

See discussions, stats, and author profiles for this publication at: <https://www.researchgate.net/publication/231346153>

Oxygen atom transfer in the oxidations of dimethyl sulfide and dimethyl sulfoxide by bis(bipyridine)oxo(pyridine)ruthenium(2+)

ARTICLE *in* INORGANIC CHEMISTRY · MARCH 1987

Impact Factor: 4.76 · DOI: 10.1021/ic00252a029

CITATIONS

72

READS

11

4 AUTHORS, INCLUDING:



Lee Roecker

Northern Michigan University

35 PUBLICATIONS 715 CITATIONS

SEE PROFILE

Notice to Authors

(Revised May 2015)

Contents (click on the topic)

General Information – **Articles and Communications** – **Manuscript Preparation** – Table of Contents Synopsis and Graphic – Safety Notes – Nomenclature – Characterization of New Compounds – Footnotes – Citing by DOI – Tables – Graphics – Chemical Structures – Supporting Information – Revised Manuscripts – ACS Policies for E-prints and Reprints – **Structure Reports** – Crystal Structure Studies – Powder Diffraction Data – Corrections – **Computational Reports** – **Magnetic Measurements** – **NMR Spectra**

IMPORTANT MANUSCRIPT SUBMISSION REQUIREMENTS

1. The names of all coauthors of a manuscript must be entered into Paragon Plus upon submission.
2. If relevant, authors are required to (a) submit a CIF file (as SI for Publication), (b) check the quality of their CIFs through the checkCIF website, (c) upload the checkCIF output file (as a PDF, for reviewers' use only), and (d) address any high-level alerts.
3. Manuscripts in the form of Communications must be in the communications template and should not exceed three pages, plus TOC page as the fourth.
4. TOC graphic AND synopsis must be on a separate page at the end of the submitted manuscript file. Synopsis can contain up to 75 words.

General Information

Inorganic Chemistry publishes fundamental studies, both experimental and theoretical, in all phases of inorganic chemistry, including the related fields of catalysis, metalloprotein and bioinorganic chemistry, energy and photochemistry research, organometallic chemistry, and solid-state, materials, and nanoscale chemistry. Emphasis is placed on the synthesis, structure, thermodynamics, reactivity, spectroscopy, and bonding properties of significant new and known compounds.

Manuscripts should be submitted electronically via the ACS Paragon Plus Environment

(<http://paragonplus.acs.org/>). Authors must also submit revised manuscripts via this website. Manuscripts submitted as e-mail attachments will not be accepted. The ACS submission website employs security mechanisms to ensure the privacy of all electronically submitted manuscripts.

Templates are provided for the preparation of manuscripts; their use is required for communications and optional for articles. All Supporting Information including X-ray data, CIF, and cited preprints must be provided at the time of Web manuscript submission. **A table of contents graphic and synopsis must be included on the last page of the submitted manuscript.**

A properly completed and signed **Journal Publishing Agreement** must be submitted for each manuscript. ACS Paragon Plus provides an electronic version of the Agreement that will be available on the **My Authoring Activity** tab of the corresponding author's Home page once the manuscript has been assigned to an Editor. A PDF version of the Agreement is also available, but **authors are strongly encouraged to use the electronic Journal Publishing Agreement**. If the PDF version is used, **all pages of the signed PDF Agreement must be submitted**. If the corresponding author cannot or should not complete either the electronic or PDF version for any reason, another author should complete and sign the PDF version of the form. Forms and complete instructions are available at <http://pubs.acs.org/page/copyright/journals/index.html>.

The name of the author to whom inquiries regarding the paper may be addressed should be marked with an asterisk. Contributions must be original and must not have appeared elsewhere, except as a preliminary communication (preprints must accompany submission). Manuscripts accepted for publication in *Inorganic Chemistry* may not be republished elsewhere in any form. Only contributions in English will be considered.

The prime criteria utilized to judge the quality of contributions will be their originality, significance, and novelty. **Routine work and studies of narrow scope will not be published. Fragmentation of related work is unacceptable.** At the start of the review process, the Editor will determine whether the manuscript is suitable for assessment by external reviewers. Reasons for declining publication prior to external review may include, but are not restricted to, inappropriate subject matter, insufficient novelty or significance, or poor manuscript preparation. Once the paper is judged suitable for external review, the Editor will typically seek the advice of at least three reviewers. Authors must provide in their submission the names and e-mail addresses of at least four possible reviewers who are experts in the research area covered by the manuscript and have no professional connections with the authors. The Editor will also use reviewers of his or her own choice. The final decision to accept or reject a manuscript rests solely in the hands of the Editor.

If a substantial amount of material from the manuscript has been previously submitted to this or another journal, whether or not it was sent to reviewers, the author should include this information in the cover letter. The author should provide the name of the journal, the name of the handling Editor, a copy of the decision letter, copies of the reviews, and a detailed explanation of the revisions made in response to the reviewers' comments. The Editor may request the names of the original reviewers from the previous Editor if the manuscript was reviewed by another American Chemical Society journal. The Editor may accept the manuscript on the basis of the previous reviews, seek additional reviews, or reject the paper without further review.

Cover Letter. 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*.

Conflict of Interest Disclosure. A statement describing any financial conflicts of interest or lack thereof is published with each manuscript. During the submission process, the corresponding author must provide this statement on behalf of all authors of the manuscript. The statement should describe all potential sources of bias, including affiliations, funding sources, and financial

or management relationships, that may constitute conflicts of interest (please see the [ACS Ethical Guidelines](#)). The statement will be published in the final article. If no conflict of interest is declared, the following statement will be published in the article: “The authors declare no competing financial interest.”

Funding Sources. When submitting a manuscript to the Journal via ACS Paragon Plus, the submitting author is asked to identify the funding sources for the work presented in the manuscript. Identifying funding sources is optional during submission of an original manuscript. Funding source information is required when a revised manuscript is submitted.

Professional Ethics. In publishing only original research, ACS is committed to deterring plagiarism, including self-plagiarism. ACS Publications uses CrossCheck's iThenticate software to screen submitted manuscripts for similarity to published material. Note that your manuscript may be screened during the submission process. Further information about plagiarism can be found in Part B of the [Ethical Guidelines to Publication of Chemical Research](#).

Author List. During manuscript submission, the submitting author must provide contact information (full name, email address, institutional affiliation and mailing address) for all of the co-authors. Because all of the author names are automatically imported into the electronic Journal Publishing Agreement, the names must be entered into ACS Paragon Plus in the same sequence as they appear on the first page of the manuscript. (Note that co-authors are not required to register in ACS Paragon Plus.) The author who submits the manuscript for publication accepts the responsibility of notifying all co-authors that the manuscript is being submitted. Deletion of an author after the manuscript has been submitted requires a confirming letter to the Editor-in-Chief from the author whose name is being deleted. For more information on ethical responsibilities of authors, see the [Ethical Guidelines to Publication of Chemical Research](#).

Assistance with English Language Editing. Authors may want to have their manuscripts edited professionally before submission to improve clarity. The ACS ChemWorx English Editing Service can assist you in improving and polishing the language in your manuscript. You can learn more about the services offered, at <http://es.acschemworx.acs.org>.

Proofs. The corresponding author of an accepted manuscript will receive e-mail notification and complete instructions when page proofs are available for review via a secure website. Authors will access the secure site through ACS ChemWorx and will need an ACS ID. To obtain an ACS ID or to reset your password, go to www.acschemworx.org.

Patent Activities and Intellectual Property Issues. Authors are responsible for ensuring that all patent activities and intellectual property issues are satisfactorily resolved prior to first publication (ASAP or in issue). Acceptance and publication will not be delayed for pending or unresolved issues of this nature.

Articles ASAP. Accepted manuscripts will be published on the “Articles ASAP” page on the Journal website as soon as page proofs are corrected and all author concerns are resolved. Publication on the Web usually occurs within 1–4 working days of receipt of page proof corrections, and this can be anywhere from 2 to 11 weeks in advance of the cover date of the issue.

ORCID. All authors are encouraged to register for an ORCID iD, a unique researcher identifier. With this standard identifier, you can create a profile of your research activities to distinguish yourself from other researchers with similar names and make it easier for your colleagues to find your publications. Learn more at <http://www.orcid.org>.

Authors and reviewers can add their ORCID iD to, or register for an ORCID iD from, their account in ACS Paragon Plus. Submitting authors have the option to provide existing ORCID iDs for coauthors during submission, but they cannot create new ORCID iDs for coauthors.

Additions and Corrections. Additions and Corrections may be used to address important issues or correct errors and omissions of consequence that arise after publication of an article. Additions and Corrections may be requested by the author(s) or initiated by the Editor after discussions with the corresponding author. Readers who detect errors of consequence in the work of others should contact the corresponding author of that work. All Additions and Corrections are subject to approval by the Editor, and minor corrections and additions will not be published. Additions and Corrections from authors should be submitted via the ACS Paragon Plus environment by the corresponding author for publication in the “Addition/Correction” section of the Journal. The corresponding author should obtain approval from all of the article coauthors prior to submitting an Addition and Correction or provide evidence that such approval has been solicited. The Addition and Correction should include the original article title and author list, citation including DOI, and details of the correction. For proper formatting, see examples in a current issue of the Journal.

Retractions. Articles may be retracted for scientific or ethical reasons. Articles that contain seriously flawed or erroneous data such that their findings and conclusions cannot be relied upon may be retracted in order to correct the scientific record. Retractions may be requested by the article author(s) or by the journal Editor(s) but are ultimately published at the discretion of the Editor. When an article is retracted, a notice of Retraction will be published containing information about the original article title, author list, and the reason for the Retraction. Retracted articles will be accompanied by the related Retraction notice and will be marked as “Retracted”. The originally published article will remain on the web except in extraordinary circumstances (e.g., where deemed legally necessary or if the availability of the published content poses public health risks). The American Chemical Society follows guidance from the Committee on Publication Ethics (COPE) when considering retractions; for more information, see <http://publicationethics.org/>.

Articles and Communications

***Inorganic Chemistry* publishes Articles, Communications, invited Award Articles, Viewpoints, and Forums.** Articles represent complete studies and are not restricted in length. However, authors are urged to be as concise as possible and to place in Supporting Information material that, while of importance for practitioners in the same area, is of significantly less interest to the general reader.

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. Supporting Information with additional documentation is also 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. **Communications are restricted in length to the equivalent of three journal pages. This three-page limit will be strictly followed.** The ACS-provided template for a Communication can help authors to determine the manuscript length and *must be used for Web submission*.

In all 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. In Articles, experimental results should be presented clearly and carefully in a separate section, whereas in Communications, *complete* experimental work should appear in the Supporting Information. **The description of experimental work must be presented accurately and in sufficient detail to allow the work to be duplicated in other laboratories.**

Manuscript Preparation

General information on the preparation of manuscripts for ACS journals may be found in the *ACS Style Guide*, 3rd ed. (2006), available from Oxford University Press, Order Department, 201 Evans Road, Cary, NC 27513, or at <http://pubs.acs.org/books/styleguide>. Access the full text ACS Style Guide for free from the ACS ChemWorx Publishing Center (pc.acschemworx.acs.org). Manuscripts prepared with currently acceptable software packages will be used for production.

It is best to use the fonts “Times” and “Symbol”. Other fonts, particularly those that do not come bundled with the system software, may not translate properly. Ensure that all special characters (e.g., Greek characters, math symbols, etc.) are present in the body of the text as characters and not as graphic representations.

Tables may be created using a word processor’s text mode or, preferably, the table format feature. Ensure that each data entry is in its own table cell. If the text mode is used, separate columns with a single tab and use a line feed (return) at the end of each row.

Manuscripts of full Articles should include:

1. Title page
2. Abstract
3. Introduction
4. Experimental Section
5. Results
6. Discussion
7. Footnotes (including explanatory notes and literature references)
8. Tables
9. Schemes
10. Charts
11. Captions for Figures
12. Figures

13. Table of Contents Synopsis

14. Table of Contents Graphic

Tables, charts, figures, and schemes may be embedded in the manuscript where initially referenced and should be labeled with Arabic numerals.

The abstract of each manuscript should not exceed 300 words for an article and 150 words for a communication.

Table of Contents Synopsis and Graphic

For all categories of papers, authors must submit a TOC graphic and synopsis, carefully following these instructions:

- Label the graphic “For Table of Contents Only” and provide it on a separate page at the end of the submitted manuscript (not as Supporting Information).
- The graphic should be in the form of a structure, graph, drawing, photograph, or scheme—or a combination.
- Submit the graphic at the actual size to be used for the TOC so that it will fit in an area no larger than 3.25 inches by 1.75 inches (approx. 8.5 cm by 4.75 cm).
- Synopsis can contain up to 75 words.

For the greatest impact, authors must create an image that represents the work while adhering to size constraints. Keeping in mind that various devices may be involved, some of the best images are simple, are relatively free of text and technical characters, and make use of color for visual impact. It is best to stay away from complex structure schemes and small-sized details.

Safety Notes

Authors must emphasize any unexpected or new hazards encountered in the reported experimental work.

Perchlorate salts of metal complexes with organic ligands are potentially explosive. In general, when noncoordinating anions are required, every attempt should be made to substitute species such as the fluorosulfonates for the perchlorates. Authors must place a cautionary note regarding perchlorate complexes or other highly energetic materials known to be potentially hazardous and should reference pertinent documentation.

Nomenclature

It is the responsibility of the authors to provide correct nomenclature. All nomenclature must be consistent and unambiguous and should conform with current American usage. Insofar as possible, authors should use systematic names similar to those used by Chemical Abstracts Service (CAS), the International Union of Pure and Applied Chemistry (IUPAC), and the International Union of Biochemistry and Molecular Biology.

Chemical Abstracts nomenclature rules are described in Appendix IV of the *Chemical Abstracts Index Guide*. A list of ring systems, including names and numbering systems, is found in the

Ring Systems Handbook, American Chemical Society, Columbus, OH, 1993, and its latest cumulative supplement.

For CA nomenclature advice, consult the Manager of Nomenclature Services, Chemical Abstracts Service, P.O. Box 3012, Columbus, OH 43210-0012. A name generation service is available for a fee through CAS Client Services, 2540 Olentangy River Road, P.O. Box 3343, Columbus, OH 43210-0334. Telephone: (614) 447-3870. Fax: (614) 447-3747. E-mail: answers@cas.org.

Selected IUPAC recommendations can be found on the Web at <http://www.chem.qmw.ac.uk/iupac/iupac.html>. In addition, the ACS website has links to nomenclature recommendations at <http://chemistry.org>.

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.

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.

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.

Footnotes

References to the literature and all explanatory notes should be numbered in one consecutive series. Footnote numbers in the text should be entered as superscripts, and footnotes should be listed at the end of the text. Journal abbreviations must conform to those used in the *Chemical Abstracts Service Source Index*. The following formats for journals (1) and books (2) must be used:

(1) Doe, J. S.; Smith, J.; Roe, P. *J. Am. Chem. Soc.* **1968**, *90*, 8234–8241.

(2) Smith, A. B. *Textbook of Chemistry*; American Chemical Society: Washington, DC, 1972.

Multiple references, preferably related and identified by letters, may be given under a single citation number.

Citing by DOI

For work published online (ASAP) and work submitted for publication (e.g., submitted; in press), the DOI should be furnished in addition to the standard bibliographic information. Authors are given instructions for citing work by DOI in an email communication when

manuscript proofs are made available. A DOI is assigned to each manuscript and should be in the form <http://dx.doi.org/10.1021/ic000000a>. DOI is an accepted form of citation before and after the article appears in an issue.

It is the authors' responsibility to provide accurate references so that readers can easily retrieve cited articles.

Tables

Tables should be used only if they present information more effectively and more efficiently than running text. If possible, they should occupy a single journal column (8.5 cm). Column heads should be as small as possible. Columns should not contain only one or two entries, nor should the same entry be repeated numerous times.

Graphics

To facilitate the publication process, please submit manuscript graphics using the following guidelines:

1. The preferred submission procedure is to embed graphic files in a Word document. It may help to print the manuscript on a laser printer to ensure all artwork is clear and legible.
2. Additional acceptable file formats are TIFF, PDF, EPS (vector artwork), or CDX (ChemDraw file). If submitting individual graphic files, in addition to them being embedded in a Word document, ensure the files are named based on graphic function (i.e., Scheme 1, Figure 2, Chart 3), not the scientific name. Labeling of all figure parts should be present and the parts should be assembled into a single graphic. For EPS files, ensure that all fonts are converted to outlines or embedded in the graphic file; the document settings should be in RGB mode.
3. TIFF files (either embedded in a Word doc or submitted as individual files) should have the following resolution requirements:
 - Black & White line art: 1200 dpi
 - Grayscale art (a monochromatic image containing shades of gray): 600 dpi
 - Color art (RGB color mode): 300 dpi
 - The RGB and resolution requirements are essential for producing high-quality graphics within the published manuscript. Graphics submitted in CMYK or at lower resolutions may be used; however, the colors may not be consistent, and graphics of poor quality may not be able to be improved.

- Most graphic programs provide an option for changing the resolution when you are saving the image. Best practice is to save the graphic file at the final resolution and size using the program used to create the graphic.
4. Graphics should be sized at the final production size when possible. Single-column graphics are preferred and can be sized up to 240 points wide (3.33 in.). Double-column graphics must be sized between 300 and 504 points (4.167 in. and 7 in.). All graphics have a maximum depth of 660 points (9.167 in.) including the caption (please allow 12 pts for each line of caption text). Consistently sizing letters and labels in graphics throughout your manuscript will help ensure consistent graphic presentation for publication.

Chemical Structures

Structures should be produced with the use of a drawing program such as ChemDraw, ChemIntosh, and ChemWindows. Desired parameters for structure drawings may be found at <http://paragonplus.acs.org>.

Authors using other drawing packages should, insofar as possible, modify their program's parameters so that they reflect the above guidelines.

Supporting Information

Supporting Information such as extensive tables, graphs, spectra, detailed descriptions of experimental procedures, and calculations will be included in the Web edition of the journal and must accompany the manuscript for review purposes. A [list of acceptable file types](#) is available on the Web. *All Supporting Information files of the same type such as CIFs should be prepared as a single file (rather than submitting a series of files containing individual images or structures). For example, all Supporting Information available as PDF files should be contained in one PDF file.*

DO NOT UPLOAD FIGURES AND TABLES THAT ARE TO BE PUBLISHED IN THE ARTICLE INTO THE SUPPORTING INFORMATION FILE.

If the manuscript is accompanied by any supporting information for publication, a brief description of the supplementary material is required in the manuscript. The appropriate format is as follows:

Supporting Information. Brief statement in nonsentence format listing the contents of the material supplied as Supporting Information.

Referenced work that is in press or has been submitted for publication must be submitted as Supporting Information for review purposes only.

Revised Manuscripts

A manuscript returned to an author for revision must be returned to the Editor within the following timeline: minor revision of an Article, 30 days; major revision of an Article, 45 days;

minor revision of a Communication, 21 days; major revision of a Communication, 45 days. If a revised manuscript cannot be returned within the allotted time, the Editor should be contacted. Failure to do so will result in the inactivation of the manuscript. Authors should send a detailed reply to the comments of the reviewers and identify all changes. Revisions of inactivated manuscripts must be uploaded as new manuscripts via the ACS Paragon Plus Environment.

ACS Policies for E-prints and Reprints

Under the ACS Articles on Request policy, the Society will provide (free of charge) to all contributing authors a unique URL within the ACS website that they may e-mail to colleagues or post on external websites. These author-directed links are designed to facilitate distribution of an author's published work to interested colleagues. The ACS Articles on Request policy allows 50 downloads within the first year after web publication and unlimited access via the same author-directed links 12 months after web publication.

For paper reprints, when authors are sent the proof of their paper, they will receive a link to a website where they may order author reprints. They may also call Cierant Corporation at 866-305-0111 from 9AM to 5PM EST. Reprints will be shipped within 2 weeks after the issue publication date. Neither the Editors nor the Washington ACS Office keeps a supply of reprints; requests for single copies of papers should be addressed to the corresponding author of the paper concerned.

ACS AuthorChoice Open Access

[ACS AuthorChoice](#) options establish fee-based mechanisms for authors or their research funding agencies to sponsor the open availability of final published articles on the Web. ACS *AuthorChoice* offers authors a wide range of open access license options, such as Creative Commons licenses and provisions for immediate or 12-month embargoed open access, and includes [ACS Certified Deposit](#). Authors will find useful information about compliance with open access policies available [here](#) and FAQs [here](#). Corresponding authors who published with ACS during 2014 may have access to [ACS Author Rewards](#), a \$60M stimulus program ACS provided to help authors transition to new open access publishing models.

Authors must sign the Journals Publishing Agreement. Forms and complete instructions are available [here](#). After acceptance, authors will be presented with the opportunity to purchase an *ACS AuthorChoice* option, and authors who do so will be presented with the appropriate license at that time. For a review of all license options available, see [here](#). For questions or further assistance with *ACS AuthorChoice*, please reach out to support@services.acs.org.

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 (http://pubs.acs.org/userimages/ContentEditor/1223613982745/inocaj_checklist.pdf) and any editorial office. 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 *printed* 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 must be present for the print version of the manuscript. In addition, important bond lengths and angles (with esd's) should be supplied in tabular form for the printed text. *Inorganic Chemistry* does not publish refined positional parameters in the printed text except in cases where such information is essential to the clarity of the manuscript. However, **complete sets of refined positional coordinates as well as anisotropic thermal parameters and complete tabulations of bond lengths and angles are required in the Supporting Information. Authors must provide this information at the time of manuscript submission using the crystallographic information file (CIF) format** (see part d below).

(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. Supplementary X-ray data submitted in CIF format will appear in the Supporting Information section of the manuscript. The CIF when prepared with a standard set of crystallographic analysis programs will include the following: complete information on collection of data and refinement of the structure; final values of all refined atomic coordinates (with esd's) including all calculated atomic coordinates (especially calculated positions for hydrogen atoms and positions of atoms calculated from refinement of rigid groups); all anisotropic thermal parameters, which should be provided as U_{ij} 's or B_{ij} 's rather than β_{ij} 's; and all bond lengths and angles. Common problems found with CIFs include incorrect absorption correction, space group, and crystal size information. The CIF should be examined and corrected by authors prior to submission. Authors are **required** to check the quality of their CIFs through the checkCIF website of the International Union of Crystallography (<http://checkcif.iucr.org>), to

upload the checkCIF output file (in PDF format, for reviewers' use only) upon submission, and to address any high-level alerts. In addition to the crystallographic data supplied in the CIF, other information such as least-squares planes and atomic deviations therefrom; closest intermolecular contacts including, if relevant, 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 text enumerating the contents of the Supporting Information.

Authors are required to provide crystallographic data in the crystallographic information file (CIF) format at the time of manuscript submission. Details on the preparation, validation, and submission of this material are available from the Journal's website (<http://pubs.acs.org/page/inocaj/submission/cif.html>). Reviewers will have access via the Web to an electronic copy of the CIF associated with a manuscript. After review and acceptance, the CIF will become part of the general Supporting Information and will be available free of charge at <http://pubs.acs.org>. Structure factor tables are no longer required for deposit *but may be requested by the Editor to assist reviewers*.

Inorganic Chemistry discourages the submission of crystallographic Supporting Information in a format other than CIF. If, however, a CIF is not readily available for a structure under review, copies of Supporting Information in tabular form must be submitted along with the manuscript.

Authors are encouraged to submit their crystallographic data to the Cambridge Structural Database and indicate the CCDC Deposition Number if known. Authors may also consider depositing structural information in the Crystallography Open Database, which desires open access to all structural reports. Regardless, CIF files submitted to *Inorganic Chemistry* will continue to reside in the Supporting Information on the ACS Publications website.

(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 paper 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. All other information that would be included in a structure report should be provided in the Supporting Information, deposited as a CIF.

(B) Powder Diffraction Data

The presentation of X-ray powder diffraction data for new materials or for materials previously uncharacterized by this technique is encouraged. Data from X-ray powder measurements should be accompanied by details of the experimental technique: source of X-rays, the radiation, its wavelength, filters or monochromators, camera diameter, the type of X-ray recording, and the technique for measuring intensities. In cases of unindexed listing of the data, the d spacings of all observed lines should be listed in sequence, together with their relative intensities. In cases where filtered radiation is used, every effort should be made to identify residual β lines. Where resolution into α_{1-2} doublets occurs, the identification of the d spacing for each line as da_1 , da_2 , etc., gives a measure of the quality of the diffraction pattern. When an indexing of the data is offered, the observed and calculated $1/d^2$ values should be listed along with the observed relative

intensities (it is superfluous to give d spacings in this instance). All calculated $1/d^2$ values should be listed (exclusive of systematic absences), to the limit of the data quoted. If possible, the crystal system should be specified. Possible space groups may also be listed if the data warrant it. Relevant information about the specimen used should be included.

(C) 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.**

Comparison of methods, studies of various levels of theory, basis set effects, etc., are considered to be technically oriented computational papers and are not encouraged. In addition, studies simply confirming results already present in the literature 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:

- a. Description of specific programs and the release or version. If the author's own or a modified version of a commercially available program is used, it is encouraged that the program/code/modification be made available to the scientific community (QCPE, publication in a computational journal, commercially, etc.), if the license permits. 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.
- b. Details of the calculations including input coordinates along with input keywords. 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.
- c. Certain data of the output files such as absolute energies, gross orbital populations, atomic spin densities, etc. Where feasible, critical checkpoint/restart files should be saved and made available upon request. If the paper discusses a reaction mechanism in terms of its potential energy surface, optimized molecular structures should be

provided in Cartesian atomic coordinates for each calculated molecule, intermediate, transition state, etc., as separate plain-text files in standard .xyz file format. More information about the .xyz file format is available at <http://openbabel.sourceforge.net/wiki/XYZ>.

Magnetic Measurements

Fits of magnetic data such as $\chi(T)$, $\chi^{-1}(T)$, $\chi T(T)$, $\mu(T)$, $M(H)$, 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) at <http://pubs.acs.org/page/4authors/tools/index.html>.