Tantalum−Gold and Tantalum−Copper Trihydride Complexes [Cp‘ 2 TaH 3 MPPh 3][PF 6] (Cp‘ = C 5 H 4 C(CH 3) 3). Structure Determination from 1 H T 1 Relaxation Studies

ARTICLE *in* INORGANIC CHEMISTRY · MARCH 1999

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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

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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.

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13. Table of Contents Synopsis
14. Table of Contents Graphic

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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.

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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.*

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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.

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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 $d\alpha_1$, $d\alpha_2$, 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.

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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:

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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.