detector								
(*i*) Sensitivity to test sample	Score maximum for best sensitivity to test compound (usually lindane).	VI	Guide to over-all sensitivity of detector.	PS WF ST				
(*ii*) Resistance to contamination	Avoidance of cold or hot spots in detector which cause analyte deposition or degradation, respectively. It is difficult to score this feature except on reputation/experience.	I	Contamination gives increased background and reduces standing current. Because of radiation hazards ECDs are difficult to clean.	PS WF ST				
(*iii*) Carrier gas options	Score according to provision to use nitrogen and/or argon–methane.	I	Appropriate selection of carrier gas can alter sensitivity.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
(*iv*) Pulsing modes of controller	Score maximum for ability to use both variable pulse rate and constant current modes.	I	Can alter linear range and sensitivity.	PS WF ST				
(*vi*) Equilibration time	Score maximum for shortest equilibration time before stable standing current is obtained.	I	Extended equilibration times reduces availability of instrument and prolongs start-up time.	PS WF ST				
(*g*) Thermionic ionisation detector (nitrogen–phosphorous detector)								
(*i*) Ease of mode selection	Score according to ease of mode selection, usually by switching electronic configuration and changing hydrogen flow-rate.	NVI	Different modes can alter selectivity or specificity to analytes containing P, N or other elements.	PS WF ST				
(*ii*) Discriminatior.	Score according to proven selectivity to different groups of compounds.	I	Can make system more specific or selective.	PS WF ST				
(*ii*) Sensitivity	Score maximum for highest sensitivity to test compound such as malathion.	VI	Guide to sensitivity and selectivity.	PS WF ST				
(*iv*) Lifetime of source	The time before there is a significant change in response. Scoring of this may be difficult, unless the manufacturers data is accepted or previous experience with the detector is available.	I	Some source materials may age over a relatively short time, which may be dependent on temperature and causes a reduction in response and discrimination.	PS WF ST				
(*h*) Flame photometric detector								
(*i*) Linearizer built into amplifier	Score for the provision of a linearizer built into the amplifier or data processing system and for evidence of satisfactory performance with test compounds.	VI (for sulfur compounds)	Sulfur compounds give a non-linear response with this detector.	PS WF ST				
(*ii*) Selectivity of filters	Score according to efficiency of filters to discriminate between emission signals due to sulfur and phosphorus and interference from the emission resulting from carbon compounds.	VI	Determines the over-all selectivity of the detector.	PS WF ST				
(*iii*) Capability of simultaneous detection of sulfur and phosphorus	Depending on proposed use, score additionally for a dual detector capability permitting simultaneous sulfur and phosphorus determination.	I	Increases analytical productivity, *e.g.*, for the analysis of oils and pesticides.	PS WF ST				
6. *Auto Sampler*								
(*a*) General	Where the number of analyses justifies automated operation, score the capability of the recommended autosampler according to the availability of sub-features (*i*)–(*iv*) listed below.		Importance is application dependent.	PS WF ST				
(*i*) Compatibility with chromatograph	Ability of auto sampler to control integrator and chromatograph programmes.		Needed for reliable automatic operation and data collection. The use of the chromatograph manufacturer's auto-sampler should ensure compatibility with instrument.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
(*ii*) Interchange-ability between sample injection ports	Ability of autosampler to inject into each of the available ports.		Needed in dual-column instruments so that either column position can be used.	PS WF ST				
(*iii*) Carousel control	Number of sample positions.		More sample positions means that longer sets of runs can be carried out unattended.	PS WF ST				
(*vi*) Carousel temperature	Temperature control of sample awaiting injection.		Permits pre-column derivatization or cooling for thermally labile or volatile samples.	PS WF ST				
(*b*) Injection system								
(*i*) Injection volumes	Score maximum for greatest range of injection volumes that can be programmed.	I	If different volumes can be programmed for each injection this increases versatility so that different levels of analyte concentration can be handled.	PS WF ST				
(*ii*) Minimum sample size	Score maximum for system requiring minimum amount of sample in vial to flush needle and make injection.	VI	Sample size may be limited. Amount can be dependent on position of needle tip in vial and hence shape of vial.	PS WF ST				
(*iii*) Sample carry over	Score highest for most convenient mode of operation avoiding presence of residue which can contaminate next injection. Score additionally if needle wash is available.	VI	Avoidance of cross contamination; alternatively, intermediate blank samples may be needed which will increase analysis time.	PS WF ST				
(*iv*) Injection modes available	Score for provision of hot needle–cold needle injection and for on-column injection.	I	Use of hot or cold needle and on-column injection can alter discrimination and reproducibility.	PS WF ST				
(*v*) Needle residence time	Score maximum for shortest needle residence time in injection port.	I	To minimize sample degradation of sensitive samples within the needle during injection.	PS WF ST				
(*vi*) Automatic one-shot injection	Score for facility to inject single sample automatically.	VI	Can be used to increase repeatability compared with manual operation, particularly by semi-skilled personnel or multiple users.	PS WF ST				
(*vii*) Manual injection	Score for facility for manual injection without removing auto injection.	VI	Improves flexibility of apparatus for non-routine samples.	PS WF ST				
(*viii*) Multiple injections	Score for facility to make a number of injections from a single sample vial.	VI	Used to obtain repeatability measurements.	PS WF ST				
(*c*) Auto sample controller	Score according to ability to programme operation of auto sampler. Score additionally if control can be effected *via* an external computer and if different conditions can be used for specified samples.	I	Improves versatility of operation. Enables use of wash solutions on repeating standard reference solutions within run.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
7. *Data handling* The selection of a data system is outside the scope of this study as many software packages are available for data handling which are interchangeable between personal computers. Providing the instrument can output the data to a suitable computer, it should not affect the choice of the instrument, so scoring is therefore inappropriate. However, the following sub-features should be taken into consideration.								
(*a*) Dedicated system	Facility to carry out data collection, integration and evaluation supplied with the instrument.		These systems are fully compatible with the chromatograph but may require an interface for data storage or more complex manipulation.	PS WF ST				
(*b*) Interfacing requirements								
(*i*) Connections	Standard connections/RS232/ parallel.		Data system can be linked to external computer (or LIMS) using standard protocols.	PS WF ST				
(*ii*) Control links	Ability of data system to control chromatograph.		Required if there is a need for the external computer system to be able to control one or more chromatographs.	PS WF ST				
8. *Additional features and accessories* These features may be required for specific analytes or applications, and enquiries should be made as to the availability of suitable accessories. These features should only be scored when appropriate.								
(*a*) Column switching	Ability to transfer eluent gas flow to second column and to reverse flow through column.		Can be used to facilitate heart-cut and back flush methods for complex samples.	PS WF ST				

Feature	Definition and/or test procedures and guidance for assessment	Importance	Reason	Score				
(*b*) Headspace sampling unit	Extraction and injection of headspace vapour from above solid, liquid or complex matrices.		Used for volatile analytes in comparatively less volatile matrix.	PS WF ST				
(*c*) Pyrolysis unit	Ability to thermally degrade sample rapidly in inlet carrier gas flow.		Used to analyse involatile samples as characteristic volatile fragments.	PS WF ST				
(*d*) Connections to mass spectrometer of FTIR spectrometer	Ability to link the chromatograph to the spectrometer with heated transfer line.		Used to give additional structural information about separated analytes.	PS WF ST				
(*a*) Thermal desorption unit	Ability to interface the chromatograph to thermal desorption unit.		Thermal desorption units are often required for the analysis of volatile toxins in environmental air samples.	PS WF ST				
				Sum of sub-totals				
9. *Value for money* (points per £)	Sum of the previous sub-totals divided by the 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 more costly.	PS WF ST				
				Grand Total				