

Thoughts on Scientific Writing

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Outline

0 Background on scientific publication

0 Writing guidance

0 Collaborative writing

0 The editorial process

Why do we write scientific papers?

0 Extrinsic reasons

- 0 Contribute to the body of scientific knowledge and thought
- 0 Document results in a reproducible way
- 0 Promotes one's reputation in a field

0 Intrinsic reasons

- 0 Forces one to organize thoughts
- 0 Breaks research into finite chunks
- 0 Vets our work with the community

How is scientific publishing changing?

0 In the “old” days (1999)

- 0 32 American Chemical Society journals
- 0 Published 19,582 articles
- 0 90 Journals classified as “physical chemistry”

0 Today (2012)

- 0 46 American Chemical Society journals
- 0 Published 38,536 articles – double!
- 0 135 Journals classified as “physical chemistry”

0 *J. Phys. Chem. C* published more articles in 2012 than all of *J. Phys. Chem.* did in 1999

Source: Web of Science

Where do you find such exciting information?

0 <http://admin-apps.webofknowledge.com.proxy.library.nd.edu/JCR/JCR?PointOfEntry=Home&SID=1BNkQHVGQZMqQGLtH6x>

Publication 1989

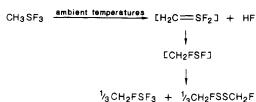
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Inorg. Chem. 1989, 28, 3292-3296

distinction has already been partially eliminated in a C_{2v} molecule like SF_4 or $(\text{CF}_3)_2\text{S}^+$ (with $2a_1 + b_1 + b_2$ σ -type 1-electron bonding MO's, where the a_1 orbitals span both axial and equatorial ligands), and relaxed still further in a C_s molecule like CF_3SF_3 (with $3a' + a''$ σ -type bonding MO's, where the a' orbitals span both axial and equatorial ligands).

We are unsure of the significance to be attached to the C–H bond length in CH_2SF_2 , which, according to our analysis of the electron-diffraction pattern, is 4.5 pm longer than the corresponding distance in other methyl-sulfur compounds, e.g. CH_3SH ,^{37a} CH_2SSCH_3 ,^{37c} and $(\text{CH}_3)_2\text{S}$.³⁹ Such an attenuation is anticipated neither by our ab initio calculations nor by the vibrational properties displayed by the CH_2SF_2 molecule¹¹ that parallel quite closely those of CH_3SH ,⁴⁰ at least with respect to the vibrations localized mainly within the CH_3 group. Moreover, there is no echo of anything similar in the dimensions of the CF_3 group as it occurs in the molecules CF_3SF_2 and CF_3SX ($\text{X} = \text{F}, \text{Cl}, \text{Br}$, etc.).³⁹ Otherwise, it would be tempting to link a weak C–H bond in CH_2SF_2 to the facility of HF elimination in accordance with the following scheme:^{11,41}

- (39) Typke, V. Z. *Naturforsch.*, A 1978, 33, 842.
 (40) May, I. W.; Pace, E. L. *Spectrochim. Acta, Part A* 1968, 24A, 1605.
 Barnes, A. J.; Hallam, H. E.; Howells, J. D. R. *J. Chem. Soc., Faraday Trans. 2* 1972, 68, 737.



With the dimethyl derivative $(CH_3)_2SF_2$, the susceptibility to HF elimination is such that the compound cannot be vaporized without decomposition.^{11,42}

Acknowledgment. We thank the SERC for the award of a research studentship (to G.S.M.), for financial support of the Edinburgh Electron-Diffraction Service, and for provision of the microdensitometer facilities. We are grateful also to Professor Dr. mult., A. Braat for the provision of a sample of Cf₂SiCl₄ and to Dr. J. C. Bradbury for assistance with the gas-phase measurements at Cf₂SiCl₄. The computational portion of the work was supported by a grant from the Robert A. Welch Foundation. Computing resources for computation with the GAUSSIAN-93 program were provided by the University of Texas System Center for High Performance Computing.

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Electronic Structure of Asymmetric Metal-Metal Multiple Bonds: The d²-d⁶ Complexes X₄Mo-Mo(PH₃)₄ (X = OH, Cl)

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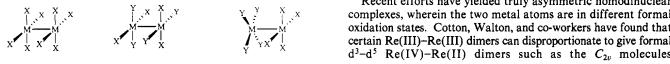
Received November 29, 1988

The electronic structure of complex organic molecules

distribution is investigated with the SCF-X_n-SW method. Such systems are known for mixed phosphine-alkoxide ligand systems. Strong δ -donor ligands such as the alkoxides inhibit the formation of a polar σ bond between the two metal centers and lead to a sterically induced staggered ligand conformation. These complexes contain a formal Mo-Mo triple bond. Weaker σ -donor ligands such as halides permit the δ charge transfer to occur and should lead to a stable, eclipsed ligand conformation with a net Mo-Mo quadruple bond. Comparisons are made to the electronic structure of more conventional Mo(I)₂-Mo(II) dimers, particularly those with bidentate phosphorus ligands and with a twisted ligand conformation about the dimeric unit.

The majority of complexes that contain multiple metal–metal bonds are homodinuclear molecules with symmetry-equivalent metal atoms. With reference to quadruple metal–metal bonds, the best studied systems are the d^4-d^4 dimers of Mo(II) or Ra(III).² The electronic structure of these d^4-d^4 complexes is fairly well understood in terms of the “usual” quadrupole-bond description: one σ metal–metal bond, two π metal–metal bonds, and one δ metal–metal bond, each of which is symmetrically disposed between the two metal atoms.

Most complexes with d^4-d^4 quadruple bonds conform to two common coordination geometries, namely M_2X_8 systems with D_{4h} symmetry (1) or $M_2X_4Y_4$ complexes that are D_{2d} (2). The



eclipsed orientation of the ligands on each metal center, even when it would appear to be sterically unfavorable, is, of course, attributed

- (1) Camille and Henry Dreyfus Teacher-Scholar (1984-1989).
 (2) Cotton, F. A.; Walton, R. A. *Multiple Bonds Between Metal Atoms*; Wiley: New York, 1982.

0020-1669/89/1328-2202\$01.50/0

to the presence of the δ bond, which is sensitive to variations in the rotational angle between the two metal fragments. The eclipsed orientation maximizes the δ interaction and the metal–metal bonding.

The symmetry equivalence of the two metal centers is removed in the heterodinuclear complexes that are based on $\text{Cr}(\text{II})\text{-Mo}(\text{II})$ or $\text{Mo}(\text{II})\text{-W}(\text{II})$ dinuclear fragments.³ These lower symmetry systems do not demonstrate any significant chemical or spectroscopic differences from the homodinuclear ones, however; apparently the differences between the two metal centers are not great enough to induce a sizably different electronic structure, and they are best considered as "slightly polarized" $d^4\text{-}d^4$ systems.

Recent efforts have yielded truly asymmetric homodinuclear complexes, wherein the two metal atoms are in different formal oxidation states. Cotton, Walton, and co-workers have found that certain $\text{Re}(\text{III})\text{-Re}(\text{III})$ dimers can disproportionate to give formal $d_3^2\text{-}d_5^3$ $\text{Re}(\text{V})\text{-Re}(\text{III})$ dimers such as the C_2 -molecules

¹ See also the discussion of the relationship between the two in the section on the "Economic Crisis."

- 0 Written in WordPerfect
- 0 Printed out multiple hard copies

0 Mailed to the Journal office

0 Mailed to reviewers

0 Ultimately printed in
thick journals

0 Kept on a dusty shelf

Publication 2015

- 0 Process entirely electronic
 - 0 Writing
 - 0 Submitting
 - 0 Reviewing
 - 0 Publishing
- 0 Much easier and faster to create today
- 0 Plus...many more people doing it!

- 0 Much harder to get heard above the noise

Publication 2015

0 Emergence of “social networking” in publication

- 0 LinkedIn
- 0 ResearchGate
- 0 Orcid
- 0 Google Scholar
- 0 CiteULike
- 0 ...

0 Someday, Facebook-like comments on all papers

Writing 2015

- 0 To be heard above the noise papers must:
- 0 Have a clear, specific, interesting message
 - 0 Discernable from the title onward
- 0 Be placed in the proper context of the field
 - 0 Reference work that connects to the right literature
- 0 Be easily digestible

General thoughts on scientific writing

0 Be honest

- 0 Take responsibility for anything you co-author
- 0 Your scientific reputation is precious

0 Tell a compelling story

- 0 Research seldom unfolds the way we expect
- 0 The story that makes the most sense is not necessarily the story as it really happened

Good resource from a master

0 <http://doi.wiley.com/10.1002/adma.200400767>

General thoughts on scientific writing

0 Writing is part of the scientific process

0 Start outlining early in a project

- 0 I often do this in the form of a presentation
- 0 Ponder in the shower

0 Expect the outline to evolve

- 0 Understanding evolves, gaps emerge
- 0 New hypotheses
- 0 New literature appears

Initial Organization

0 Results

- 0 Compile the figures, graphs, tables of what you did
- 0 Paper will be written around these.
- 0 Need to be **complete, self-contained**, and clear to your audience.

0 Key insights/conclusions

- 0 What message do you want your readers to get?

0 Introduction

- 0 What questions did you set out to answer?
- 0 Why? What's the context?
- 0 What's the relevant literature?

Full organization

- 0 **Title** – Descriptive, concise, promotes your work
- 0 **Abstract** - write last. Self-contained summary.
- 0 **Introduction**
 - 0 Context of your work, relevant literature
 - 0 End with, “In this work, we show...”
- 0 **Methods**
 - 0 Technical details of the work
- 0 **Results**
 - 0 Organize around Figures and Tables.
 - 0 Follow logical progression of ideas
 - 0 Distinguish Results from Inference.
- 0 **Discussion**
 - 0 Analysis and, interpretation of results, compare/contrast to literature
- 0 **Conclusions**
 - 0 Not a summary! What are main insights and implications of this work?

Writing tips

0 Be **precise**. Say exactly what you mean in words understandable to the readership.

0 Be **concise**.

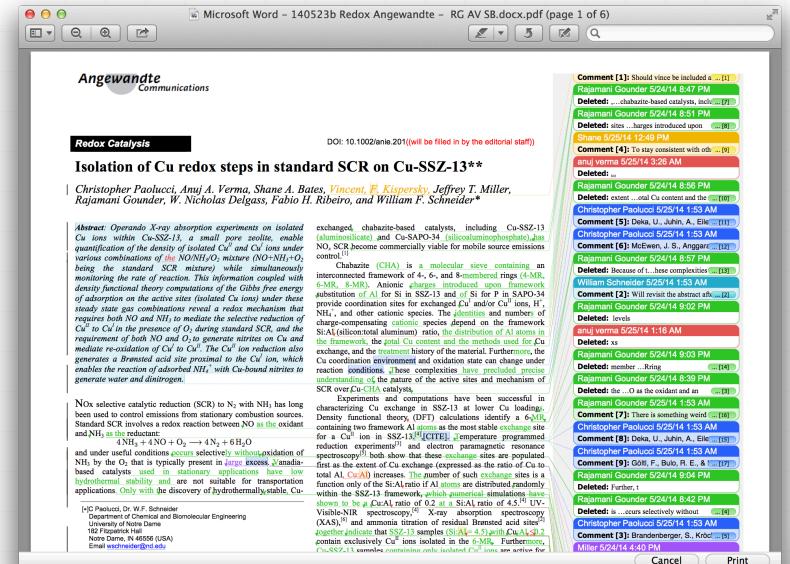
- 0 If you can find ways to remove extra explanatory words while retaining the same identical meaning, then do so.
- 0 Make each point in as few words as possible.
- 0 Do not repeat yourself!
- 0 And don't be repetitious!

0 Use the **active voice**.

0 See <https://owl.english.purdue.edu/owl/>

Collaborative Writing

- 0 Nearly all scientific papers have multiple authors
 - 0 People earn authorship in various ways
- 0 Author order convention varies by community
 - 0 starts with the people who did most of the work
 - 0 ends with the most senior authors, usually brought the \$\$
- 0 Take ownership!
- 0 Will invariably involve iteration
 - 0 Software
 - 0 File sharing
 - 0 Version control
 - 0 Editing and responses



“Office” style software

0 Microsoft Word and similar

- 0 Full featured
- 0 WYSIWIG
- 0 Low barrier to entry
- 0 Very common but closed format
- 0 Least friendly to collaborative writing

0 File sharing

- 0 E-mail or shared folder

0 Editing

- 0 One at a time
- 0 Internal “track changes” and “comments” tools

0 Version control

- 0 Rename files, e.g. with dates 140715-greatpieceofwriting.docx

“Mark up” style software

0 LaTeX and similar

- 0 Plain text file with formatting codes
- 0 Encourages structured writing
- 0 Simplifies, standardizes formatting
- 0 Have to be “compiled”
- 0 High barrier to entry – frustrating

0 File sharing

- 0 Email or shared folder
- 0 Version control repository

0 Editing

- 0 One at a time

0 Version control

- 0 Rename files
- 0 Check-in, check-out

“Cloud” software

- 0 Google Docs, ShareLatex, and similar
 - 0 Browser-based and “free”
 - 0 Very low barrier to entry
 - 0 Least full featured of the bunch
 - 0 References, figures, tables
 - 0 Not (yet) widely accepted
- 0 File sharing
 - 0 One version shared with all
- 0 Editing
 - 0 Many at once
- 0 Version control
 - 0 Automatically keeps track of previous versions and who made changes
 - 0 Infinitely reversible

How to write collaboratively

- 0 Take ownership!
- 0 Look for the meaning in every comment
- 0 Respond constructively to every comment
- 0 Make it easy for your co-authors to remember the old comments and to see your answers

The Publishing Process

0 Choose your target Journal wisely

- 0 Relevant to your work
- 0 Correct format
- 0 Impact factor!?!?

0 Carefully follow all the directions for preparing a manuscript

- 0 Manuscript style, length
- 0 Abstract
- 0 Supplementary material
- 0 TOC material
- 0 Key words
- 0 Cover letter to editor

The view from the editor's office

0 Manuscript received by office and initially triaged

- 0 Does submission have all the required pieces?

- 0 Are the authors all fully identified?

0 Assigned to an editor

- 0 *JPC* has 1 Editor-in-Chief, 3 Deputy Editors, and 25 Senior Editors

0 My editorial dashboard

The Cover Letter

- 0 Who are you?
- 0 Why is your work significant?
- 0 Why is it relevant to this *Journal*?
- 0 Who is qualified to review this work?

A good example

0 Cover_letter-43.pdf

Bad examples

0 Cover_letter-45.pdf

0 Cover_letter-44.pdf

Suggested reviewers

- 0 Very important to suggest reviewers who are competent to evaluate the work
- 0 Are not your colleagues
- 0 Published on similar topics, preferably in the Journal you are submitting to
- 0 Are not the “usual suspects”
- 0 Suggest more than you are required to. Give the editor options!

A Good Review

0 Is written with an eye to helping the authors present their material better

0 Concisely summarizes the content

0 Identifies the

Ask your advisor to let you review papers
Practice by reviewing your own group's/friends papers

0 Recommends an action to the editor

BTA-Major

0 Opportunity to improve the content of a manuscript

0 Every comment indicates that something was not clear to a reviewer

0 Response letter

- 0 Is respectful of the editor and reviewers
- 0 Reproduces every comment from every reviewer
- 0 Responds to every comment
- 0 Identifies what exactly was modified in the text in response to the comment

Publication

- 0 Iterate with editor/reviewer to convergence
- 0 or, submit elsewhere.
 - 0 Perhaps 50% of papers submitted to *JPC* ultimately appear in the journal
- 0 ASAP
- 0 Proofs
- 0 On-line!
- 0 Hard copy?

Conclusions

- 0 Very satisfying to do great research
- 0 Much more satisfying to have that research preserved in a publication
- 0 What else in life persists with your name on it forever?
- 0 Be patient. Good research takes time. Good writing takes time. Do them together.