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### 13. Table of Contents Synopsis

### 14. Table of Contents Graphic

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#### **(A) Crystal Structure Studies**

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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).

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### (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>.