### APPLIED SPECTROSCOPY

## AIMS AND SCOPE: Reporting High-Quality Research in Spectroscopy

Applied Spectroscopy is an international journal for the publication of original research and review articles covering all aspects of spectroscopy. The journal seeks to be comprehensive in scope, with its primary aim the publication of papers on both the fundamentals and applications of photon-based spectroscopy. These include, but are not limited to, ultraviolet-visible absorption, fluorescence and phosphorescence, mid-infrared, Raman, near-infrared, terahertz, and microwave, and atomic absorption, emission, laser-induced breakdown spectroscopies (and ICP-MS), as well as cutting-edge hyphenated and interdisciplinary techniques.

Fundamental topics include, but are not restricted to, the theory of optical spectra and their interpretation, instrumentation design, and operational principles. Reports of spectral processing methodologies such as 2D correlation spectroscopy (2D-COS), baseline correction, and chemometric methods applied to spectra are also strongly encouraged. Application papers are intended to feature novel, innovative applications of spectroscopic methods and techniques. Papers from all fields of scientific endeavor in which applied spectroscopy can be utilized will be considered for publication. Representative fields include chemistry, physics, biological and health sciences, environmental science, materials science, archeology and art conservation, and forensic science.

In addition to full papers, the journal publishes Rapid Communications, Spectroscopic Techniques, Notes, and Correspondence related to previously published papers. A regular feature of the journal, Focal Point Reviews, provides definitive, comprehensive free-to-view reviews of spectroscopic techniques and applications. The journal encourages the submission of proposals for consideration for Focal Point articles.

# The Benefits of Submitting to Applied Spectroscopy:

- Fast times to publication
- Early online publication of articles ahead of print (preprints)
- No page charges
- No color figure charges for SAS members
- Electronic articles available on three separate online platforms:
  - SAS website, for SAS members: http://www.s-a-s.org
  - SAGE Publishing: https://mc.manuscriptcentral.com/asp
  - Optics Infobase: http://www.opticsinfobase.org/as/home.cfm
- Utilization of CrossRef, allowing readers to link directly to a reference from within the PDF of an article, with DOIs (digital object identifiers) assigned and available immediately upon acceptance

- Free high-resolution PDF reprint made available to corresponding authors after publication (this file is for personal use only and may not be distributed outside of fair use guidelines without written permission from the Society for Applied Spectroscopy)
- Applied Spectroscopy is abstracted and/or indexed in
  - PubMed
  - EBSCO Academic Search
  - BIOSIS Previews
  - Chemical Abstracts Service/CASSI
  - Current Contents
  - Science Citation Index

#### **SUBMISSIONS**

All manuscript submissions are handled electronically through the journal's online ScholarOne submission system with SAGE Publishing. Manuscripts can be submitted by visiting **https://mc.manuscriptcentral.com/asp** and following the instructions. A link to our submission site can also be found on the Society for Applied Spectroscopy website at **http://www.s-a-s.org**, on the journal home page.

Submission and peer review questions should be addressed to:

Sergei G. Kazarian, Professor Editor-in-Chief, Applied Spectroscopy Professor of Physical Chemistry Department of Chemical Engineering South Kensington Campus Imperial College London London SW7 2AZ United Kingdom

Phone: +44 (0)20 7594 5574 Email: s.kazarian@imperial.ac.uk

http://www.imperial.ac.uk/people/s.kazarian

Submitted manuscripts should contain original material that has not been previously published and must not be under simultaneous consideration for publication elsewhere. Submissions should be accompanied by a cover letter outlining the findings of the paper and their significance in terms of novelty and importance. Every paper submitted to *Applied Spectroscopy* that is judged by the editors to be within the Aims and Scope and of suitable quality for *Applied Spectroscopy* will be peer reviewed. Manuscripts that are deemed inappropriate in terms of subject matter, completeness, or quality of the written language may be declined.

### Types of Articles

**Original research papers** should be detailed reports of the authors' work in a particular research area. The work, or a substantial and identifiable portion of the work, should be complete.

**Rapid Communications** may report significant results originating from research that is not yet complete.

**Spectroscopic Techniques** should address a specific new, novel, and useful technique as applied to an area of spectroscopy.

**Notes** are brief communications, usually of no more than 2000 words, describing a new instrument, a particularly interesting finding, or a novel application.

**Correspondence** should address an author's questions or concerns regarding a specific paper and may be answered by the authors of that paper in the same or a subsequent issue of *Applied Spectroscopy*.

## Form and Preparation of Manuscripts

Manuscripts must be submitted as editable word-processing files. MS Word files (.doc, .docx, .rtf) are preferred. Files will be accepted in LaTeX (.tex); however, because of the difficulty and expense of translating files in this format to the SAGE Publishing typesetting system, it is discouraged. All LaTeX submissions must be accompanied by a PDF of the submission in which all symbols and equations appear correctly.

To be acceptable for submission to *Applied Spectroscopy*, a manuscript must adhere to certain formatting standards. These standards assist our reviewers in their reading of your material:

- (I) Please use Times or Times New Roman, I2-point font, double-spaced throughout. This requirement holds for abstracts, body of the text, references, footnotes, tables, and all captions.
- (2) All tables and figures must be numbered consecutively, tables with Roman numerals and Figures with Arabic numerals. Tables and figures may be integrated into the first draft of the text, which simplifies the review process, but figures should also be uploaded as individual files.
- (3) Refrain from using section numbering.
- (4) References should be collected in a list at the end of the document, following the conventions described later in these instructions. References should never appear as footnotes and footnotes should never appear in the reference list.

### **Title**

A manuscript should have a straightforward title that adequately describes the primary area of research and the technique or methodology utilized. We follow the ACS Style Guide, 3rd ed., with regard to titles:

"The title serves two main purposes: to attract the potential audience and to aid retrieval and indexing" (for more information on this retrieval and indexing, see https://us.sagepub.com/en-us/nam/help-readers-find-your-article#Title).

- (I) Choose terms that are as specific as the text permits, e.g., 'a vanadium—iron alloy' rather than 'a magnetic alloy'. Avoid phrases such as 'on the', 'a study of', 'research on', 'regarding', and 'use of'. In most cases, omit 'the' at the beginning of the title. Avoid nonquantitative, meaningless words such as 'rapid' and 'new'.
- (2) NOTE: Spell out all terms in the title, avoid jargon, symbols, formulas, and abbreviations. Whenever possible, use words rather than expressions containing superscripts, subscripts, or other special notations.

#### **Abstract**

An abstract must accompany each submitted article. The abstract should mention the subjects studied and new methods used, new observations, and conclusions. Brief numerical results and their accuracy are encouraged. Introductory material should not be placed in the abstract.

- (1) Avoid using abbreviations or acronyms without prior definition.
- (2) References are not allowed in the abstract; if other work must be cited, please give the entire citation in parentheses.
- (3) Index headings should be included after the abstract. These should contain at least four and no more than ten key words that best describe the classification of the paper. Both written-out terms and abbreviations should be included (i.e., NIR spectroscopy; near-infrared spectroscopy). This facilitates the process of searching for articles on the Internet. Each term should be capitalized and separated by a semi-colon.

## **Spectroscopic Nomenclature**

The spectroscopic nomenclature must comply with the conventions recommended by the International System of Units (SI) and the International Union of Pure and Applied Chemistry (IUPAC). A brief summary of acceptable terms and their accurate use appears periodically on the back page of *Applied Spectroscopy* and is available on the journal's website at https://www.s-a-s.org/4DCGI/cms/review.html?Action=CMS\_Document&DocID=107&MenuKey=Journal.

- (I) Define acronyms and abbreviations on first use, followed by the acronym or abbreviation in parentheses.
- (2) Please do not begin a paragraph with an acronym or abbreviation and avoid their use in headings where possible and practical.
- (3) Provide names of manufacturers in parentheses for instruments, equipment, and materials.
- (4) Latin terms (i.e., et al., in vivo, ca.) should not be italicized.

# **Mathematical Expressions**

Take great care with mathematical equations and expressions. Math that is not properly set may be re-keyed, increasing the possibility of error:

- (I) "Display" equations must be in an editable format using MS Word Equation Editor or MathType and should be set apart by line breaks and should be created. They should have no ending punctuation, should be numbered consecutively in parentheses (i.e., (I), (2), (3), etc.), and should not be linked as fields or images within the manuscript.
- (2) Display equations should be immediately followed by a description of the variables used.
- (3) Shorter mathematical expressions should appear in the text ("in-line"). These should be created using standard keyboard characters and the "Insert Symbol" palette whenever possible. Equation Editor or MathType should only be used when absolutely necessary, i.e., for stacked subscripts and superscripts,  $\lambda_{\max}^2$ .
- (4) Conventions for publishing mathematics should be followed. All Greek characters should appear in normal face (i.e., Roman, not italic). All variables represented by a Latin letter should be in *italics*. All constants and designators (i.e.,  $\lambda_{max}$ ) should be in normal (Roman) face. Vectors should be **lowercase bold** and matrices should be **uppercase bold** (both in normal, Roman, face).
- (5) Refer to equations using "Eq. #" in the body of the text or "Equation #" when beginning a sentence. Do not use the abbreviation "Eqn."
- (6) Do not repeat mathematical derivations that are easily found elsewhere in the literature; merely cite the references.

# **Figures**

Color figures where necessary to provide clarity are encouraged and are printed without charge for members of the Society. There is a fee of £300 for the first figure and £150 per figure thereafter for non-members. A one-year complimentary membership to the Society for Applied Spectroscopy is included for the corresponding author, should they desire it, upon payment of the color-figure fee. Please note, however, that color should be used appropriately. Color should not be used to specify multiple lines and points in simple x,y plots when different line styles (solid, dashed, dotted) or plotting symbols in a black-and-white figure are equally effective.

- (1) For the first draft of a submitted manuscript, figures may be submitted in two ways. Each figure may be embedded in the text with the caption located immediately underneath the image or the figures may be located in separate files. PDFs of figures are not acceptable upon first submission of a paper. **No more than six (6) to eight**
- **(8) figures per paper.** Additional figures, tables, and images may be submitted as Supplemental Material to be hosted online.
- (2) When a revised manuscript is uploaded or upon acceptance of a manuscript, high-resolution figure files must be uploaded individually to ScholarOne. The following high-resolution formats are preferred: .tif, .eps, and .jpg. The following formats are not

preferred but are acceptable if the resolution is high enough: .pdf, .gif, .ppt, and .doc. Halftone and color images should be a minimum of 200 pixels per inch (ppi), and ideally 350 ppi. Line art must be a minimum of 600 ppi, and ideally 1200 ppi.

- (3) The majority of figures will appear in the journal at a width of 8.8 cm (one column wide). Larger images requiring greater detail or figures containing multiple panels may be printed at up to 18 cm wide. Axis labels, symbols, and line widths should be clearly visible at this size. Letters and numbers, for example, should be no less than 1.5 mm high, and symbols should be no less than 1.0 mm high.
- (4) If a figure consists of multiple panels or parts, all parts should be provided together in one image arranged as you wish them to appear in print.
- (5) A caption must be included at the end of the manuscript for each figure. Captions should not be included in the figure image. However, the inclusion in a figure of line or symbol legends that are not easily reproduced in text is encouraged. Captions should provide a detailed description of the figure content.
- (6) Every figure must be referred to in the main text in consecutive numerical order.
- (7) For figures that have been published elsewhere, the author must obtain written permission from the publisher/copyright owner to reproduce them. Proper acknowledgment at the end of the figure caption is made as follows: [Reproduced with permission from Society/Journal.<sup>18</sup>] where "Society/Journal" is the copyright holder and "18" is the appropriate full citation in the reference list.
- (8) Important spectra that are necessary for the proper development of the paper will be published. Large collections of routine spectra will not be published in *Applied Spectroscopy*. However, supplemental electronic files such as spectra or video can be published and maintained through the Society for Applied Spectroscopy website. Please see the Supplemental Material section below for more information.

#### **Tables**

- (I) For the first draft of a submitted manuscript, tables (up to four [4]) may be submitted in two ways. Each table may be embedded in the text with the caption located immediately above the table, or the tables may be located at the end of the manuscript. When the final version of the manuscript has been accepted for publication, each embedded table must be removed from the text and placed at the end of the manuscript. Uploading separate table files is discouraged. Additional tables must be included as Supplemental Material.
- (2) Tables must be in an editable format, such as .xls or .doc. Pictures or images of tables that cannot be edited are not acceptable.
- (3) Each table must be numbered (with a Roman numeral) consecutively in order of appearance.
- (4) Each table must carry a caption at its head.
- (5) Table footnotes, including definitions of abbreviations or terms, should be included after the table (not *in* the table) and they must be lettered consecutively, with a

superscript a, b, etc. If a reference is cited in a table, it should be numbered consecutively with regard to the table's first mention in the text and the reference should be included in the reference list and not in the table footnotes.

#### **Footnotes**

- (I) All comments or ancillary information should be included as footnotes and should not appear in the list of references.
- (2) References should not be formatted as footnotes or endnotes.
- (3) Footnotes other than table footnotes should be inserted using MSWord's "Insert Footnote" tool (or alternately, placed on the bottom of the page of the paper on which they appear).
- (4) Footnotes other than table footnotes should be designated using the following symbols: \*, †, ‡  $\S$ , \*\*, ††, ‡‡, and  $\S\S$  in that order.
- (5) Care must be taken that footnote material is not overly long. Footnotes longer than two or three sentences should be reworked for inclusion within the text, possibly as a separate paragraph or as a parenthetical statement.

## **Supplemental Material**

New methods of electronic publishing allow *Applied Spectroscopy* to provide additional materials to its readers that would not normally be feasible in print. The Journal maintains an archive of supplemental material online through its host platform, SAGE Publishing, with each file directly linked to the online version of the primary article. Supplemental material should support and enhance the existing article or supply further information that is of too limited interest to be included in the Journal. Examples of such material include tables of raw data, additional figures, including routine spectra, that are not essential to the primary manuscript, repetitive details of experimental procedures, and detailed mathematical derivations.

Please note that supplemental material will be peer reviewed. However, it will not normally be edited for content, style, or format by the editorial staff. Authors are solely responsible for the content of supplemental material. This also means that the data will be made available free of charge to any interested user. Text documents will normally be converted to PDFs, as these are easily downloadable and readable on most computing platforms. Figures should be embedded within text documents, either in the text or at the end. Tables provided in Excel format will also typically be converted to PDF. If you wish to provide a table of raw data in a form that can be easily used by other researchers, or some other native format, such as a .jpg from which color/intensity information can be extracted, please include a note with your cover letter stating that you wish that material to remain in its native format. Please note that files should not exceed 10 MB in size in order to facilitate downloading.

The existence of supplemental material should be noted briefly in the text, usually parenthetically or in a footnote. After the Acknowledgements, include a brief statement describing the nature of the material, using the following example as a guideline:

### **SUPPLEMENTAL MATERIAL**

All supplemental material mentioned in the text, including <enter brief description of Supplemental Material here>, is available in the online version of the journal.

#### References

All references cited in the text should be collected in a reference list at the end of the manuscript, but before figure captions and tables. Citation formats are given below.

- (I) References should consist solely of citations to material that has been published elsewhere, i.e., in journals, books, technical reports, etc.
- (2) Papers that have been submitted or accepted for publication may be cited using the authors, the full title of the article, and the journal title, followed by "paper submitted" or "paper in press," and the year. If a DOI is available for papers that are in press but not yet published, it should be included after the year. "In preparation" and "To be submitted" citations are generally unacceptable.
- (3) References to "unpublished data" or "private communications" are acceptable, but they should be cited as footnotes in the text and should identify the source of the information cited, such as name, institution, type of communication, and year.
- (4) Electronic publications, such as web pages, databases, or on-line reports, may be cited by including the author or authoring organization, the name of the page or database if available, the date the page was created, if available, the full URL, and the date the material was accessed by the author.
- (5) All references must be numbered consecutively in order of appearance in the text. Reference citations in the text should appear as Arabic numerals (without parentheses or brackets), placed as superscripts, outside punctuation marks. Ranges of references should be shown using a dash (2–5) rather than written out (2,3,4,5,)

Example of reference citations in the text:

The equipment used<sup>8</sup>—inexpensive and easily constructed in the laboratory—met the criteria established by Smith et al.<sup>9,10</sup> In later experiments, Jones and Percy,<sup>11–13</sup> who perfected the technique, found modifications unnecessary.

- (6) Each reference number should refer to only one article, chapter, or book; multiple citations within one reference are not acceptable.
- (7) Direct quotes from other sources must be cited, including the page number where the quoted material appears.

## **Formats and Samples for Citations**

All references should be double-spaced and in 12-point font, collected in a list at the end of the manuscript. Journal titles should be abbreviated using the standard ACS/CASSI abbreviations

(http://cassi.cas.org/search.jsp). A searchable database of titles and their abbreviations is also available at http://scieng.library.ubc.ca/coden/#TOP.

# **PERIODICALS**—the ordering is as follows:

Authors. "Title of the Article". Full journal name (abbreviated). Year. Volume number(issue number): page range.

- E.C. Navarre, J.M. Goldberg. "Design and Characterization of a Theta-Pinch Imploding Thin Film Plasma Source for Atomic Emission Spectrochemical Analysis". Appl. Spectrosc. 2010. 65(1): 26-35.
- 2. A. Vrij. "Possible Mechanism for the Spontaneous Rupture of Thin, Free Liquid Films". Discuss. Faraday Soc. 1966. 42: 23-33.
- 3. C. Xu, B.A. Maxwell, J.A. Brown, L. Zhang, Z. Suo. "Global Conformational Dynamics of a Y-Family DNA Polymerase during Catalysis". PLoS Biol. 2009. 7(10): e1000225. doi:10.1371/journal.pbio.1000225.

# **BOOKS**—the ordering is as follows:

Authors. "Title of chapter". In: Editor Names, editor. Title of Book. Location of Publisher: Name of Publisher, Year. Vol. #, Chap. #, Pages cited.

- P.R. Griffiths. "Introduction to the Theory and Instrumentation for Vibrational Spectroscopy". In: E.C.Y. Li-Chan, J.M. Chalmers, P.R. Griffiths, editors. Applications of Vibrational Spectroscopy to Food Science. Chichester, UK: John Wiley and Sons, 2010.
- 2. Y. Ozaki. "Application in Chemistry". In: H.W. Siesler, Y. Ozaki, S. Kawata, H.M. Heise, editors. Near-Infrared Spectroscopy: Principles, Instruments, Applications. Weinheim, Germany: Wiley-VCH, 2002. Pp. 179-211.
- 3. W.H. Press, S.A. Teukolsky, W.T. Vetterling, P.B. Flannery. Numerical Recipes in C: The Art of Scientific Computing. Cambridge, UK: Cambridge University Press, 1999. 2nd ed.

### **THESES**—the ordering is as follows:

Author. Title of Thesis. [M.S. or Ph.D. Thesis/Dissertation]. Location of institution: Name of institution, year.

I. A.-M. Saariaho. Resonance Raman Spectroscopy in the Analysis of Residual Lignin and Other Unsaturated Structures in Chemical Pulps. [Doctor of Science in Technology Dissertation]. Espoo, Finland: Helsinki University of Technology, 2005.

### **EXTRANEOUS MATERIAL**

#### Patents:

Inventor name. Item description. Patent number. Filed Year. Issued Year.

I. M. Foquet, P. Peluso, S. Turner, D. B. Roitman, G. Otto. Zero Mode Waveguide Substrate. US Patent 7486865. Filed 2007. Issued 2009.

# Papers, posters, or workshops presented at a meeting:

- 1. S. Student. "Title of My Paper". Paper (poster) presented at: FACSS 2011. Reno, NV; Sept 30-Oct 5 2011.
- S.M. Clegg, J.E. Barefield, R.C. Wiens, C.R. Quick, S.K. Sharma, A.K. Misra, M.D. Dyar, M.C. McCanta, L. Elkins-Tanton. Workshop on Venus Geochemistry: Progress, Prospects, and New Missions. Workshop presented at: Venus Geochemistry: Progress, Prospects, and New Missions. Gilruth Center, NASA Johnson Space Center, Houston, TX; February 26–27, 2009.

### Websites:

At a minimum, provide the URL and the date that the reference was last accessed. Any further information, particularly the author of a page, the host organization, copyright dates, or a DOI, should also be provided. A few examples follow:

- I. Unicef. "Health: Malaria". 2009. http://www.unicef.org/health/index\_malaria.html [accessed Oct 15 2011].
- 2. United States Department of Labor, OSHA. "Safety and Health Topics: Laser Hazards". Page last reviewed Jan 10 2008. http://www.osha.gov/SLTC/laserhazards/ [accessed Jan 11 2011].

#### **CrossRef and DOIs**

Applied Spectroscopy participates in the digital object identifier (DOI) initiatives of CrossRef (http://www.crossref.org). DOIs of cited material should be included in references whenever possible. Please include the DOI as the last element in a citation, followed by a period, i.e., DOI: 10.1366/11-06598.

## **REVISED MANUSCRIPT**

A manuscript sent back to an author for revision should be returned within three months; otherwise, it will be considered a new manuscript and must be resubmitted. Revised manuscripts and figures should be submitted online, as noted above, and accompanied by a letter listing the responses to the reviewers' concerns.

### **PROOFS**

Proofs are provided to the corresponding author via email as a PDF. The author must respond within 48 hours with approval of the manuscript or with corrections to the manuscript. Corrections can be marked directly on the PDF and may be accompanied by a written list detailing the corrections, either in the email or in a separate document.

Take great care that revised manuscripts are accurate and complete. All editing for style and clarity should be included in the final submitted revision. Some alterations in the proof stage are unavoidable, but the cost of extensive alterations in proof will be charged to the author. There is no charge for correction of errors made during copy-editing or typesetting, but corrections to author's errors in the original manuscript in excess of five will be billed to the corresponding author at a rate of US\$5.00 per alteration.

Authors are reminded to read the proof very carefully. Final proofreading responsibility resides with them. Papers will not be published without final approval of the proof by the author.

### **STYLE MANUAL**

The ACS Style Guide: A Manual for Authors and Editors, 3rd ed., Janet S. Dodd, Ed. (American Chemical Society, Washington, D.C., 2006) contains much valuable information on the proper preparation of manuscripts, illustrations, and tables, as well as lists of acceptable abbreviations, spectroscopic nomenclature, etc.

#### CORRESPONDENCE

All correspondence should be addressed to: Sergei Kazarian, Editor-in-Chief, Department of Chemical Engineering, Imperial College London, South Kensington Campus, London, UK SW7 2AZ. Queries and comments can be sent by e-mail to s.kazarian@imperial.ac.uk or applied\_spectroscopy@chem.ubc.ca. Reference must be made to author(s), article title, and manuscript number.