



*Chinese Journal of Structural Chemistry*

Instructions for Authors

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## 1 General

The *Chinese Journal of Structural Chemistry* is an international peer-reviewed journal published in English. It publishes original research works about the structure and property of matter, including but not limited to coordination chemistry, organometallic chemistry, nanoscale chemistry, heterogeneous catalysis, homogenous catalysis, energy chemistry, environment science, and life science in the form of Articles, Communications, Reviews, Perspectives, and News & Views. The journal is published twelve issues a year by Fujian Institute of Research on the Structure of Matter, CAS, and is available online at <http://www.cjsc.ac.cn>.

Authors are solely responsible for the contents of their contribution. It is assumed that they have the necessary authority for publication. The contents of manuscripts submitted to the *Chinese Journal of Structural Chemistry* have not been submitted to any other journal in parallel or published previously. Any manuscript available on personal/group web pages will be considered by the Editors as already published and will not be accepted. The authors must inform the Editors of manuscripts submitted to, soon to be submitted to, or in press at other journals that have a bearing on the manuscript being submitted. All submissions must adhere to the Ethical Guidelines for Publication in Journals and Reviews of the European Association of Chemical and Molecular Sciences (EuCheMS). In particular, authors should reveal all sources of funding for the work presented in the manuscript and should declare any conflict of interest.

All articles must be written in English. A well-written paper helps share your results most clearly. Manuscript must be “spell checked” and “grammar checked” before submission, and our English editor will edit your manuscript for grammar, spelling, and other language errors so that your ideas could be presented at their best.

All submitted manuscripts that are suitable for consideration will be sent to independent referees. Manuscripts which are clearly inappropriate for the journal can be rejected without consulting referees. Authors are encouraged to suggest suitable referees (full names and affiliations including e-mail address). However, the referees that are contacted will not be limited to those nominated by the authors. All accepted manuscripts are edited before printing to ensure scientific consistency,

clarity of presentation, and uniformity of style.

If authors have to or want to make their publications freely available at the moment they are published (open access), the *Chinese Journal of Structural Chemistry* offers such a service. Under the keyword Online Open you can find all the information about this subject on our homepage.

In general, we recommend that authors link on their homepage to their *Chinese Journal of Structural Chemistry* publication through the "Digital Object Identifier" (DOI). Only in this way Crossref function correctly and full-text downloads can be tallied.

## 2 Submission of Manuscripts

The *Chinese Journal of Structural Chemistry* offers web-based manuscript submission and peer-review. This service guarantees fast and safe submission of manuscripts and rapid assessment processes. Online submission is mandatory, and conventional submission of manuscripts via courier service or e-mail is no longer accepted. Please prepare your manuscript in keeping with the guidelines given below (§4).

For the submission of new, revised and final accepted manuscripts, a single Word DOC file containing graphical abstract, text, tables and all graphics should be uploaded as "Main Document" on the File Upload screen. Tables and all graphics need to be embedded in the text of the DOC file where they belong (not collected at the end).

Note: Do not choose the file designation "Image" to upload graphics as separate files when uploading new manuscripts. Supporting Information is uploaded as a single, separate PDF file with all graphics embedded by choosing the file designation "Supporting Information".

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Authors are asked to make their manuscripts suitable for a heterogeneous readership. Please use a simple, clear style, and avoid jargon. In some cases, it might be helpful for manuscripts to be checked by a third party, such as Wiley English Language Editing Services for correct language usage before submission.

### 3 Types of Manuscripts

Articles represent complete studies and are not restricted in length. However, authors are urged to be as concise as possible, presenting experimental results clearly and carefully in a separate section and placing material in the Supporting Information file that, while of importance for practitioners on the topic, is of significantly less interest to the general reader.

Reviews are generally on *progress in rapidly developing fields*. Reviews are generally invited by the editor. Submission without invitation is welcome with the consent of the editor, which can be granted on the basis of a pre-submission with a table of contents and a summary, as well as a list of major references. A review is required to present clear, complete, and objective review and depiction of the historical background, problems and current status, recent progress and future perspectives in a research field. A review is not expected to be a reference report. Personal accounts with unique and critical assessments and perspectives are generally encouraged.

### Short Communications

Provide a rapid and significant report of a new finding that is brief but is originality, mechanistic insight, and interest to a broad readership. The introduction should concisely provide sufficient background information that help the reader understand the importance of the work. Short Communications without abstract and keywords. should be less than 3 printed pages with 1–2 displayed items including chemical formulae, Figures, Schemes, and Tables. Other additional information (if necessary) should be submitted as Supplementary materials. Each paper will begin with “Short Communication:” followed by the title. Short Communications will appear at the end of the topical sections in the journal table of contents.

### Perspectives

Provide fresh insights on new advances in a specific research field of science and technology or scientific policy and other issues related to the science community. Perspective authors are asked to assess the current status of the field with an emphasis on identifying key advances being made or those advances that are needed, and with an eye to the future. Authors should not primarily discuss their work. While snapshotting the issue or problem, perspectives are expected to propose a solution in detail. Perspectives should be less than 3000 words with a maximum of 15 references and 1–2 displayed items. An abstract is required.

## Research Highlights

Research Highlights mainly describe the latest important progress. It focuses on the main findings, emphasizes their significance, and provides a further discussion on the research topic. The results should be presented clearly without the comprehensive details required for an original article. Highlights should be limited to approximately 2000 words with 1 displayed item and 15 references within 2 pages. Highlights should have no more than three authors (at the discretion of the editor), who should not have affiliations with the author(s) of the work being highlighted.

## 4 Manuscript Preparation

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.

### **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.

### **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.

### **Numbered sections**

Divide your article into clearly defined and numbered sections. Subsections should be numbered 1.1 (then 1.1.1, 1.1.2, ...), 1.2, etc. (the abstract is not included in section numbering). Use this numbering also for internal cross-referencing: do not just refer to 'the text'. Any subsection may be given a brief heading. Each heading should appear on its own separate line.

### **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 proofreading 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.

### **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.

### **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.

### **References**

The author is responsible for correct citations. Please ensure that every reference cited in the text is also present in the reference list (and vice versa). Any references cited in the abstract must be given in full. Unpublished results and personal communications are not recommended in the reference list, but may be mentioned in the text. If these references are included in the reference list they should follow the standard reference style of the journal and should include a substitution of the publication date with either 'Unpublished results' or 'Personal communication'. Citation of a reference as 'in press' implies that the item has been accepted for publication.

### **Reference links**

Increased discoverability of research and high quality peer review are ensured by online links to the sources cited. In order to allow us to create links to abstracting and indexing services, such as Scopus, Crossref and PubMed, please ensure that data provided in the references are correct. Please note that incorrect surnames, journal/book titles, publication year and pagination may prevent link creation. When copying references, please be careful as they may already contain errors. Use of the DOI is highly encouraged.

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As a minimum, the full URL should be given and the date when the reference was last accessed. Any further information, if known (DOI, author names, dates, reference to a source publication, etc.), should also be given. Web references can be listed separately (e.g., after the reference list) under a different heading if desired, or can be included in the reference list.

### Data references

This journal encourages you to cite underlying or relevant datasets in your manuscript by citing them in your text and including a data reference in your Reference List. Data references should include the following elements: author name(s), dataset title, data repository, version (where available), year, and global persistent identifier. Add [dataset] immediately before the reference so we can properly identify it as a data reference. The [dataset] identifier will not appear in your published article.

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Where a preprint has subsequently become available as a peer-reviewed publication, the formal publication should be used as the reference. If there are preprints that are central to your work or that cover crucial developments in the topic, but are not yet formally published, these may be referenced. Preprints should be clearly marked as such, for example by including the word preprint, or the name of the preprint server, as part of the reference. The preprint DOI should also be provided.

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### ***Reference style***

**Text:** Indicate references by number(s) in square brackets in line with the text. The actual authors can be referred to, but the reference number(s) must always be given.

**Example:** '..... as demonstrated [3,6]. Barnaby and Jones [8] obtained a different result ....'

**List:** Number the references (numbers in square brackets) in the list in the order in which they appear in the text.

**Examples:**

Reference to a journal publication:

[1] J. van der Geer, J.A.J. Hanraads, R.A. Lupton, The art of writing a scientific article, *J. Sci. Commun.* 163 (2010) 51–59. <https://doi.org/10.1016/j.Sc.2010.00372>.

Reference to a journal publication with an article number:

[2] J. van der Geer, J.A.J. Hanraads, R.A. Lupton, 2018. The art of writing a scientific article. *Heliyon*. 19, e00205. <https://doi.org/10.1016/j.heliyon.2018.e00205>.

Reference to a book:

[3] W. Strunk Jr., E.B. White, *The Elements of Style*, fourth ed., Longman, New York, 2000.

Reference to a chapter in an edited book:

[4] G.R. Mettam, L.B. Adams, How to prepare an electronic version of your article, in: B.S. Jones, R.Z. Smith (Eds.), *Introduction to the Electronic Age*, E-Publishing Inc., New York, 2009, pp. 281–304.

Reference to a website:

[5] Cancer Research UK, Cancer statistics reports for the UK. <http://www.cancerresearchuk.org/aboutcancer/statistics/cancerstatsreport/>, 2003 (accessed 13 March 2003).

Reference to a dataset:

[dataset] [6] M. Oguro, S. Imahiro, S. Saito, T. Nakashizuka, Mortality data for Japanese oak wilt disease and surrounding forest compositions, *Mendeley Data*, v1, 2015. <https://doi.org/10.17632/xwj98nb39r.1>.

Reference to software:

[7] E. Coon, M. Berndt, A. Jan, D. Svyatsky, A. Atchley, E. Kikinzon, D. Harp, G. Manzini, E. Shelef, K. Lipnikov, R. Garimella, C. Xu, D. Moulton, S. Karra, S. Painter, E. Jafarov, S. Molins, *Advanced Terrestrial Simulator (ATS) v0.88 (Version 0.88)*, Zenodo, March 25, 2020. <https://doi.org/10.5281/zenodo.3727209>.

Reference to patents:

[8] 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.

Journal abbreviations source

Journal names should be abbreviated according to the [List of Title Word Abbreviations](#).

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

## 5 Format of Figure and Others

We recommend that you create **all figures** as **vector-based graphics**, such as those produced by Adobe Illustrator. Vector files can be properly resized without losing resolution, as they can be altered in size while maintaining high print-quality resolution. The symbols and words in the figures should be large enough to be clearly visible when the picture is reduced (reduced size is about 2 mm). We **cannot** accept files that are not readable by PowerPoint, Adobe Photoshop, Macromedia Freehand, or Adobe Illustrator. To keep file sizes reasonable, please save art at a resolution of 300



dots per inch (dpi) or higher for initial submission. Digital color art is best submitted in **CMYK** (cyan, magenta, yellow, black) rather than RGB (red, green, blue).

- 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.
- Use capital letters for part labels in multipart figures – A, B, C, etc. These letters should be 9 pt and bold in figure. Place part labels at the upper left-hand corner of each figure part; if a part is an image, set labels inside the perimeter to avoid waste space.
- The symbols and words in the figures should be large enough to be clearly visible when the picture is reduced (reduced size is about 2 mm).
- Avoid using colors that are close in hue to identify different parts of a figure.

Note: The *Chinese Journal of Structural Chemistry* does not use charts, which should be converted into figures or schemes.

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.

### **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.

### **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. The width of a picture will be 5.5 cm or 12.0 cm when printed. Use solid symbols for plotting data if possible (unless data overlap or there are multiple symbols). Line widths should be legible upon reduction (minimum of

0.5 pt at the final reduced size).

### 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.

### 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. Abbreviations, symbols, Nomenclature and units used in a figure should match those used in the text.

### 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.

### 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 and units

Nomenclature must be consistent, clear, and unambiguous. Follow internationally accepted rules and conventions: use the international system of units (SI). If other quantities are mentioned, give their equivalent in SI or refer to 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).

### Formulae, Equations and Schemes

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.

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

### 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 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.

## 6 Crystal Structural Analysis

Authors are required to (a) check the quality of their CIFs through the checkCIF website *prior to submission of their manuscript*, (b) submit CIFs and structure factor tables to the Cambridge Crystallographic Data Centre (CCDC) prior to submission and provide the CCDC access code(s) upon submission, (c) provide the checkCIF output file (as a PDF uploaded as Supporting Information for Review Only), and (d) address any A and/or B level alerts in the checkCIF PDF and consider inserting their comments directly into CIFs.

Submitting a copy of the output as Supporting Information for Review is mandatory. Authors with appropriate software may alternatively use IUCRVAL or the CHECK validation tool in PLATON. Prior to manuscript submission, the author(s) must deposit their data or update data already available, so that referees can retrieve the information electronically directly from the database. Crystallographic data should be deposited with either the Cambridge Crystallographic Data Centre (CCDC) for organic and organometallic compounds or with the Fachinformationszentrum Karlsruhe (FIZ) for inorganic compounds, elements, metals, and minerals. Guidelines for depositing data can be found on the *Chinese Journal of Structural Chemistry* homepage. If a crystal structure analysis is an essential part of the paper, crystallographic data should be given in an order as follows: triclinic, space group  $P\bar{1}$ ,  $a = 11.1348(7)$ ,  $b = 12.2599(7)$ ,  $c = 20.2479(13)$  Å,  $\alpha = 82.448(2)^\circ$ ,  $\beta = 76.433(2)^\circ$ ,  $\gamma = 74.5025(19)^\circ$ ,  $V = 2582.3(3)$  Å<sup>3</sup>,  $Z = 2$ ,  $\mu = 0.585$  mm<sup>-1</sup>.

## 7 Supporting Information

Supporting Information may be included for deposition on the WWW. The author bears full responsibility for the content of the Supporting Information, and must keep a copy to make available to readers who do not have access to the WWW. Supporting Information may consist of original data that relate to the paper, e.g., additional or color illustrations, tables, supplemental experimental details, and characterization data, or may include information that is more convenient in electronic form, such as coordinates, spectral data, etc., or that cannot be printed: animations, audio recordings, and videos. This material should be included in the original submission for peer-review. After acceptance, succinct text and the necessary graphics should be sent as a separately saved single MS Word file with the final revised version of the manuscript. The graphics should be embedded in the file rather than as separate files. Color and animated multimedia applications in the Supporting Information are welcome and published online at no cost to the author or reader.

Note: Experimental procedures for crystallographic studies can be included, but do not include the complete crystallographic data that are available from CCDC or FIZ.

## 8 Final/Revised Version

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