Pure & Appl. Chem., Vol. 63, No. 6, pp. 887–893, 1991.
Printed in Great Britain.

ADONIS 206922209100098V

INTERNATIONAL UNION OF PURE
AND APPLIED CHEMISTRY

PHYSICAL CHEMISTRY DIVISION
COMMISSION ON MOLECULAR STRUCTURE AND SPECTROSCOPY*

ENGLISH-DERIVED ABBREVIATIONS FOR EXPERIMENTAL TECHNIQUES IN SURFACE SCIENCE AND CHEMICAL SPECTROSCOPY

(Recommendations 1991)

Prepared for publication by

N. SHEPPARD

School of Chemical Sciences, University of East Anglia, University Plain, Norwich NR4 7TJ, UK

*Membership of the Commission during the preparation of this report (1985–89) was as follows:

Chairman: J. R. Durig (USA; 1985–89); *Secretary*: H. A. Willis (UK; 1985–87); J. G. Grasselli (USA; 1987–89); *Titular Members*: A. M. Bradshaw (FRG; 1985–89); R. D. Brown (Australia; 1987–89); B. G. Derendjaev (USSR; 1985–89); J. G. Grasselli (USA; 1985–89); E. Hirota (Japan; 1985–89); J. F. J. Todd (UK; 1985–89); *Associate Members*: R. D. Brown (Australia; 1983–87); S. Forsen (Sweden; 1985–87); R. K. Harris (UK; 1985–89); H. Kon (USA; 1985–87); S. Leach (France; 1987–89); G. J. Martin (France; 1985–89); L. N. Masalov (USSR; 1987–89); Yu. N. Molin (USSR; 1985–87); W. B. Person (USA; 1985–89); C. J. H. Schutte (RSA; 1985–1989); M. Tasumi (Japan; 1985–87); S. Tsuchiya (Japan; 1987–89); *National Representatives*: J. E. Collin (Belgium; 1985–89); S. L. Spassov (Bulgaria; 1987–89); G. Herzberg (Canada; 1985–87); J. Lu (Chinese Chemical Society; 1985–89); G. Varsányi (Hungary; 1985–89); M. Chowdhury (India; 1986–89); Z. Luz (Israel; 1985–89); S. Ng (Malaysia; 1985–89); B. Jezowska-Trzebiatowska (Poland; 1985–89); T. A. Ford (RSA; 1987–89); C. Pascual (Spain; 1987–89); M. Cebe (Turkey; 1987–89).

English-derived abbreviations for experimental techniques in surface science and chemical spectroscopy (Recommendations 1991)

Abstract - Surface science and the chemical spectroscopies have led in the literature and in oral presentation, etc., to the use of a large number of abbreviations for different experimental techniques. In some cases several different abbreviations have been used for the same technique and in many cases the abbreviations are understood by only a small part of the Surface Science/Spectroscopy community. Such a situation causes particular difficulties in communication for those with interdisciplinary interests. The present document suggests a systematic procedure for the generation of abbreviations which accords with many of those previously adopted. A survey is given of current principal abbreviations in these fields and recommendations are made which are either in accord with the systematic principles, or are so well-established that it would be unrealistic to suggest alternatives.

INTRODUCTION

It is a natural and common practice to use short abbreviations for lengthy names of experimental techniques that have to be repeated many times in a scientific paper. When these abbreviations are listed prominently near the beginning of the paper in question, and are not used in the title or abstract in accordance with previous IUPAC recommendations (Pure and Applied Chemistry, 52, 2229, 1980), little difficulty is caused. Increasingly, however, such abbreviations become more generally and less carefully used, not only in publications but also in posters and oral presentations when professional editorial scrutiny is not feasible. They can then cause substantial communication difficulties for a worker with interdisciplinary interests whose expertise is in one discipline but who wishes to be conversant with the literature, and possibly to make use of the results or experimental capabilities, of adjacent disciplines.

The field of Surface Science is one which has seen a particularly large-scale proliferation of often inconsistent abbreviations. In a recent IUPAC survey of the field (Pure and Applied Chemistry, 59, 1343, 1987) no less than 139 different abbreviations were listed (!), some of them repetitive in meaning and most of them undoubtedly obscure to most readers other than those in a narrow field. As many of the Surface Science techniques are spectroscopic in nature, this situation has also been reflected in abbreviations in Chemical Spectroscopy as a whole.

This document makes recommendations in an attempt to simplify the abbreviations field in Surface Science and Chemical Spectroscopy by proposing abbreviations for many of the more commonly-used techniques taking into account some systematic principles. In most cases the resulting preferred choice corresponds to one of the common abbreviations already in use. However, where a long-established abbreviation is not consistent with the proposed principles, but nevertheless has very widespread usage, this will continue to be recommended on grounds of practicality. It is to be hoped that the principles themselves will stimulate systematic choices for future new abbreviations.

A SUGGESTED SYSTEM FOR THE GENERATION OF ABBREVIATIONS

We recommend, as principles for constructing an abbreviation for a given technique, the assemblage of a sequence of letters, starting from the right-hand side, as follows:

(i) a letter or letters relating to the general type of technique used, e.g. spectroscopy or diffraction;

(ii) a letter or letters relating to the types of probes/particles involved in the experiment (e.g. photons, electrons, etc.);

(iii) letters relating to descriptive adjectives or phrases; these can sometimes be selected from alternatives to give convenient acronyms.

Examples of some abbreviations which do essentially conform to these principles are as follows:

	(iii)	(ii)	(i)
Low Energy Electron Diffraction	LE	E	D
Auger Electron Spectroscopy	A	E	S
Transmission Electron Microscopy	T	E	M

Notes

(a) Where under (ii) more than one probe/particle is involved, the abbreviation for the incident particle should be given on the left, followed by that of the emitted particle.

e.g. photo(n)electron spectroscopy	PE	S
	(ii)	(i)

(b) When solely electromagnetic radiation is involved, long-established usage shows that there are almost invariably adjectives which make it obvious that photons are involved, e.g. ultraviolet (UV); infrared (IR), etc., so that the symbol P, for photon, is not normally required.

(c) As mentioned in the Introduction, on practical grounds preference should nevertheless be given to abbreviations which are already very well established, even if these conflict with those derived systematically as described above. For example, it would be absurd at this stage to propose a change from

Nuclear Magnetic Resonance	N	M	R
	(ii)	(iii)	(i)

to the alternative

Magnetic Nuclear Resonance	M	N	R
	(iii)	(ii)	(i)

which would be based on the above principles.

ALPHABET OF SYMBOLS FOR USE IN SPECTROSCOPY AND SURFACE SCIENCE

In order to carry out the above program, it is necessary first of all to choose letters as symbols for consistent use. Bearing in mind common English usage, suggestions are given below using the various headings listed in the section on the Suggested System for the Generation of Abbreviations.

(i) Type of Technique

Spectroscopy, S; resonance, R; diffraction, D; microscopy, M; ionization, I; scattering, S.

(ii) Type of Probe/Particle

Photon, P (usually unnecessary, see NOTE (b) above); electron, E; neutron, N; atom, A; ion, I; field, F; potential, P; radiation, R.

(iii) Descriptive Adjectives or Phrases

(a) Pertaining to the type of technique:

Absorption, A; emission, E; reflection, R; transmission, T; far, F; mid, M; near, N; high, H; low, L; inelastic, I; scanning, S; surface, S; tunnelling, T; angle-resolved, AR; Fourier-transform, FT.

(b) Pertaining to the types of probe/particles:

X-rays, X or XR; ultraviolet, U or UV; infrared, IR; etc. (see Table 2 below).

RECOMMENDATIONS FOR ABBREVIATIONS IN SURFACE SCIENCE AND CHEMICAL SPECTROSCOPY

The overall list of selected techniques and their abbreviations have been subdivided under the following principal headings.

(1) The electron, photoelectron and related spectroscopies

(2) The photon spectroscopies resulting from the use of electromagnetic radiation

(3) Neutron and ion scattering

(4) Mass spectroscopy

(5) Other spectroscopic techniques

(6) Desorption and related techniques

(7) Diffraction techniques

(8) Spectroscopy/Diffraction hybrids

(9) Microscopy techniques in Surface Science

A series of tables follows, in order of the above principal headings. Within a given table the various techniques are listed in the left-hand column, where necessary with alternative names. Three columns of abbreviations are given in the table with entries opposite each technique listed. The first one is the abbreviation that would relate to the name of the technique using the systematic procedures described above; the second lists abbreviations that have been widely used; the final entry gives the abbreviation recommended for future use from amongst those given in the previous two columns.

At this stage no attempt has been made to suggest abbreviations for other than fairly well-established techniques, but elaborations on those given can be generated by adding letters to the left of the basic abbreviation using the recommendations for descriptive adjectives or phrases given in (iii) of the section Alphabet of Symbols for Use in Spectroscopy and Surface Science, e.g. X-ray excited Auger electron spectroscopy (XAES) or angle-resolved Auger electron spectroscopy (ARAES). For this purpose it is even more important that the abbreviations for the basic techniques become well-established.

In the Tables those descriptions of the techniques which are in accord with the systematic principles outlined in the section on the Suggested System for the Generation of Abbreviations are given in italics.

TABLE 1. The Electron, Photoelectron and Related Spectroscopies

This is a major group of spectroscopies that is used in Surface Science. In some cases systematic names have been added when they differ from common usage.

	Systematic	Common Usage	Recommended
Auger Electron Spectroscopy	AES	AES	AES
Electron Energy Loss Spectroscopy *Energy-loss Electron Spectroscopy*	ELES	EELS	EELS
High-resolution Energy-Loss Electron	HRELES	HREELS	HREELS
Spectroscopy; Vibrational Energy-Loss Electron Spectroscopy	VELES		or VEELS*
Inelastic Electron Tunnelling Spectroscopy *Inelastic Tunnelling Electron Spectroscopy*	ITES	IETS	IETS
Photo(n)electron Spectroscopy	PES	PS	PS
Photoemission Spectroscopy		PES§	or PES§
Ultraviolet Photoelectron Spectroscopy	UVPES	UPS	UPS
Outer-shell Photoelectron Spectroscopy	OSPES		or UPES§
X-ray Photoelectron Spectroscopy	XRPES	XPS	XPS
Inner-shell Photoelectron Spectroscopy	ISPES	XPES§	or XPES§
Electron Spectroscopy for Chemical Analysis	ESCA	ESCA	
Angle-resolved Photoelectron Spectroscopy	ARPES	ARPS	ARPS
Angle-dispersed Photoelectron Spectroscopy	ADPES	ADES	or ARPES§

*The EELS technique for studying vibrational spectra of adsorbed species is of low resolution in comparison with the vibrational photon (infrared) technique for obtaining such information (RAIRS in Table 2). Hence the abbreviation HR for 'high resolution' is increasingly seen as inappropriate. VEELS, although not yet well-established, has been preferred by most of the practitioners consulted about this document.

§The abbreviation PS for photoelectron spectroscopy, as in UPS or XPS, is more common but the previous IUPAC recommendation of PES (Pure and Applied Chemistry, 45, 221, 1976) is used substantially and involves only a slight modification with little change in pronunciation. It has the substantial advantage of symbolizing the involvement of electrons as well as photons in the experiment.

TABLE 2. The Photon Spectroscopies Resulting From the Use of Electromagnetic Radiation

As discussed earlier (in the section on A Suggested System for the Generation of Abbreviations, Note (b)) the use of the word (or the symbol P) for photon, under principle (ii), is usually unnecessary in the electromagnetic spectroscopies. Also for the most part the common usage of abbreviations is long-standing and clear-cut. For these reasons only the recommended abbreviations are listed in this Table.

	Recommended
Mössbauer (γ-ray) Spectroscopy	*
X-ray Spectroscopy	§
Vacuum Ultraviolet Spectroscopy	VUV
Ultraviolet Spectroscopy	UV
Visible Spectroscopy	VIS
Near-Infrared Spectroscopy	NIR
Mid-Infrared Spectroscopy	MIR
Far-Infrared Spectroscopy	FIR
Microwave Spectroscopy	MW
Electron Paramagnetic Resonance	EPR
Electron Spin Resonance	ESR
Nuclear Magnetic Resonance	NMR
Nuclear Quadrupole Resonance	NQR
Raman Spectroscopy	RS
Resonance Raman Spectroscopy	RRS
Surface-enhanced Raman Spectroscopy	SERS

General Notes:

* No well-established abbreviation is in use for this branch of electromagnetic spectroscopy.

§ The most commonly encountered abbreviation is XRF, standing for X-ray fluorescence. XRS for X-ray spectroscopy is also used.

(a) S, for spectroscopy, is not usually added to the above abbreviations in the literature of general Chemical Spectroscopy. However, in Surface Science it is common to do so and the additional letter may be added where appropriate. M for 'mid' is also often omitted for the principal infrared region.

(b) Other abbreviations in common use in infrared spectroscopy include:

attenuated total (internal) reflection	ATR
diffuse reflectance infrared (FT) spectroscopy	DRIFT
reflection/absorption infrared spectroscopy	RAIRS
photoacoustic spectroscopy	PAS

(c) The magnetic resonance spectroscopies have generated a particularly wide range of additional abbreviations, e.g., for free induction decay, FID; magic-angle rotation, MAR (or magic-angle spinning, MAS); cross polarization, CP; nuclear Overhauser effect, NOE; etc.

TABLE 3. Neutron and Ion Scattering (elastic, inelastic)

	Systematic	Common Usage	Recommended
Ion Neutralization Spectroscopy *Neutralization Ion Spectroscopy*	NIS	INS	INS*
Ion Scattering Spectroscopy	ISS	ISS	ISS
Rutherford (Ion) Back Scattering	RIBS	RBS	RBS
Inelastic Neutron Scattering	INS	INS	INS*

*Both these abbreviations are well-established, but the context will resolve ambiguities.

TABLE 4. Mass Spectroscopy

	Systematic	Common Usage	Recommended
Mass Spectroscopy	MS	MS	MS
Secondary Ion Mass Spectroscopy	SIMS	SIMS	SIMS
Field-Ion Mass Spectroscopy	FIMS	FIMS	FIMS
Fast-atom Bombardment (Mass Spectroscopy)	FAB(MS)	FAB	FAB(MS)

TABLE 5. Other Spectroscopic Techniques

	Systematic	Common Usage	Recommended
*Metastable Deexcitation Spectroscopy**	MDS	MDS	MDS
Penning Ionization (Electron) Spectroscopy	PIES	PIS	
Inverse Photoelectron Spectroscopy	IPES		
Inverse Photoemission Spectroscopy	IPES		IPES§
Bremsstrahlung Isochromat Spectroscopy	BIS		

*This is preferred as the more general term; Penning ionization is one of two possible mechanisms.

§See corresponding footnote in Table 1.

TABLE 6. Desorption and Related Techniques

	Systematic	Common Usage	Recommended
Thermal Desorption Spectroscopy	TDS	TDS	
Temperature Programmed Desorption	TPD	TPD	TPD
Temperature Programmed Reaction Spectroscopy	TPRS	TPRS	TPRS
Electron-stimulated Desorption	ESD	ESD	ESD
Photon-stimulated Desorption	PSD		PSD

TABLE 7. Diffraction Techniques*

	Systematic	Common Usage	Recommended
Low-Energy Electron Diffraction	LEED	LEED	LEED
Transmission High-Energy Electron Diffraction	THEED	THEED	THEED
Reflection High-Energy Electron Diffraction	RHEED	RHEED	RHEED
X-Ray Diffraction	XRD	XRD	XRD

*The abbreviation ED for electron diffraction is rarely used in isolation.

TABLE 8. Spectroscopy/Diffraction Hybrids

	Systematic	Common Usage	Recommended
Photoelectron Diffraction	PED		PED
Extended X-Ray Absorption Fine Structure	EXAFS	EXAFS	EXAFS
Surface Extended X-Ray Absorption Fine Structure	SEXAFS	SEXAFS	SEXAFS
Near-Edge X-Ray Absorption Fine Structure	NEXAFS	NEXAFS	NEXAFS
X-Ray Absorption Near-Edge Fine Structure		XANES	

TABLE 9. Microscopy Techniques in Surface Science

	Systematic	Common Usage	Recommended
Transmission Electron Microscopy	TEM	TEM	TEM
Reflection Electron Microscopy	REM		REM
Scanning Transmission Electron Spectroscopy	STEM	STEM	STEM
Scanning (Reflection) Electron Microscopy	SREM	SEM	SEM
Field Emission (Electron) Microscopy	FEEM	FEM	FEM
Scanning Tunnelling (Electron) Microscopy	STEM	STM	STM
Field-Ion Microscopy	FIM	FIM	FIM
X-Ray Microscopy	XRM	XRM	XRM