Instructions to Authors

Editorial Policies

X-ray Structure Analysis Online is an international journal published monthly by The Japan Society for Analytical Chemistry (JSAC), which appears only at the JSAC website. The journal presents unpublished X-ray structure data and structural discussion from academic and industrial research laboratories to make this information available to the public to be used in various fields, including analytical sciences, pharmacology, theoretical chemistry, etc. All classes of compounds will be accepted: organic, organometallic, inorganic compounds and metal complexes. We hope that this journal will be successful through receiving strong response from the society members.

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(1) Manuscripts should be submitted by e-mail or by conventional mail, but will not be accepted by fax. E-mail submission is strongly preferred. Please select a single method for submission. For e-mail submission, a single electronic file of all the manuscript materials (including text, figures and tables) should be prepared in Adobe PDF file. A cover letter should be sent as a separate file.

Manuscripts should consist of a text, references, tables and figures all contained within 2 printed pages; moreover, a CIF format file must be attached to the manuscripts, which should contain necessary information for refereeing. Also, the CIF format file will be treated as Supporting Information of the article. It should be sent as a separate attached file in e-mail submission or as a diskette in normal mail submission.

Before submission, the CIF format file should be carefully checked and deposited to the CCDC (organic, metal-organic; http://www.ccdc.cam.ac.uk/) or the FIZ-Karlsruhe (inorganic; http://www.fiz-karlsruhe.de/) as a Pre-Publication deposition. The deposition number should be listed in Table 1.

An acknowledgment of paper receipt will be made to the corresponding author *via* e-mail. In the case that the author does not receive it within 10 days after submission, please contact the Editorial Office *via* e-mail or fax as soon as convenient.

(2) Page charge of 150USD or 15000JPY for a two-page article is requested. This charge does not cover any reprint offer. As for the reprints, please contact the editorial office.

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(4) A cover letter should specify the following information:

The reason why the authors think their work should be published in *X-ray Structure Analysis Online*.
The title of the article.
The name, affiliation, postal address, e-mail address, telephone number, and fax number for the corresponding author.

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Preparation of Manuscripts

(1) The manuscript materials (title, abstract, text, references, tables, figures, and captions) must be written in English, double-spaced, on A4 or 8 1/2 × 11 page size with ample margins. All of the pages should be consecutively numbered starting with the title page. The recommended fonts used are Times or Times New Roman and Symbol, and the font size should be 11 point. Do not use non-English fonts, otherwise the PDF files cannot be reproduced perfectly. For the authors' convenience, a template can be downloaded from *X-ray Structure Analysis Online* website.

(2) The title page should contain the title of the article, the names, affiliations, and addresses of all the authors. The title should be informative enough to make the content readily understandable. Avoid unnecessary use of vague expression, such as "novel" and "new". Also avoid use of abbreviations of analytical methods and chemicals.

(3) The abstract should be self-contained, describing what was done and concluded. The length should be less than 80 words.

(4) The text should contain the purpose of the study, preparative method of sample, experimental condition such as temperature, polymorphism, main results, disorder, absolute configuration, and treatment of hydrogen atoms. The routine crystallographic experimental data and other analytical data such as IR, NMR can be included in the Supporting Information and omitted from the text.

(5) Tables and figures should include:

Table 1 Crystal and experimental data
Table 2 Selected bond distances and angles
Table 3 Other values of interest
Fig. 1 Chemical structure drawing
Fig. 2 Tertiary structure with an ORTEP-style drawing and atom-labeling scheme

Table 1 Crystal and experimental data

Chemical formula: $C_{60}H_{62}Mn_2N_8O_8$	
Formula weight = 1452.70	
T = 293 K	
Crystal system: triclinic	Space group: $P\bar{1}$
a = 10.269(1)Å	α = 111.821(1)°
b = 10.994(1)Å	β = 93.270(1)°
c = 14.136(2)Å	γ = 91.562(1)°
V = 1477.2(2)Å^3	Z = 1
D_x = 1.631g/cm^3	D_m (floatation) = 1.62 g/cm^3
Radiation: Mo K_α (λ = 0.71073 Å)	
μ(Mo K_α) = 3.194 mm^{-1}	F(000) = 732
Crystal size = 0.25 × 0.08 × 0.07 mm^3	
No. of reflections collected = 9156	
No. of independent reflections = 6542	
θ range for data collection: 1.56 to 30.00°	
Data/Restraints/Parameters = 6542/0/370	
Goodness-of-fit on F^2 = 1.100	
R indices [$I > 2\sigma(I)$]: $R1$ = 0.0447, $wR2$ = 0.0640	
R indices (all data): $R1$ = 0.1128, $wR2$ = 0.1640	
$(\Delta/\sigma)_{max}$ = 0.001	
$(\Delta\rho)_{max}$ = –0.38 eÅ^{-3}	$(\Delta\rho)_{min}$ = –0.21 eÅ^{-3}
Measurement: Bruker SMART CCD	
Programs system: SHELXTL-97, SADABS	
Structure determination: SHELXS-97	
CCDC deposition number: *nnnnnn*	

The authors should prepare Table 1 according to the format shown below, although D_m is optional.

"Measurement" indicates the name of diffractometer. "Program system" indicates the name of software for X-ray analysis, including any private package. "Structure determination" indicates the heavy atom method, direct method, Patterson method, or names of well-known programs.

Figure 1 should be a chemical structure, not an ORTEP drawing. For the molecular or crystal structure drawings, authors are encouraged to present color figures that require no additional expense.

Tables 2 and 3 may not be printed if space is not available. The authors are encouraged to utilize the Supporting Information to include additional tables and figures for readers.

(6) References must be numbered consecutively in the order that they are cited in the text and designated by a superscript. A list should be included on separate double-spaced pages at the end of the text. The number of references should usually be less than 10. The references for crystallographic software are not included in this number. For the proper abbreviations of the journal titles, refer to "Chemical Abstracts". Examples are shown below.

Journals

1. M. Harada, M. Shibata, T. Kitamori, and T. Sawada, *Anal. Sci*., **1999**, *15*, 647.
2. Y. Yoshikawa, P. S. Dahr, and H. Yamatera, *Chem. Lett*., **1984**, 841.
3. H. Nakamura and Z. Tamura, *Bunseki Kagaku*, **1988**, *37*, 35.
4. T. Buehrer, P. Gehrig, and W. Simon, *X-ray Struct. Anal. Online*, in press.

Books.

5. A. J. Bard and L. R. Faulkner, "*Electrochemical Methods: Fundamentals and Applications*", **1980**, John Wiley and Sons, New York, Chichester, Brisbane, Toronto.
6. R. S. Houk, H. J. Svec, and V. A. Fassel, "*Dynamic Mass Spectrometry*", ed. D. Price and J. F. J. Todd, **1981**, Vol. 6, Chap. 19, Heyden, London, 234.

Supporting Information

Extensive tables, figures, and other materials (including high-resolution color photographs, crystallographic drawings, *etc*.) may be included in the Web edition as Supporting Information (SI). The SI can be accessed separately on the Web by readers. At the time the manuscript is first submitted, the authors should provide the SI as a single PDF file. The total size of the files should not exceed 2 MB. A statement of the availability of SI should appear in the text before the references section as Supporting Information: (Describe concisely what is in the material). This material is available free of charge on the Web at http://www.jsac.or.jp/xraystruct/. Figures, tables, equations, *etc*. provided in SI should be labeled as Fig. S1, Table S2, Eq. (S3), *etc*., and should be cited in the text as "Fig. S1 (Supporting Information)" or "Tables S2−S4 (Supporting Information)".

Accepted Manuscripts

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