

## Manuscript Preparation and Writing Standard

General Authors are encouraged to consult recent issues of the *Chinese Journal of Structural Chemistry* for examples of format. We recommend the use of the manuscript templates (MS Word for Win/Mac). Supporting Information should be submitted as a separate file. For clarity, manuscripts should be subdivided into sections such as Introduction, Experimental, Results and Discussion, Conclusion, Acknowledgement and References.

### Titles

Titles should be as short as possible, clearly and accurately indicate the contents of the paper and be expressed in adequate scientific terms. Titles are often used in information-retrieval systems. Avoid abbreviations and formulae where possible.

### Author names and Affiliations

Please clearly indicate the given name(s) and family name(s) of each author and check that all names are accurately spelled. You can add your name between parentheses in your own script behind the English transliteration. Present the authors' affiliation addresses (where the actual work was done) below the names. Indicate all affiliations with a lower-case superscript letter immediately after the author's name and in front of the appropriate address. Provide the full postal address of each affiliation, including the country name and the e-mail address of each author.

▲ **Corresponding author** Clearly indicate who will handle correspondence at all the stages of refereeing and publication, also post-publication. This responsibility includes answering any future queries about Methodology and Materials. Ensure that the e-mail address is given and that contact details are kept up to date by the corresponding author.

▲ **Present/permanent address** If an author has moved since the work described in the article was done, or was visiting at the time, a 'Present address' (or 'Permanent address') may be indicated as a footnote to that author's name. The address at which the author actually did the work must be retained as the main, affiliation address. Superscript Arabic numerals are used for such footnotes.

### Abstract

All manuscripts must contain a concise and factual abstract, which should summarize the purpose for the work, the most significant results, and the major conclusions. An abstract is often presented separately from the article, so it must be able to stand alone. For this reason, References should be avoided, but if essential, then cite the author(s) and year(s). Also, non-standard or uncommon abbreviations should be avoided, but if essential they must be defined at their first mention in the abstract itself. The abstract should not exceed about 250 words. Pasting the abstract in the text box on the Web submission page does not replace the need for including an abstract in the manuscript document.

### Keywords

Immediately after the abstract, provide 3–7 keywords, using American spelling and avoiding general and plural terms and multiple concepts (avoid, for example, 'and', 'of'). Be sparing with abbreviations: only abbreviations firmly established in the field may be eligible. These keywords

will be used for indexing purposes.

### ***Abbreviations***

Define abbreviations that are not standard in this field in a footnote to be placed on the first page of the article. Such abbreviations that are unavoidable in the abstract must be defined at their first mention there, as well as in the footnote. Ensure consistency of abbreviations throughout the article.

### ***Acknowledgements***

Collate acknowledgements in a separate section [at the end of](#) the article before the references and do not, therefore, include them on the title page, as a footnote to the title or otherwise. List here those individuals who provided help during the research (e.g., providing language help, writing assistance or proof reading the article, etc.). All dedications must appear in the Acknowledgment section and are subject to approval by the Editor.

### ***Formatting of funding sources***

List funding sources in this standard way to facilitate compliance to funder's requirements:

Funding: This work was supported by the National Institutes of Health (grant numbers xxxx, yyyy); the Bill & Melinda Gates Foundation, Seattle, WA (grant number zzzz); and the United States Institutes of Peace (grant number aaaa).

It is not necessary to include detailed descriptions on the program or type of grants and awards. When funding is from a block grant or other resources available to a university, college, or other research institution, submit the name of the institute or organization that provided the funding.

### ***Nomenclature and units***

Follow internationally accepted rules and conventions: use the international system of units (SI). If other quantities are mentioned, give their equivalent in SI. You are urged to consult [IUPAC: Nomenclature of Organic Chemistry](#) for further information.

### ***Math formulae***

Please submit math equations as editable text and **not as images**. Present simple formulae in line with normal text where possible and use the solidus (/) instead of a horizontal line for small fractional terms, e.g., X/Y. In principle, variables are to be presented in italics. Powers of e are often more conveniently denoted by exp. Number consecutively any equations that have to be displayed separately from the text (if referred to explicitly in the text).

### ***Footnotes***

Footnotes should be used sparingly. Number them consecutively throughout the article. Many word processors can build footnotes into the text, and this feature may be used. Otherwise, please indicate the position of footnotes in the text and list the footnotes themselves separately at the end of the article. Do not include footnotes in the Reference list.

### **Formulae and Equations**

Subscripts and especially superscripts should be written with care, and exponents should be

arranged on a single line. Organic structural drawings should be submitted in a form suitable for direct photographic reproduction and should fill space economically. Do not use structures when a simple formula will suffice. Do not use multiple lines unnecessarily. Please type formulae and equations as normal text in the body of the text as far as possible.

### **Background and Originality Content**

Background and Originality Content should describe the significance and novelty of this work, and it should include relevant references. A color picture describing the main observation of this contribution is strongly suggested.

### **Experimental**

Experimental section should be given in [sufficient detail](#) to enable others to repeat your work. This should provide source of the chemical reagents, instruments used in the study and should provide sufficient technical information to allow the experiments to be repeated. New method or modifications to existing methods should be described in detail.

The synthesis of all new compounds must be clearly described. Synthetic procedures must include the specific reagents, products and solvents and must give the amounts (g, mmol, L, mL) for all of them, as well as clearly stating how the percentage yields are calculated. They must also include all the characterization data for the prepared compounds or materials. For multistep synthesis papers, spectra of key compounds and the final product should be included.

Figures, schemes, and equations must be cited in the text and numbered in order of appearance with Arabic numerals. All graphics (including chemical structures) must be provided at the actual size that they are to appear (single-column width is 8.4 cm, double-column width is 17.7 cm). Please arrange schematics so that they fill the column space (either single or double), so as not to leave a lot of unused white space. Please ensure that all illustrations within a paper are consistent in type, quality, and size. Color figures may be printed in the journal, provided that the editor considers the color necessary to convey scientific information.

All tables should be cited in the text, and numbered in order of appearance with Arabic numerals. All table columns should have a brief explanatory heading and, where appropriate, units of measurement. Vertical lines should not be used. Footnotes to tables should be typed below the table and should be referred to by superscript letters. Each table should have a descriptive heading, which, together with the individual column headings, should make the table, as nearly as possible, self-explanatory. In setting up tabulations, authors are requested to keep in mind the column widths (8.4 cm and 17.7 cm), and to make the table conform to the limitations of these dimensions.

### **Safety**

Authors must emphasize any **unexpected, new, and/or significant hazards or risks** associated with the reported work. This information should be in the Experimental Section of the full article or the main text of a Communication.

### **Formulae Analyses and Spectral Data**

The physical and chemical parameters of new compounds should be given in the following order and style: m.p. 157–240 °C, UV-vis (EtOH)  $\lambda_{\text{max}}$ : 238, 258 nm;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz)  $\delta$ : 0.78 (t,  $J = 8$  Hz, 3H), 1.07 (d,  $J = 8$  Hz, 3H), 2.96 (s, 1H), 3.80–4.00 (m, 1H), 6.90–7.10 (m, 1H); IR (KBr)  $\nu$ : 3420, 3380, 1675, 1683, 1610, 1588, 1500  $\text{cm}^{-1}$ ; MS (70 eV)  $m/z$  (%): 525 ( $\text{M}^+$ , 46), 507 (30), 43 (100). Anal. calcd. for  $\text{C}_{12}\text{H}_{11}\text{N}$  (%): C, 85.70; H, 6.55; N, 8.27. Found (%): C, 85.24; H, 6.56; N, 8.15 (HRMS calcd. for  $\text{C}_{17}\text{H}_{20}\text{O}_2$  266.1458, found 266.1460). Note that the correct order of characterization data should be as follows: UV, NMR, IR, MS and elemental analysis.

### **Computer-aided image enhancement**

Computer-aided image enhancement is often unavoidable. However, such manipulation cannot result in data that are less relevant or unrepresentative being shown and/or genuine and significant signals being lost. A clear relationship must remain between the original data and the electronic images that result from those data. If an image has been electronically modified, the form of the modification shall be given in the Figure caption. If computer-aided processing or modification of an image is a fundamental part of the experimental work, the form this processing takes must be clearly described in the Experimental Section.

### **Results and Discussion**

Results should be clear and concise, and Discussion should explore the significance of the results of the work, not repeat them. A combined Results and Discussion section is often appropriate. Avoid extensive citations and discussion of published literature.

### **Conclusion**

Conclusion should summarize the results obtained, propose further improvements and predict possible applications. It may be presented in a short Conclusions section, which may stand alone or form a subsection of a Discussion or Results and Discussion section.

### **References**

The author is responsible for correct citations. In the text the numbers should be typed as superscripts (e.g., Smith<sup>[3]</sup>) and, if applicable, after punctuation. All references mentioned in the Reference List are cited in the text, and vice versa. Journal titles should be abbreviated according to the Chemical Abstracts Service Source Index (CASSI). Unpublished results and lectures should only be cited for exceptional reasons. If a paper has been published online but has not appeared in print yet, it is cited by listing the author names and then the abbreviated title of the journal and year followed by the DOI number.

All the references must be placed together in a list at the end of the manuscript text. In the Web edition, many of them will have links to other Web resources, such as the corresponding abstracts in Chemical Abstracts and the full text on publisher Web sites. Because of this electronic linking, and to aid scientific research, it is crucial that authors verify the accuracy of all reference citations and footnotes.

Unnecessarily long lists of references should be avoided, and excessive self-citation is not permitted. However, authors must reference all previous publications in which portions of the present work

have appeared. Literature references and short explanatory footnotes must be numbered with Arabic numerals in the order of their first citation in the text and the corresponding numbers placed at the appropriate locations in the text as superscripted numerals.

Literature references should be arranged and formatted as follows:

### **1 Journals in English**

Kong, D. L.; Jiang, J.; Wu, L. Y.; Wang, X. H.; Shi, Z. M.; Wu, M. S.; Wang, X.; Lin, Q. Synthesis, structure and antimicrobial activity of 9,9-dimethyl-9,10-dihydrospiro- [benzo[a]-xanthene-12,3'-indoline]-2',11(8H)-dione. *Chin. J. Struct. Chem.* **2016**, 35, 1849–1854.

### **2 Journals in Chinese**

Shen, R. Z.; Cao, X.; Yu, B. Total synthesis of dammarane-type saponins ginsenoside Re and notoginsenoside R1. *Acta Chim. Sinica* **2018**, 76, 278–285 (in Chinese).

### **3 Books (without editor)**

(a) Sun, S. G.; Chen, S. L. *Electrocatalysis*, Chemical Industry Press, Beijing, **2018** (in Chinese).

Books (with editor):

(b) *Synthetic Chemistry*, Eds.: Bai, C. L.; Li, J. H.; Qin, D. H., Science Press, Beijing, **2018**, pp. 188–189 (in Chinese).

### **4 Conferences**

Chiba, S. In *Metal-Mediated Radical Reactions for Synthesis of Nitrogen-Heterocycles*, the 12<sup>th</sup> International Symposium on Organic Free Radicals, Shanghai, China, **2016**, p. 18.

### **5 Patents**

Crosby, S. R.; Jennison, M.; Brennan, J. New thermally-cleavable protecting group-and-linker group-containing heterocyclic compound used in composition for e.g. purification of proteins and peptides. *WO2018189546-A1*, **2018**.

### **6 Theses**

Dissertations: Li, L. C. Ph.D. *Dissertation*, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, **2015**, pp. 90–91 (in Chinese).

**Note:** All authors and titles of the cited papers should be listed and CA numbers of patents should also be provided.

### **Graphical Abstract**

Authors are required to provide a separate sheet containing a small diagram or other informative illustration (scheme or figure), showing the most important aspect of the paper. The words or sentences in the diagram must be concise. The height of the scheme or figure is 6 cm.

### **Legends**

Each figure and scheme should have a legend. In the final accepted manuscript, the legends should be listed together after the reference section of the text file and not be included with the drawings in the separate graphic files.

### **Tables**

All tables must have a **brief title** and should only be subdivided by **three horizontal lines** (head rule,

neck rule, and foot rule). Footnotes in the tables are denoted as superscripts by a, b, etc., and presented at the bottom of the table. Tables should be constructed using the table function in Word; do not make tables using the tabulator. Tables should be prepared to fit the page format of the journal (width of the columns is 8.55 cm; width of the pages is 17.6 cm). When a table consists mainly of graphic elements, the entire table should be prepared with Word DOC file rather than a drawing program. At this time, graphic elements linked to ChemDraw programs should be inserted to the table.

### **Illustrations**

Illustrations including figures and schemes should be designed for reduction to a one-column (8.55 cm wide) or two-column format (17.6 cm wide) with a resolution of **300 dpi or higher**. **Note: The *Chinese Journal of Structural Chemistry* does not use charts**, which should be converted into figures or schemes. Illustrations should be stored as the format of TIFF.

### **Figures of chemical structures**

Figures of chemical structures should be drawn using ChemDraw according to the ACS-1996 standard as follows: chain angle, 120°; bond spacing, 18% of length; fixed length, 0.508 cm (14.4 pt); bold width, 0.071 cm (2.0 pt); line width, 0.021 cm (0.6 pt); margin width, 0.056 cm (1.6 pt); hash spacing, 0.088 cm (2.5 pt).

### **Curve graphics**

Curve graphics should be drawn by Origin and their parameters are as follows: font, Arial; letter size, 8.0 pt; curve line width, 0.5 pt; symbol, 3.0 pt; width of graphics, 5.5 cm.

### **Figures of crystal structures**

Figures of crystal structures should present all atomic labeling using Arial, a size of 7.5 pt with parentheses such as N(2), O(3), etc. If the table of the parameters of anisotropic displacements is not printed, at least one figure should show the displacement ellipsoids. Figures showing the crystal packing should not be overcrowded and should not show sections larger than necessary. Usually, one unit cell and a few adjacent atoms are sufficient. Include and label the outlines of the unit cell. Avoid the depiction of several translation-equivalent atoms in the viewing direction. If lines intersect, it should be clear which one is in front of the other.

### **Schemes**

Multiple-step reactions should be regarded as Schemes, and their reaction conditions should be given above the arrows rather than in the caption.

### **Scanned pictures or color pictures**

These pictures should be readable with a resolution of 300–600 dpi. Color: Printing of Figures and Schemes in color is expensive, so we request that part of the additional costs be carried by the author (RMB 1500 per figure or scheme). If color is essential and the author does not have access to funds for publication costs, the editor can make an exception. Because the web and print versions of the manuscript need to be identical, it is not possible for the manuscript to contain color only in the web version.

## Symbols

Use only characters from the Symbol and Normal Text fonts, especially when inserting Greek letters and characters with umlauts, accents, tildes, etc.:  $\alpha$ ,  $\ddot{a}$ ,  $\grave{a}$ ,  $\tilde{a}$ ,  $\text{\AA}$ . Symbols of physical quantities, stereochemical information (cis, Z, R, etc.), locants (N-methyl,  $\alpha$ -amino), symmetry designations ( $C_{2v}$ ) should be italicized. Chemical formulae should be numbered with boldface Arabic numerals (e.g., 1). If physical quantities are listed as numerical values without their units, e.g., in tables or for labels of axes in figures, the units must be specified after a slash or with a power of  $-1$ , e.g.,  $T/K$ ,  $c/(\text{mol}\cdot\text{L}^{-1})$ . Abbreviations such as Me, Et, *n*-Bu, *i*-Pr, *s*-Bu, *t*-Bu and Ph may be used in formulae. General substituents should be indicated by R1, R<sup>2</sup> (not R<sub>2</sub>, which means 2R) or R, R'. The spatial arrangement of the substituents should be indicated by hatched lines and a wedge. The Symbol font should be used for minus signs.

## Abbreviations and acronyms

Abbreviations and acronyms should be used sparingly and consistently, following the system of abbreviations and symbols recommended by the International Union of Pure and Applied Chemistry. Where they first appear in the text, they should be defined (apart from the most common ones such as NMR, HPLC, and THF).

## Nomenclature

Nomenclature must be consistent, clear, and unambiguous, and in keeping with the rules established by the International Union of Pure and Applied Chemistry, the International Union of Biochemistry, and Chemical Abstracts Service.