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Inorganic Chemistry

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Scope of the Journal

Inorganic Chemistry publishes fundamental studies, both experimental and theoretical, on all topics of inorganic chemistry from across the periodic table, including but not limited to coordination chemistry, main-group chemistry, bioinorganic chemistry, organometallic chemistry, solid- state/materials/nanoscale chemistry, energy and photochemistry, catalysis, and theory/computation.

The journal places emphasis on scientifically rigorous studies of the synthesis and mechanisms, structure, thermodynamics, kinetics, reactivity, spectroscopy, bonding, and functional properties of new and significant known compounds. Only those manuscript submissions that sufficiently emphasize inorganic chemistry aspects will be considered. Illustrative examples of manuscripts that will not be considered include ones that describe poorly defined or characterized compounds or materials, or that are deemed to emphasize morphological, nanoscale, or larger scale attributes of materials, biological phenomena, analytical methods, speculative or predominantly technical aspects of theory, or technological applications. Reports of routine research describing incremental additions to the scientific literature are discouraged. More detailed discussion (organized by topic) of submissions that will be considered are presented below.

Coordination and Organometallic Chemistry: Fundamental studies of the design and synthesis of new coordination and organometallic complexes incorporating main group, transition metal, and/or lanthanide/actinide elements with tailored reactivity and/or functional electronic, optical, and magnetic properties are welcome. These studies should include details of coordination environment, electronic structure, bonding, magnetic properties, and/or reactivity probed through experimental and/or computational methods and involving spectroscopy, electrochemistry, and other characterization means. The added value to general knowledge in inorganic chemistry should be clearly visible, for example in the description of uncommon structures, bonding, reactivity, and/or proven potential for new molecular or materials applications (such as catalysis, sensing, and optics). Articles that focus solely on solid-state structures or synthetic organic applications are discouraged.

Bioinorganic Chemistry: Studies in the area of bioinorganic chemistry should emphasize new inorganic structures, solution chemistry, detailed mechanisms of biological efficacy or reactions, or spectroscopic properties. The inorganic chemistry must be central and contribute new perspectives to the field, for example in areas of biomimetic and bioinspired coordination chemistry, metalloproteins and metallodrugs, and metal-based probes. Manuscripts with a focus on biology that lack in-depth studies of inorganic chemistry aspects will not be considered.

Solid State, Materials, and Nanoscale Chemistry: *Inorganic Chemistry* encourages submissions that contribute significant new synthetic, mechanistic, or structural insight on well-characterized new or known molecular, nanostructured, or extended inorganic compounds (clusters and supramolecular compounds) and push the frontiers of functional inorganic chemistry-dependent materials properties, characterization techniques, or theoretical description. Manuscripts that emphasize technological applications or that describe routine syntheses and characterization, incremental advances for well-known families of compounds, routine formulations of known components, or phenomenological work that does not provide new inorganic chemistry insight will not be considered. For further guidance, see: (Nano)materials Chemistry: What

Belongs at Inorganic Chemistry?

Energy and Photochemistry: Studies in the area of energy and photochemistry should emphasize new inorganic structures or coordination compounds with properties and functions related but not limited to electrical, redox, luminescence, excited states, photoredox sensitization, and energy-transfer chemistry or to applications in solar-energy conversion and storage. Contributions that focus on applications, including analytical techniques and photophysics, or on speculative theoretical aspects, will not be considered.

Catalysis: Studies on heterogeneous and homogeneous catalysis using inorganic or organometallic compounds and/or inorganic-organic hybrid compounds and materials as well as metallosupramolecules are welcome. The focus should be on inorganic chemistry aspects, in particular new complexes with interesting structures, bonding, coordination numbers, or electron configurations, rather than applications to organic synthesis or industrial process development with well-known compounds, for example.

Theory and Computation: *Inorganic Chemistry* welcomes studies that use state-of-the art theoretical/computational methods to contribute to conceptual advances in all areas of inorganic chemistry, especially those that combine experiment and theory. Studies that focus on technical aspects, for example the choice of density functionals and/or basis sets, or are largely speculative, that is, make predictions that cannot reasonably be subjected to experimental testing, will not be considered.

If you are a new *Inorganic Chemistry* author, or if you have not submitted a manuscript during the past year, please read and familiarize yourself with these complete Author Guidelines to ensure you are up to date with all of the journal's manuscript preparation and submission requirements.

Editors, Authors, and Reviewers should read the ACS Ethical Guidelines.

Emphasis on Chemical Safety

In 2021, in support of ACS's core value of "Professionalism, Safety, and Ethics," ACS Publications added a Safety Considerations requirement to the Author Guidelines of every ACS journal (Appendix 1):

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 a full article and included in the main text of a letter. Statement examples can be found in the Safety Statement Style Sheet and additional information on communicating safety information from the *ACS Guide to Scholarly Communication* is freely available here.

Inorganic Chemistry is participating in a pilot program to further encourage use of Safety Statements in manuscripts, including details on how to mitigate hazards and risks. Reviewers and Editors will be more carefully checking manuscripts to determine whether an existing Safety Statement is accurate and complete, and if there is no Safety Statement in a manuscript whether there are any hazards or risks that require a Safety Statement be added. If a Safety Statement is needed, authors will be asked to include one in their manuscript at revision and before acceptance.

Manuscript Types

Inorganic Chemistry publishes Articles, Communications, invited Viewpoint Articles, and invited Reviews.

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.

Featured Articles are submitted Articles selected by the editors for their quality, interest, and importance, and have also received especially strong positive comments from reviewers. These articles are expedited during journal production and appear at the beginning of the Articles section in the Table of Contents of each issue. They are also highlighted in a special section on the Journal's website.

Communications are reports of unusual urgency, significance, and interest originating in all areas of inorganic chemistry. A statement from the authors describing why their manuscript meets these criteria is required in the cover letter. Communications must convey the scientific findings concisely in 2,200 words or less, which includes the abstract, main text, and figure captions, plus approximately four graphics (each typically 5 cm/2 inches long in a single column) and the TOC graphic. References and the TOC synopsis are not included in the word count. Communications must meet these length requirements before acceptance. *Complete* experimental work should appear in the Supporting Information; additional documentation in the Supporting Information is encouraged. Communications that contain X-ray crystallographic information must be accompanied by full documentation to be used as Supporting Information in the editorial and review process.

Viewpoints are personalized discussions of a developing subject or field, firmly based in science, with the intent of inspiring future research efforts. In each Viewpoint, authors introduce the topic, provide insight and critical assessment of recent advances, and discuss new directions and future outlook for the field. The manuscript length should fit within 5–10 final published journal pages. While Viewpoints are typically invited by the Editor-in-Chief, proposals for Viewpoint submissions are welcome.

Reviews are currently by invitation only from the Editor-in-Chief. Suggestions for both authors and topics as well as uninvited proposals are welcome (Email: eic@inorg.acs.org). Formal requirements are minimal: The length is flexible with an upper limit of 10,000 words; the manuscript should contain an abstract, a Table of Contents graphic, and author biographies and photographs; references can be provided in any style, but they must be complete, including titles; Supporting Information may be included as needed.
A good review should be timely (not merely another in a line of reviews on the same topic) with historical context to lay out challenges and forward-looking to discuss opportunities. The manuscript should be firmly based in science, critically evaluating the recent work of multiple groups (not just the work of the authors) in an inorganic chemistry field or across disciplines with a clear connection to inorganic chemistry aspects. The Review should be a concise survey of the literature with a logical organization and written at a level that makes the material easily accessible to a wide readership through clear text and figures—authors are free to present the topic with their own personal flavor. Authors should be judicious in citing the literature, focusing on the most seminal or recent articles, limiting the overall number of their own publications, being mindful of personal biases, and striving to provide an inclusive perspective.

In all types of submissions, authors should present their material as clearly and concisely as possible. Introductions should contain sufficient background material to show why the work was done and how it relates to the subject. However, extensive reviews of the literature and/or numerous general references are inappropriate. **The description of experimental work must be presented accurately and in sufficient detail to allow the work to be duplicated in other laboratories.**

ACS Researcher Resources

While this document will provide basic information on how to prepare and submit the manuscript as well as other critical information about publishing, we also encourage authors to visit ACS Researcher Resources for additional information on everything that is needed to prepare (and review) manuscripts for ACS journals and partner journals, such as

- Mastering the Art of Scientific Publication, which shares editor tips about a variety of topics including making your paper scientifically effective, preparing excellent graphics, and writing cover letters.
- Resources on how to prepare and submit a manuscript to ACS Paragon Plus, ACS Publications' manuscript submission and peer review environment, including details on selecting the applicable Journal Publishing Agreement.
- Sharing your research with the public through the ACS Publications open access program.
- ACS Reviewer Lab, a free online course covering best practices for peer review and related ethical considerations.
- ACS Author Lab, a free online course that empowers authors to prepare and submit strong manuscripts, avoiding errors that could lead to delays in the publication process.
- ACS Inclusivity Style Guide, a guide that helps researchers communicate in ways that recognize and respect diversity in all its forms.

Manuscript Preparation

Submit with Fast Format

All ACS journals and partner journals have simplified their formatting requirements in favor of a streamlined and standardized format for an initial manuscript submission. Read more about the requirements and the benefits these serves authors and reviewers here.

Manuscripts submitted for initial consideration must adhere to these standards:

- Submissions must be complete with clearly identified standard sections used to report original research, free of annotations or highlights, and include all numbered and labeled components.
- Figures, charts, tables, schemes, and equations should be embedded in the text at the point of relevance. Separate graphics can be supplied later at revision, if necessary.
- When required by a journal's structure or length limitations, manuscript templates should be used.
- References can be provided in any style, but they must be complete, including titles. For information about the required components of different reference types, please refer to the ACS Style Quick Guide.
- Supporting Information must be submitted as a separate file(s).

Document Templates and Format

The templates facilitate the peer review process by allowing authors to place artwork and tables close to the point where they are discussed within the text. Learn more about document templates here.

General information on the preparation of manuscripts may also be found in the ACS Guide to Scholarly Communication.

Acceptable Software, File Designations, and TeX/LaTeX

See the list of Acceptable Software and appropriate File Designations to be sure your file types are compatible with ACS Paragon Plus. Information for manuscripts generated from TeX/LaTeX is also available.

Cover Letter

A cover letter must accompany every manuscript submission. During the submission process, you may type it or paste it into the submission system, or you may attach it as a file.

Authors must explain clearly and convincingly in their cover letter how their manuscript is original, significant, and novel and why it will be of interest to the readers of *Inorganic Chemistry*.

Manuscript Text Components

1. Title
2. Abstract
3. Introduction
4. Experimental and/or Computational Section
5. Results and Discussion
6. Conclusions
7. Tables, Schemes, and Figures with captions
8. Synopsis
9. Table of Contents Graphic

For full articles, authors may decide to place the Experimental and/or Computational Section after the Introduction or after the Conclusions. For Communications, section headings are optional and the Experimental and/or Computational Section may be placed in the Supporting Information so long as it is accurate and complete.
Tables, Schemes, and Figures should be placed as near as possible to where first mentioned in the main text and not at the end of the manuscript.
The use of manuscript titles or descriptions in the abstract or text to make claims of priority, originality, convenience, effectiveness, or value should be avoided or used with great restraint. For example, the words “boost,” “concise,” “convenient,” “efficient,” “elegant,” “expedient,” “exciting,” “facile,” “first,” “new,” “novel,” “practical,” “simple,” “unique,” “unprecedented,” and “versatile” should not be used. The use of “free” should also be avoided, that is “metal-free,” “catalyst-free,” “light-free,” and so on, as these terms can be misleading. In addition, editors may ask authors to moderate or remove what they judge to be excessive use of subjective evaluative language elsewhere in the manuscript.

In addition to emphasizing safety hazards or risks associated with the reported work and how to mitigate them, the Editorial Team encourages authors to include comments on the use of toxic and/or environmentally persistent reagents and solvents, and provide a rationale on choice of these reagents and solvents. This acknowledgement is especially important in cases of “dual use” potential when the reported work could be directly misapplied by others to pose a threat to public health and safety. *Inorganic Chemistry* further encourages authors to consider the Principles of Green Chemistry in carrying out their research and consider reporting metrics such as atom economy, mass efficiency, E-factor, or others. For more information, please consult Research Tools provided by the ACS Green Chemistry Institute.

Title. The title should be descriptive of the topic of the article and as short as possible, using easily searchable keywords and minimizing hyphenation. Avoid using abbreviations and acronyms unless they are more commonly used than spelled out words. Also avoid complex compound names as much as possible in the title by using generic names, and spell out elements rather than using symbols unless part of a compound name. Neither the title nor any other text should indicate that the manuscript is part of a numbered series on a broader research topic, or a numbered contribution from a particular institution or research group.

Abstract and Abstract/Table of Contents Graphic. The abstract should briefly state the purpose of the research, principal results, and major conclusions and not exceed 200 words. Undefined nonstandard abbreviations and reference citation numbers should be avoided. A graphic must be included with each manuscript for display in the Abstract and Table of Contents (TOC), fitting in an area no larger than 8.25 cm by 4.45 cm (3.25 inches by 1.75 inches). (See TOC/Abstracts Graphics guidelines). The graphic should capture the reader’s attention and, in conjunction with the manuscript title, should give a quick visual impression of the content of the manuscript. *The TOC graphic should not exactly duplicate a graphic appearing within the text of the manuscript.* In preparing an Abstract/TOC graphic, creativity is welcome, but avoid images of people living or from the past and avoid caricatures or parodies that could be socially/culturally insensitive or considered racist or discriminatory, especially when taken out of context. Ensure that cartoon depictions of machinery, nature, and processes do not indicate actions or settings that are improbable. See Appendix 2 for full details on graphics requirements.

Synopsis. For all article types, authors must submit a Synopsis, which can contain up to 75 words, that describes in simple terms what the article is all about.

A well-written Title, Abstract/TOC graphic, and Synopsis can attract the attention of potential readers and increase the likelihood that the published article will be cited by other researchers.

Introduction. The introduction should include sufficient background information to provide appropriate context as to the novelty and importance of the new work and clearly state the purpose and objectives of the research, including how it fits within the scope of *Inorganic Chemistry*. An extensive review of prior work is not appropriate, and documentation of the relevant background literature should be selective rather than exhaustive, particularly if reviews can be cited.

Abbreviations, Symbols, Units, Compound Names. Authors should use abbreviations and acronyms in the text to conserve space. A list of standard abbreviations is provided in the ACS Guide to Scholarly Publishing. Nonstandard abbreviations and acronyms must be defined the first time they are used in the abstract, text, and Supporting Information. The use of abbreviations should be consistent throughout the manuscript text and graphics/captions. For example, either CH_3 or Me may be used for “methyl,” but not both. Full systematic names of compounds (see Part 4 and Part 5 of The ACS Guide for Scholarly Communication for guidance) should be included in

the Experimental Section on first mention and for brevity compounds should be assigned a molecule number for reference throughout the article. In other sections of the manuscript, authors should use their judgement on common usage of compound names or use a generic name or molecule numbers in lieu of full systematic names. As a courtesy to the research community, a list of abbreviations used in your manuscript if extensive can be included under Associated Content at the end of the manuscript and at the end of the Supporting Information before the References section.

References. Authors should be judicious in citing the literature; unnecessarily long lists of references should be avoided. If a number of publications are relevant to a statement in the text, not more than two or three of the most seminal or recent should be cited; if appropriate, the author may add “and references cited therein” following a reference. Authors must also cite any previously published work wherein portions of the submitted work have been disclosed. It is seldom necessary or appropriate for an author to cite more than 10 of their own publications. No reference should repeat a reference that appears elsewhere in the manuscript’s list of references. Authors are encouraged to include additional references cited in Supporting Information files in the main article reference list. Long endnotes should be avoided; peripheral discussion should be placed in the supporting information. Endnotes should not contain graphics, experimental procedures, or compound characterization data.

Author portrait for Viewpoints and Editorials. A high-resolution (300 dpi or better), in focus, color head-and-shoulders photograph and a brief one or two sentence statement of the author(s) current research interests should be included in the Author Information section. Alternatively, a group photo of the authorship team may be used. Model release and copyright forms are required for author photographs and will be provided by the Journal office.

Supporting Information

This information is provided to the reviewers during the peer-review process (for Review Only) and is available to readers of the published work (for Publication). Supporting Information must be submitted at the same time as the manuscript. See the list of Acceptable Software by File Designation and confirm that your Supporting Information is viewable.

If the manuscript is accompanied by any supporting information files for publication, these files will be made available free of charge to readers. A brief, nonsentence description of the actual contents of each file, including the file type extension, is required. This description should be labeled Supporting Information and should appear before the Acknowledgement and Reference sections. Examples of sufficient and insufficient descriptions are as follows:

Examples of sufficient descriptions: “Supporting Information: ^{1}H NMR spectra for all compounds (PDF)” or “Additional experimental details, materials, and methods, including photographs of experimental setup (DOC)”.

Examples of insufficient descriptions: “Supporting Information: Figures S1-S3” or “Additional figures as mentioned in the text”.

When including supporting information for review only, include copies of references that are unpublished or in-press. These files are available only to editors and reviewers.

Research Data Policy

All ACS journals strongly encourage authors to make the research data underlying their articles publicly available at the time of publication.

Research data is defined as materials and information used in the experiments that enable the validation of the conclusions drawn in the article, including primary data produced by the authors for the study being reported, secondary data reused or analyzed by the authors for the study, and any other materials necessary to reproduce or replicate the results.

The ACS Research Data Policy provides additional information on Data Availability Statements, Data Citation, and Data Repositories.

Data Requirements

Characterization of New Compounds

The Journal upholds a high standard for compound characterization to ensure that substances being added to the chemical literature have been correctly identified and can be synthesized in known yield and purity by the reported preparation and isolation methods. The Editors would like to point out that reported yields above 95%, isomer ratios above 200:1, and enantiomeric excesses above 99% typically aren't realistic without further explanation. The Editors also remind authors that it is unethical to modify reported data or spectra, for example to correct spectral baselines or remove solvent/impurity peaks.

Authors are responsible for retaining their original data or having available original data from collaborators or from contractors who perform analyses on their behalf. Authors may be asked to provide copies of spectra or analytical reports if an editor or reviewer raises a question about reported results. Upon publication, authors are encouraged to link the manuscript to their data housed in a repository or other location, and to make their primary data freely available to others upon request.

For all **new** compounds, evidence adequate to establish both *identity* and *degree of purity* (homogeneity) must be provided. For known compounds prepared by a new or modified synthetic procedure, the types of physical and spectroscopic data that were found to match *cited* literature data should be identified, and purity documentation should be provided. Authors are further encouraged to include additional data or revised data that was not reported in original references cited, and in doing so indicate which part of the data set is new information.

Single-crystal X-ray diffraction results are not, in general, acceptable as the *only* means of characterization of new compounds. Compounds *must* also be characterized by spectroscopic and analytical methods appropriate for the particular sample or compound. Methods may include elemental analyses to demonstrate bulk composition, NMR spectroscopy, mass spectrometry, infrared spectroscopy, and electronic spectroscopy.

Structure Reports

(A) Crystal Structure Studies

A checklist for authors derived from recommendations of the Commission on Crystallographic Data of the International Union of Crystallography (*Acta Crystallogr.* **1967**, *22*, 445) is available from the *Inorganic Chemistry* website. Authors should consult this checklist (revised 2001) before preparing manuscripts for submission. Not all data requested for review will be shown in the printed text.

This applies both to reports in which the structure study is the main thrust of the work (full structure report) and to those in which such a study plays only a supporting role (abbreviated structure report). Single-crystal X-ray diffraction results are not, in general, acceptable as the only means of characterization of new compounds. See the statement under Characterization of New Compounds given above. If electronic spectral data are employed to relate the bulk and crystallographic samples, extinction coefficients should be provided. It is possible that syntheses will occasionally produce a material that cannot be reliably analyzed, gives uninformative IR and electronic spectra, and presents no definitive NMR data because of paramagnetism or dynamic exchange processes. Cases of this sort may be acceptable if and only if the author clearly delineates the limitations of the available data.

(1) Structure Reports in Articles.

(a) Experimental Section. Every effort should be made to minimize the quantity of tabular material appearing in the published text. The collection of data and refinement of the structure are usually routine, and a concise description can be accomplished with a brief written description and a table containing crystallographic parameters and data collection and refinement information described below.

(b) Tabular Material. An abbreviated table containing unit cell constants, space group information, Z, data collection and refinement parameters, and final agreement factors may be helpful to readers and may be included in either the text or Supporting Information. In addition, important bond lengths and angles (with esd's) should be supplied for the published text when they are significant to the overall discussion. *Inorganic Chemistry* does not publish refined positional parameters in the published text except in cases where such information is essential to the clarity of the manuscript. This information can be accessed easily from the web page displaying the final published article, which links to the data deposited at the CCDC via the Accession Codes box. Note that a list of the Accession Codes will also be published in the PDF version of the final article. If relevant, other information such as least-squares planes and atomic deviations therefrom, closest intermolecular contacts (e.g., details of intermolecular hydrogen-bonding or other packing interactions), and unit cell and packing diagrams (optional if no unusual intermolecular contacts exist), stylized to emphasize packing information and drawn with right- handed axes, should be deposited in PDF format as Supporting Information. A statement should appear at the end of the printed manuscript text enumerating the contents of the Supporting Information.

(c) Figures. Drawings of crystal or molecular structures should be made with the noncrystallographer in mind. **For structures refined anisotropically, plots showing thermal ellipsoids are required rather than ball-and-stick drawings.** Stereoscopic pairs of perspective drawings and unit cell and packing diagrams should be deposited as Supporting Information unless they contribute directly to the discussion.

(d) Deposited Data. See Requirements for Depositing X-Ray Crystallographic Data. Prior to manuscript submission, authors are **required** to check the quality of their CIFs (for single-crystal data collections) through the checkCIF website of the International Union of Crystallography (http://checkcif.iucr.org) and to upload the checkCIF output files (combined into one PDF file) as Supporting Information for Review Only. Any A and/or B level alerts must be addressed prior to submission or otherwise explained in the checkCIF PDF, and authors are further encouraged to insert their comments directly into CIFs.

CIFs, structure factor tables, and CheckCIF reports must be submitted to the Cambridge Crystallographic Data Centre (CCDC) **prior to manuscript submission**. The CCDC deposition number(s) should be entered during manuscript submission**.** Any subsequent revisions to the CIFs

or structure factor tables should be deposited directly with the CCDC before uploading a revised manuscript to ACS Paragon Plus.

Reviewers will have access via the CCDC to an electronic copy of the CIF(s) associated with a manuscript. If the manuscript is accepted and published, the CIF(s) will be made available to readers via the article on the journal's website.

CCDC will accept organic, metal-organic, and inorganic compounds, including extended molecular solids and powder data where a constrained refinement has been used. Structural data for inorganic compounds will be transferred by CCDC to the Inorganic Crystal Structure Database (ICSD) after publication and will maintain the original deposition number(s). For all other crystallographic data that are not accommodated by the CCDC, authors are encouraged to deposit into a database according to instructions in the Requirements for Depositing X-Ray Crystallographic Data, in addition to uploading the data in ACS Paragon Plus during manuscript submission as Supporting Information. Please indicate whether the other crystallographic data is intended for publication or for review only.

If restraints or constraints on non-hydrogen atoms or adjustments to the structure factors are used in the refinement of a crystal structure, these should be described in detail in the experimental section and their application justified. Data from complementary experiments should be made available to resolve any ambiguities arising from problems with a refinement.

(2) Abbreviated Structure Reports in Communications and Articles. In a Communication or in the case where a structural study plays a supporting role in a full article devoted to another principal objective, a good molecular or unit cell diagram should appear as a figure. A brief summary of unit cell constants and data collection and refinement information should be given in a footnote, while selected distances and angles should be placed in the figure caption or a short table. The corresponding CIF should still be deposited with the CCDC as described above.

(B) Powder Diffraction Data

The structural determination of new materials by powder diffraction methods (laboratory X-ray, synchrotron, and/or neutron diffraction) is encouraged. Authors must include a table with the information shown below, as well as a figure showing the observed, calculated, and difference diffraction patterns and tick marks indicating the positions of the reflections for the refined phase and impurity phase(s). Authors are encouraged but not required to supply a CIF for a structure determined from powder diffraction. If a CIF file is provided for a powder diffraction structure, a checkCIF file is not required.

Crystallographic Data (Powder)

- Source (laboratory X-ray, synchrotron, neutron time of flight (TOF), neutron constant wavelength)
- Chemical formula
- Formula weight
- Temperature
- Pressure (if not ambient)
- Wavelength for constant wavelength or TOF
- Crystal system
- Space group (No.)
- *a*, *b*, *c*, , ,

- *V* (A3)
- *Z*
- *d*-space range
- 2
- *R*p
- *R*wp
- Definition of *R* factors

(C) Electron Diffraction

For reporting Electron Diffraction studies and results, please consult CCDC guidance and "Establishing Electron Diffraction in Chemical Crystallography."

(D) Corrections

Errors discovered in published structure reports should be communicated directly to the corresponding author of the work. The Editor should be kept informed by a copy of such correspondence. Upon verifying the error, the author or authors should submit a suitable correction to the Editor without delay, carrying an acknowledgment of the colleagues who brought the matter to their attention.

Computational Reports

With great advances in computational facilities and the availability of electronic structure codes (particularly DFT), there has been a significant increase in the number of computational papers being submitted to *Inorganic Chemistry*. In addition to computational competence (level of theory, basis sets, etc.), for a manuscript to be appropriate for publication in *Inorganic Chemistry*, it must be strongly correlated to experimental data, address problems of broad interest to the inorganic community, and provide significant chemical insight. Manuscripts reporting computational results are required to include appropriate references to the program packages and theoretical methods used in the main text; relegating these references to the Supporting Information is not appropriate.

Comparison of methods, studies of various levels of theory, basis set effects, etc., are considered to be technically oriented computational manuscripts and are not encouraged. In addition, studies simply confirming results already present in the literature or which are entirely speculative should be directed toward more specialized journals.

Authors should supply enough Supporting Information to reproduce the calculations or to make the results utilizable without repeating the calculations. Computational manuscripts should include at least the following Supporting Information:

1. Description of specific programs and the release or version. Authors should check and comply with citation requests of the program packages used. If the author's own or a modified version of a commercially available program is used, it is required that the program/code/modification be made available to the scientific community (QCPE, publication in a computational journal, commercially, etc.), if the license permits. Policies in this regard are identical with those of several other ACS journals, as summarized in *J. Chem. Inf. Model.* **2006,** *46,* 937.A clear exposition of any nonstandard equations and algorithms used and, where feasible, tests of the codes in various limiting cases should also be provided.
2. Details of the computations. The computed molecular model should be described clearly, possibly with a ChemDraw figure. If the model is based on an experimentally known complex/reaction, any modifications (such as truncations) should be clearly described and

justified. Final optimized coordinates and keywords are to be provided. For DFT computations, the choice of functional must be justified, or the validation of the functional provided. The choice of basis sets must be explicitly discussed including any deviation from standard basis sets. Convergence criteria, integration parameters, active space definition in multireference calculations, and, for open-shell systems, the way in which spin states are handled should be mentioned explicitly. The exact definition of any applied numerical or symmetry constraint should be indicated.

3. Details of the computational results. When relevant to the results of the study, data such as absolute energies, gross orbital populations, atomic spin densities, etc., should be supplied. Where feasible, critical checkpoint/restart files should be saved and made available upon request.

Cartesian Coordinates. Cartesian coordinates of all molecules, intermediates, transition states, etc. that are part of the manuscript must be uploaded in a single file that is formatted for convenient viewing with widely available molecular modeling packages. The .xyz and .mol formats are accepted at this time. The .xyz format is the most basic and easily prepared from computational output. More information on the .xyz file format is available at http://openbabel.sourceforge.net/wiki/XYZ.

The first line of the .xyz format file denotes the number of atoms in the molecule.

The second line of the file is a comments line, and should begin with a descriptive name of the molecule/structure consistent with the designation in the manuscript, and any other pertinent information selected by the author, such as total energy.

Next follow lines for each element in the molecule. Each line contains the element symbol followed by the x, y, and z coordinates in angstroms (Å) separated by spaces in free-field format (i.e. precise formatting not required).

Multiple structures are placed directly end-to-end in the file. The file name should have the extension ".xyz".

It is strongly recommended that authors view the structures in the file with a modeling program before uploading the file. The program Mercury (version 3.3 or later) is recommended for viewing and manipulating the multiple structures. The Cambridge Crystallographic Data Centre (CCDC) offers Mercury at no cost. Include the phrase "a text file of all computed molecule Cartesian coordinates in a format for convenient visualization" in the Supporting Information statement.

For additional guidance, see the ACS Simulations, Machine Learning, Computational Data guidelines.

Magnetic measurements

Fits of magnetic data such as (T), $^{-1}$(T), T(T), (T), M(H), etc., to an analytical expression must include both the Hamiltonian from which the analytical expression is derived and the final analytical expression and fitting parameters. When the value of an exchange coupling constant, J, is given in the abstract, the form of the Hamiltonian must also be included. The expressions may be included in the manuscript or, if long and complex, as Supporting Information; if the latter method is used, it should be noted as such in the "Supporting Information Available" paragraph at the end of the manuscript. In addition, how the sample was measured (in a gelatin capsule, Teflon capsule, etc.) and the diamagnetic correction for the sample holder, as well as the diamagnetic correction for the material, must be provided and the manner in which it was calculated (Pascal's constants) or measured stated.

NMR Spectra

Please follow the specific guidelines for presenting NMR spectroscopic data (as text and as spectra).

Primary NMR Data Files

Submission of primary NMR data files (FID files, acquisition data, processing parameters) is highly recommended. All original primary NMR data supporting a submission should be retained and provided if requested. For more information on packaging primary NMR data and metadata for submission, see the ACS Research Data Center.

When submitting FID files:

- One folder should be created for each compound
- Folder should be named clearly, using the compound number
- Include the FID files, acquisition data and processing parameters for each experiment
- Name each spectrum according to the type of nucleus measured: ^{1}H, ^{13}C, etc.
- NMR files should be compressed into zip file(s)

In a text document, include the name of the manufacturer of the spectrometer used to collect the data, the acquisition software and processing programs used to analyze the data, and the field strength used to measure each nucleus (i.e., 300 MHz ^{1}H or 50 MHz ^{13}C). Include a structure file that shows the structure and compound identifier for each provided dataset. MolFile is the recommended format and is strongly preferred.

Electrochemistry Data

For reporting Voltammetry and Amperometry measurements, and for reporting Bulk Electrolysis procedures, please see the ACS Electrochemistry Guidelines.

Biological Data

For reporting information on specimens, techniques, and data, please see the ACS Biological Data Guidelines.

Electrophoretic Gels and Blots

The practice of cropping raw gel data and inserting such cropped data into a single figure is discouraged, but it is permitted if it improves the clarity and conciseness of the presentation. In such cases, cropped blots should retain at least six band widths above and below the band of interest. The brightness and contrast should remain the same for the spliced images, and the spliced images with lanes that were non-adjacent in the gel must have a clear separation or a black line delineating the boundary between the gels. Any alteration of the images must be mentioned in the figure caption. Always have the original, unaltered files available for review upon request.

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Digital graphics pasted into manuscripts should have the following minimum resolutions:

- Black and white line art, 1200 dpi
- Grayscale art, 600 dpi
- Color art, 300 dpi

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Charts

Charts (groups of structures that do not show reactions) may have a brief caption describing their contents.

Tables

Each table must have a brief (one phrase or sentence) title that describes the contents. The title should be understandable without reference to the text. Details should be put in footnotes, not in the title. Tables should be used when the data cannot be presented clearly in the narrative, when many numbers must be presented, or when more meaningful inter-relationships can be conveyed by the tabular format. Tables should supplement, not duplicate, information presented in the text and figures. Tables should be simple and concise.

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