

Part II, Chapters 2.11-13, App. D ACS Style Guide, Chapter 14

References & Bibliography

Formats of Reference Sections and Citation of Reference in Text

*Let's start by
looking at some
Examples!*

Type(s) of Reference Sections

- Footnotes
- Endnotes
- Footnotes and Endnotes

Types of Items Cited

- Journals
- Books (several types)
- Online Resources (sites, databases)
- Software

Citing Reference in Text

- [1] By superscript numbers, which appear outside the punctuation.

Oscillations in the Belousov-Zhabotinski reaction were reported previously.⁵

- [2] By italic numbers in parentheses on the line of text and inside the punctuation.

Oscillations in the Belousov-Zhabotinski reaction were reported previously (*5*).

- [3] By author name and year of publication in parentheses inside the punctuation.

The primary structure of this enzyme has also been determined (Finnigan et al., 2004).

Citation Style Depends on Journal

Type 1 Journals

Journal of the American Chemical Society, *J. Am. Chem. Soc.*, 1

The Journal of Organic Chemistry, *J. Org. Chem.*, 1

Crystal Growth & Design, *Cryst. Growth Des.*, 1

Type 2 Journals

Biochemistry, *Biochemistry*, 2

Chemical Research in Toxicology, *Chem. Res. Tox.*, 2

Type 3 Journals

Assessment and Evaluation in Higher Education, *Assess. Eval. Higher Educ.*, 3

Citing One or More Author(s)

1 Author: The primary structure of this enzyme has also been determined (Finnigan, 2004).

2 Authors: The primary structure of this enzyme has also been determined (Finnigan and Bird, 2004).

3 or More Authors: The primary structure of this enzyme has also been determined (Finnigan et al., 2004).

Thesaurus

Legend: █ Synonyms █ Related Words █ Antonyms

Adv. 1. **et al.** - and others ('et al.' is used as an abbreviation of 'et alii' (masculine plural) or 'et aliae' (feminine plural) or 'et alia' (neuter plural) when referring to a number of people); "the data reported by Smith et al."

█ [et al.](#), [et alia](#), [et aliae](#), [et alii](#)

2. **et al.** - and elsewhere (used when referring to other occurrences in a text)

█ [et alibi](#), [et al](#)

Based on WordNet 3.0, Farlex clipart collection. © 2003-2008 Princeton University, Farlex Inc.

Citing Author(s) in Text

1 Author: The primary structure of this enzyme has also been determined by Finnigan (2004).

2 Authors: The primary structure of this enzyme has also been determined by Finnigan and Bird (2004).

3 or More Authors: The primary structure of this enzyme has also been determined by Finnigan et al. (2004).

Citing References in Text

[1] By superscript numbers: Oscillations in the Belousov-Zhabotinski reaction were reported previously.^{5-7,11}

[2] By italic numbers in parentheses on the line of text: Oscillations in the Belousov-Zhabotinski reaction were reported previously (*5-7, 11*).

[3] By author name and year of publication in parentheses: The primary structure of this enzyme has also been determined (Finnigan et al., 2004; Gerson et al., 2005).

Multiple Citation to Same Group

[1] By superscript numbers: No problem.

[2] By italic numbers in parentheses on the line of text: No problem.

[3] By author name and year of publication in parentheses: Add a, b, c... to year.

The primary structure of this enzyme has also been determined Finnigan **et al.** (2004**a**; 2004**b**).

The primary structure of this enzyme has also been determined Finnigan **and coworkers** (2004**a**; 2004**b**).

Logical Placement of Citation

Aspirin has been synthesized from oil of wintergreen (5) and by carboxylation of sodium phenoxide (6).

Aspirin has been synthesized from oil of wintergreen and by carboxylation of sodium phenoxide (5, 6).

Type 1 Example

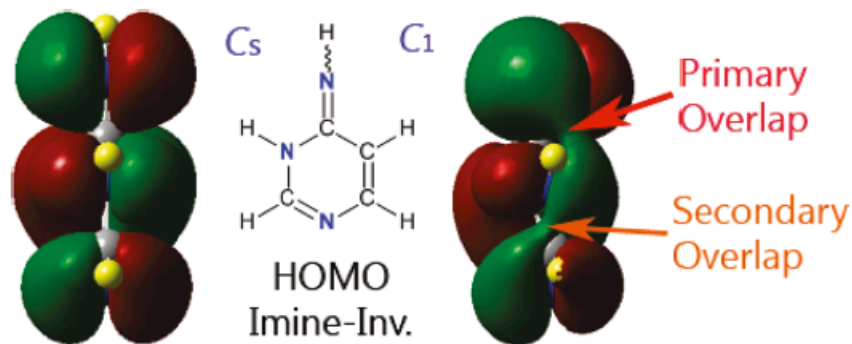
Asymmetry in the *N*-Inversion of Heteroarene Imines: Pyrimidin-4(3*H*)-Imine, Pyridin-2(1*H*)-Imine, and 1*H*-Purine-6(9*H*)-Imine

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Smets and Meas studied 4-aminopyrimidine in argon matrices; they observed exclusively the amino tautomer, and their ab initio computations showed a preference of about 21.5 kcal/mol for APM over (Z)-PMI at the RHF/6-31++G(d,p) level.² Semiempirical computations by Öğretir and Yaman also showed a clear, albeit smaller preference of 14–15 kcal/mol for the amino tautomer APM.³ Fujimoto et al. recently reported an (E)-preference energy of 2.9 kcal/mol for PMI based on using density functional computations at the B3LYP/6-311++G(d,p) level.⁴ Regarding the pyridine system, computations by Hung et al. showed a preference of 14.1 kcal/mol of the amino tautomer APY over (E)-PYI at the B3LYP/6-31+G(d',p') level.⁵ Hence, there is no doubt that the equilibria $\text{PMI} \rightleftharpoons \text{APM}$ and $\text{PYI} \rightleftharpoons \text{APY}$ lie on the side of the amino tautomer.⁶ Whether equilibrium can be reached starting from the (Z)-imine depends on the reaction rates of the imine (Z)/(E)-isomerization (i.e., (Z)-PMI \rightarrow (E)-PMI) and of the asymmetric amidine–amidine tautomerization (i.e., (E)-PMI \rightarrow APM).

(2) Smets, J.; Adamowicz, L.; Maes, G. Matrix-Isolation FT-IR Studies and ab-Initio Calculations of Hydrogen-Bonded Complexes of Molecules Modeling Cytosine or Isocytosine Tautomers. 2. 4-Aminopyridine and 4-Aminopyrimidine Complexes with H₂O in Ar Matrices. I. In *J. Phys. Chem.* **1995**, *99*, 6387–6400.

(3) Öğretir, C.; Yaman, M. AM1, PM3 and MNDO study of the tautomeric equilibria of 2-, 4- or 5-hydroxypyrimidin derivatives and their azo- and thio- analogs. In *THEOCHEM* **1999**, *458*, 217–226.

(4) Kitamura, T.; Okita, M.; Sasaki, Y.; Ishikawa, H.; Fujimoto, A. Amino-imino tautomerization reaction of the 4-aminopyrimidine/acetic acid system. In *Spectrochim. Acta A* **2008**, *69*, 350–360.

(5) Hung, F.-T.; Hu, W.-P.; Li, T.-H.; Cheng, C.-C.; Chou, P.-T. Ground and Excited-State Acetic Acid Catalyzed Double Proton Transfer in 2-Aminopyridine. In *J. Phys. Chem. A* **2003**, *107*, 3244–3253.

(6) Katritzky, A. R.; Pozharskii, A. F., Eds. *Handbook of heterocyclic chemistry*, 2nd ed.; Pergamon: New York, 2000; p 51.

(7) Johnson, J.; Morales, N.; Gorczyca, A.; Dolliver, D.; McAllister, M. For acid-catalyzed imine inversion, see for example: Mechanisms of Acid-Catalyzed Z/E Isomerization of Imines. In *J. Org. Chem.* **2001**, *66*, 7979–7985.

(8) For base-catalyzed imine inversion with deprotonation of imine-R, see for example: Cainelli, G.; Giacomini, D.; Trerè, A.; Boyd, P. Efficient Transamination under Mild Conditions: Preparation of Primary Amine Derivatives from Carbonyl Compounds via Imine Isomerization with Catalytic Amounts of Potassium *tert*-Butoxide. In *J. Org. Chem.* **1996**, *61*, 5134–5139.

(9) For base-catalyzed imine inversion with deprotonation at C_α, see for example: Gosselin, F.; Roy, A.; O'Shea, P.; Chen, C.; Volante, R. Oxazolidine Ring Opening and Isomerization to (E)-Imines. Asymmetric Synthesis of Aryl- α -fluoroalkyl Amino Alcohols. In *Org. Lett.* **2004**, *6*, 641–644.

The (Z)/(E)-isomerization of imines can proceed with acid catalysis,⁷ with base catalysis,^{8,9} or with acid and base catalysis (i.e., via enamines).^{10,11} In the present study, we are concerned with the uncatalyzed (Z)/(E)-isomerization. The barriers to (Z)/(E)-isomerization by way of *N*-inversion were measured for *N*-alkyl and *N*-aryl benzophenone imines ($\text{ArAr}'\text{C}=\text{N}-\text{R}$) in a number of seminal papers by Curtin et al.^{12,13} (in cyclohexene, heptane, ethanol) and by Jennings et al.¹⁴ (in diethyl ether, toluene, *tert*-butyl alcohol), and the activation energies are 17–30 kcal/mol depending on the arene substituents. Miller et al.¹⁵ estimated the rate constant $k = 27 \text{ s}^{-1}$ at ca. 50 °C for the (Z)/(E)-isomerization of an $\text{R}-\text{CPh}=\text{N}-\text{Ph}$ imine and this reaction rate corresponds to an activation barrier of $\Delta G^\ddagger = 16.8 \text{ kcal/mol}$. The low inversion barriers of imines are in marked contrast to the high thermal stabilities of *N*-haloimines and of oximes. Inversion barriers of formimines $\text{H}_2\text{C}=\text{N}-\text{X}$ (H, CN, F, OH) were studied by Bach et al.^{16,17} the computed barriers

(10) Morpurgo, S.; Grandib, A.; Zazzab, C.; Bossa, M. A theoretical study on the sugars' mutarotation: the epimerization of 2-tetrahydropyranol catalysed by formamide, benzamide and by the 2-aminopyridine/2-iminopyridine tautomeric couple. In *THEOCHEM* **2005**, *729*, 71–82.

(11) Includes *E/Z*-isomerization via enamines: (a) Boyd, D. R.; Jennings, W. B.; Waring, L. C. Isomerization of Chiral Imines in [²H₄]Methanol Solution. In *J. Am. Chem. Soc.* **1986**, *51*, 992–995. (b) Jennings, W.; Boyd, D. The Mechanism of Interconversion of (Z)- and (E)-Ketimines. In *J. Am. Chem. Soc.* **1972**, *94*, 7187–7188.

(12) Curtin, D.; Hausser, J. Effects of Structural Changes on the Interconversion of Stereoisomeric Imines. Isoelectronic Models for Vinyl Anions. In *J. Am. Chem. Soc.* **1961**, *83*, 3474–3481.

(13) Curtin, D. Y.; Grubbs, E. J.; McCarty, C. G. Uncatalyzed syn-anti Isomerization of Imines, Oxime Ethers, and Haloimines. In *J. Am. Chem. Soc.* **1966**, *88*, 2775–2786.

(14) Jennings, W.; Al-Showiman, S.; Boyd, D.; Campbell, R. Dynamic Stereochemistry of Imines and Derivatives. Part IX. The Mechanism of *E-Z* Isomerization in *N*-Alkylimines. In *J. Chem. Soc., Perkin II* **1976**, 1501–1506.

(15) Miller, S.; Reich, B.; Greenwald, E.; Justice, A.; Beckstead, B.; Reibenspies, J.; North, S. Phenyl-(2-phenylimino-1,2-diphenylethyl)-amine: Ene-diamine versus Imine-amine Isomeric Preferences. In *J. Org. Chem.* **2005**, *70*, 8409–8416.

(16) (a) Bach, R.; Wolber, G. Theoretical Study of the Barrier to Nitrogen Inversion in *N*-Cyano- and *N*-Diazoformimine. Mechanism of the Schmidt Reaction. In *J. Org. Chem.* **1982**, *47*, 239–245. (b) Bach, R.; Wolber, G. Theoretical Analysis of the Barrier to Nitrogen Inversion in *N*-Fluoroformimine and Formaldoxime. In *J. Org. Chem.* **1982**, *47*, 245–248.

(17) Bharatam, P.; Amita; Kaur, K. J. Electronic structure of *N*-sulfonylimines. In *Phys. Org. Chem.* **2003**, *16*, 183–188.

Type 2 Example

Reactivity of Zn-, Cd-, and Apo-Metallothionein with Nitric Oxide Compounds: In Vitro and Cellular Comparison

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Received October 21, 2009

Introduction

Mammalian metallothionein (MT¹) is a small, thiol rich protein that binds multiple metal ions in two metal–thiolate clusters (1). Numerous studies, including ones with MT knockout mice, demonstrate that the presence of MT in cells protects them from excessive exposure to metal ions such as Cd²⁺ (2, 3). Undoubtedly, this property is due to the capacity of MT with its many cysteinyl sulfhydryl ligands to bind various metal ions with high affinity and, thereby, to prevent them from interacting with sensitive sites in the cell (4). It is also likely that the high density of MT's thiolate groups reacts with and

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¹ Abbreviations: apo-MT, metal ion free or metal ion unsaturated metallothionein; Cd-MT, cadmium metallothionein without reference to the number of bound Cd ions; DEA/NO, 2-(*N,N*-diethylamino)-diazene 2-oxide; DETA/NO, 1-[*N*-(2-aminoethyl)-*N*-(2-ammonioethyl)amino]diazene-1-ium-1,2-diolate; DTNB, 5,5'-dithiobis(2-nitrobenzoate); GSH, glutathione; DTT, dithiothreitol; GS-NO, *S*-nitroso-glutathione; LMW, low molecular weight (defined in Figure 9); PAR, 4-(2-pyridylazo)resorcinol; proteome, high molecular weight band of protein defined by Sephadex G-75 chromatography (defined in Figure 9); PTIO, 2-phenyl-4,4,5,5-tetramethylimidazole-1-oxyl 3-oxide; RS-NO, general nitrosyl thiolate; MT, metallothionein; Zn-MT, metallothionein with focus on sites that have bound Zn²⁺; SH, thiol or sulfhydryl group; MTT, thiazolyl blue tetrazolium bromide; SNAP, *S*-nitrosoacetylpenicillamine; SNOC, *S*-nitrosocysteine; Zn₇-MT, fully Zn²⁺ saturated metallothionein; zincon, 2-carboxy-2-hydroxy-5-sulfoformazyl-benzene sodium salt.

In Vitro and in Vivo Metallothionein Reactions

Acknowledgment. We acknowledge the support of NIH grants ES-04184 and ES-04026, and NSF grant CHE-9977636 for the inductively coupled plasma mass spectrometer used in this research.

References

- (1) Robbins, A. H., McRee, D. E., Williamson, M., Collett, S. A., Xuong, N. H., Furey, W. F., Wang, B. C., and Stout, C. D. (1991) Refined crystal structure of Cd, Zn metallothionein at 2.0 Å resolution. *J. Mol. Biol.* 221, 1269–93.
- (2) Zheng, H., Liu, J., Choo, K. H., Michalska, A. E., and Klaassen, C. D. (1996) Metallothionein-I and -II knock-out mice are sensitive to cadmium-induced liver mRNA expression of c-jun and p53. *Toxicol. Appl. Pharmacol.* 136, 229–35.

Type 3 Example

Assessment & Evaluation in Higher Education
2009, 1–22, iFirst Article



Chemistry Is in the news: assessing intra-group peer review

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Keywords: science education; interdisciplinarity; group collaboration; peer review; accountability

The search for more effective teaching methods particularly in large lecture classes has led to the wide adoption of collaborative group work (Cooper 2005; McKeachie 2002; Smist 2004; Woolfolk 2004). Collaborative group work has been touted as providing a support network for students and increasing student retention (Gupta 2004; Tinto 1997), providing additional cognitive benefits (Bransford, Brown, and Cocking 2000) and increased learning (Slavin 1996). It is often integrated as a major

Dr Rainer E. Glaser, professor of chemistry, studied chemistry and physics in Tübingen, at Berkeley, and at Yale. He is a physical organic chemist with three major lines of research in bioorganic chemistry and toxicology, materials chemistry and astrochemistry. He has collaborated extensively with chemists, biochemists, physicists, mathematicians, astronomers, educators and journalists. In 1995, Glaser began his education research with the novel curriculum, *Chemistry Is in the News (CIITN)*, that he designed for chemistry education of science majors. He was a JSPS Fellow in 1997 and was elected AAAS Fellow in 2004 and Fellow of the Royal Chemical Society in 2006.

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- Carlone, H.B. 2004. The cultural production of science in reform-based physics: Girls' access, participation, and resistance. *Journal of Research in Science Teaching* 41, no. 4: 392–414.
- Carson, K.M., B. Hodgen, and R.E. Glaser. 2006. Teaching dissent and persuasion. *Education Research and Reviews* 1, no. 4: 115–20.

Formatting References

Type(s) of Reference Sections

- Footnotes
- Endnotes
- Footnotes and Endnotes

Types of Items Cited (Table 14-2 in ACS SG)

- Journals
- Books (several types)
- Online Resources (sites, databases)
- Software

Lots of variations
and exceptions.

Journal Article

Author 1; Author 2; Author 3; etc. Title of Article. *Journal Abbreviation* **Year**, *Volume*, inclusive pagination.

From Acc. Chem. Res.:

16 Thomä, N. H.; Evans, P. R.; Leadlay, P. F. Protection of radical intermediates at the active site of adenosylcobalamin-dependent methylmalonyl-CoA mutase. *Biochemistry* **2000**, 39, 9213-9221.

From Chem. Rev.:

(200) de Lucas, A.; Valverde, J. L.; Rodriguez, L.; Sanchez, P.; Garcia, M. T. *Appl. Catal., A* **2000**, 203, 81.

From Chem. Res. Tox.:

(12) Hatcher, L. Q., Hong, L., Bush, W. D., Carducci, T. and Simon, J. D. **(2008)** Quantification of the binding constant of copper(II) to the amyloid-beta peptide *J. Phys. Chem. B* **112**, 8160-8164.

Journal Abbreviations from CASSI

Chemical Abstract Service Source Index

ACS Style Guide, Appendix 14-1 lists >1000 journal abbreviations.
CASSI published quarterly supplements with extensive lists of journals.



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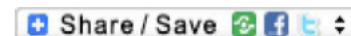
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CASSI sample record (CD-ROM)

Entry Type: Changed Title Serial
 CODEN: AASCAU
 ISSN: 0001-5121
 Abbreviated Title: Acta Agric. Scand.
 Title: Acta Agriculturae Scandinavica
 Former Title Note: Supersedes
 Former Title: Acta Agric. Suec.
 Language of Text: English
 Summaries in: English
 Language Note: Fr or Ger pap are also accepted
 History: Began v1 1950
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 Country Code: SE
 Successor Title Note: Divided into
 Successor Title(s): Acta Agric. Scand., Sect. A, which see Acta Agric. Scand., Sect. B, which see
 Availability: This title is available through CAS Document Delivery Service.
 Holdings: AAP 1950-1964; ArU 1950+; AzU 1950+; CLU-P 1950+; CU 1950+; CU-A 1950+; CoES 1950+; CtlU 1950+;

1950+; KyU-ASC 1954+; LU 1950+; MdU 1950+; MeU 1950+; MnSU 1950+; MoKL 1950+; MoU 1950+; MsSM 1950+; MtBC 1950+; NIC 1950+; NbU 1950+; NeRS 1950+; NdFA 1957+; NhD-D 1971+; NhU 1950+; NmLcU 1950+; NvU 1958-1965; OU 1950+; OkS 1951+; OrCS; PSt 1950+; RU 1950+; ScCleU 1950+; SdB 1950+; TU 1951+; TxCM 1950+; TxDaM; TxLT 1950+; ULA 1951+; ViBibV 1950+; WU-A 1950+; WaPS 1950+; WvU 1950+; WyU 1950+; AuMU 1950+; AuSU 1950+; CaAEU 1950+; CaBVaU 1950-1964; CaOOAg 1950+; FiHT 1952-1959; liNI 1967+; IreDR 1950+; ItRC 1954+; JTNDL; RuLA 1950-1962; SzZE 1950+; Uk 1950+

Journal Abbreviations

Acta Crystallogr., Sect. C: Cryst. Struct. Commun.
2005, 61, 99-102.

Acta Crystallogr., Sect. C **2005**, 61, 99-102.

Acta Crystallogr. **2005**, C61, 99-102.

Pagination Field

99-102 Inclusive pages, first to last page.

99-102 and references therein.

Use this paper as a “leading reference”.

99 f Read page 99 and 100.

99 ff Read page 99 and following pages.

99-101 ff Read pages 99 – 101 for sure and browse following pages.

Books (without Editors)

Author 1; Author 2; Author 3; etc. Chapter Title. *Book Title*, Edition Number, Series Information (if any); Publisher: Place of Publication, Year; Volume Number, Pagination.

From Chem. Rev.:

- (3) Emsley, J. *The 13th Element: The Sordid Tale of Murder, Fire, and Phosphorus*; John Wiley & Sons, Inc.: New York, 2000.
- (4) Corbridge, D. *Phosphorus: An Outline of its Chemistry, Biochemistry, and Technology*, 5th ed.; Elsevier: New York, 1994.
- (5) Engel, R. *Synthesis of Carbon Phosphorus Bonds*, 2nd ed.; CRC Press: Boca Raton, 2004.

Books (with Editors)

Author 1; Author 2; Author 3; etc. Chapter Title. In *Book Title*, Edition Number; Editor 2, Editor 2, etc., Eds.; Series Information (if any); Publisher: Place of Publication, Year; Volume Number, Pagination.

From Acc. Chem. Res.:

3 *Organic Mass Spectrometry in Art and Archaeology*; Colombini, M. P., Modugno, F., Eds.; John Wiley & Sons: Chichester, U.K., 2009.

4 Andreotti, A.; Bonaduce, I.; Colombini, M. P.; Modugno, F.; Ribechini, E. Organic paint materials and their characterization by GC-MS analytical procedures. In *New Trends in Analytical, Environmental and Cultural Heritage Chemistry*; Tassi, L., Colombini, M. P., Eds.; Transworld Research Network: Kerala, India, 2008, pp 389-423.

Web Sites

Author (if any). Title of Site. URL (accessed Month Day, Year), other identifying information (if any).

From *Energy & Fuels*:

to these standards based on a phase-in requiring 50% compliance in 2008 and 100% compliance in 2009).² These goals are nearly

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(1) Environmental Protection Agency. *A Comprehensive Analysis of Biodiesel Impacts on Exhaust Emissions*. Draft technical report. EPA 420-P-02-001 2002 (cited May 27, 2005); <http://www.epa.gov/otaq/models/analysis/biodsl/p02001.pdf>.

is approximately 60 billion gallons per year. According to EIA's International Energy Outlook 2005, the world demand for crude oil grows from 78 million barrels/day in 2002 to 103 million barrels/day in 2015 and to just over 119 million barrels/day in

(2) California Air Resources Board. *Exhaust Emission Standards and Test Procedures—1985 and Subsequent Model Heavy Duty Urban Bus Engines and Vehicles*; (cited May 27, 2005); http://www.arb.ca.gov/regs/components/pubtransit_buses.pdf.

10.1021/ef050202m CCC: \$33.50 © 2006 American Chemical Society
Published on Web 11/19/2005

(47) Corradini, M. L. *Fundamentals of Multiphase Flow*. (Available via the Internet at <http://wins.engr.wisc.edu/teaching/mpfBook/>. Accessed July 2007.)

(48) Chen, S. K.; Lefebvre, A. H. Discharge Coefficients for Effervescent Atomizers. *Atomization Sprays* **1994**, 4 (3), 275–290.

(49) Process Associates of America, *Modified Baker's map for horizontal two-phase flow with transformed coordinates*. (Available via the Internet at http://www.processassociates.com/process/fluid/2faz_xy.htm. Accessed March 2003.)

Formatting the Reference Section(s)

Articles

Communications

Reviews ; Review Articles

Mini-Reviews

Highlights

Essays

Perspectives

Book, Chapters by same Author(s)

Edited Book, Chapters by different Authors(s)

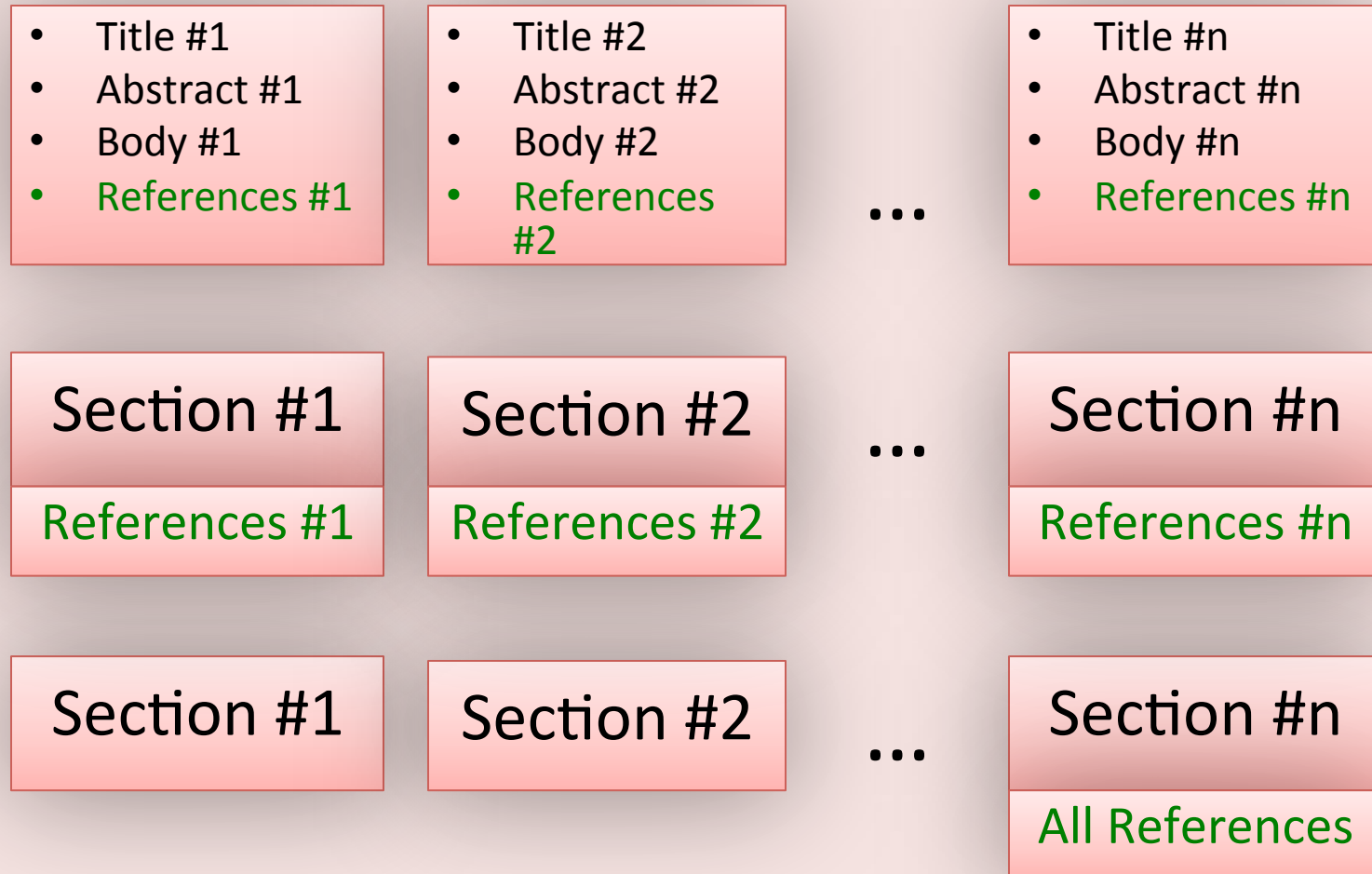
Stereotyped Format

- Title
- Abstract
- Introduction
- Materials & Methods
- Results
- Discussion
- Conclusion
- References

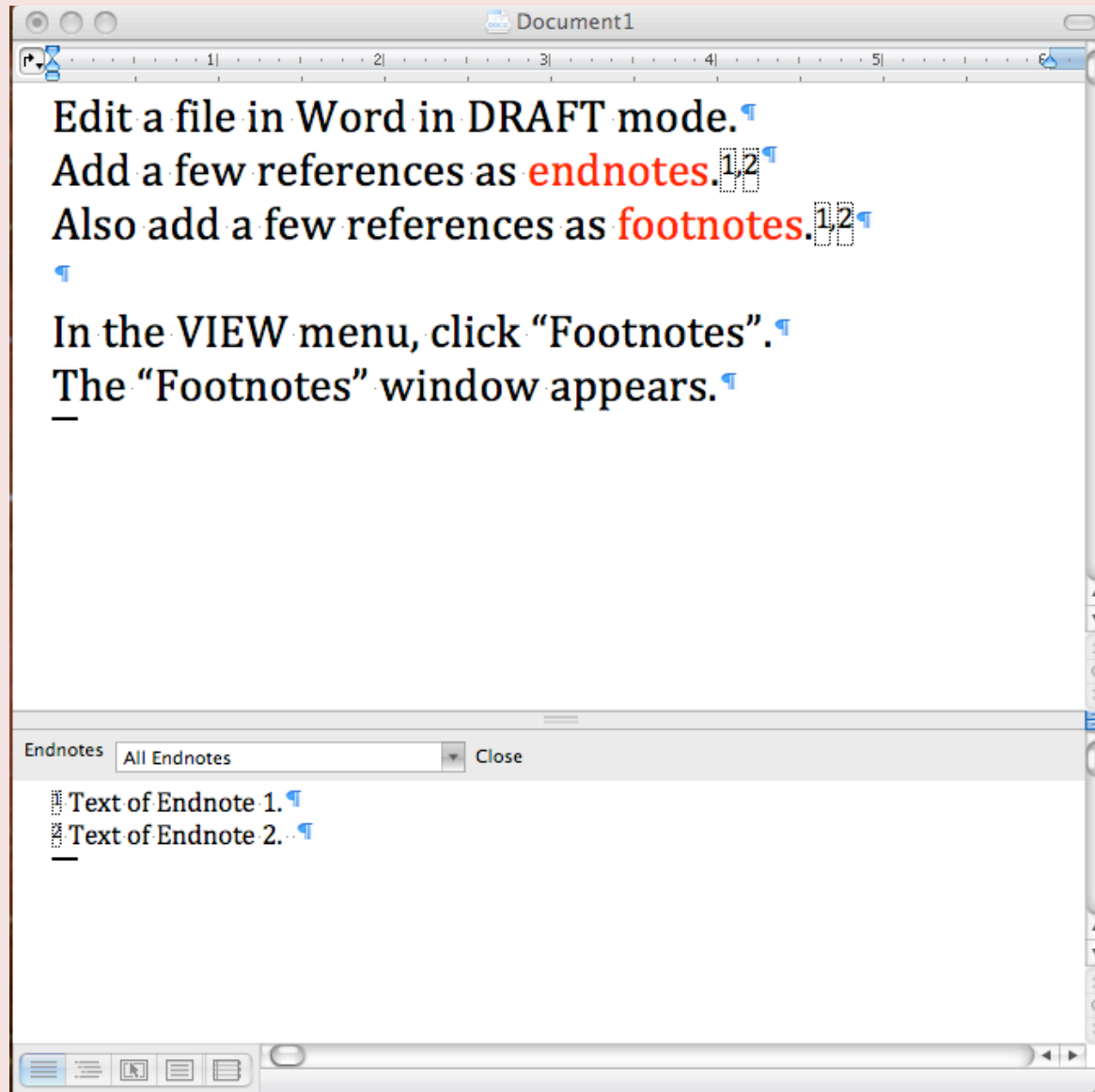
- Title
- Abstract
- Body
- References

Chapters and Sections

References End of Section vs. End of Document



Formatting References



Formatting References

Edit a file in Word in DRAFT mode.¹

Add a few references as **endnotes**.^{1,2}

Also add a few references as **footnotes**.^{1,2}

In the VIEW menu, click “Footnotes”.¹

The “Footnotes” window appears.¹

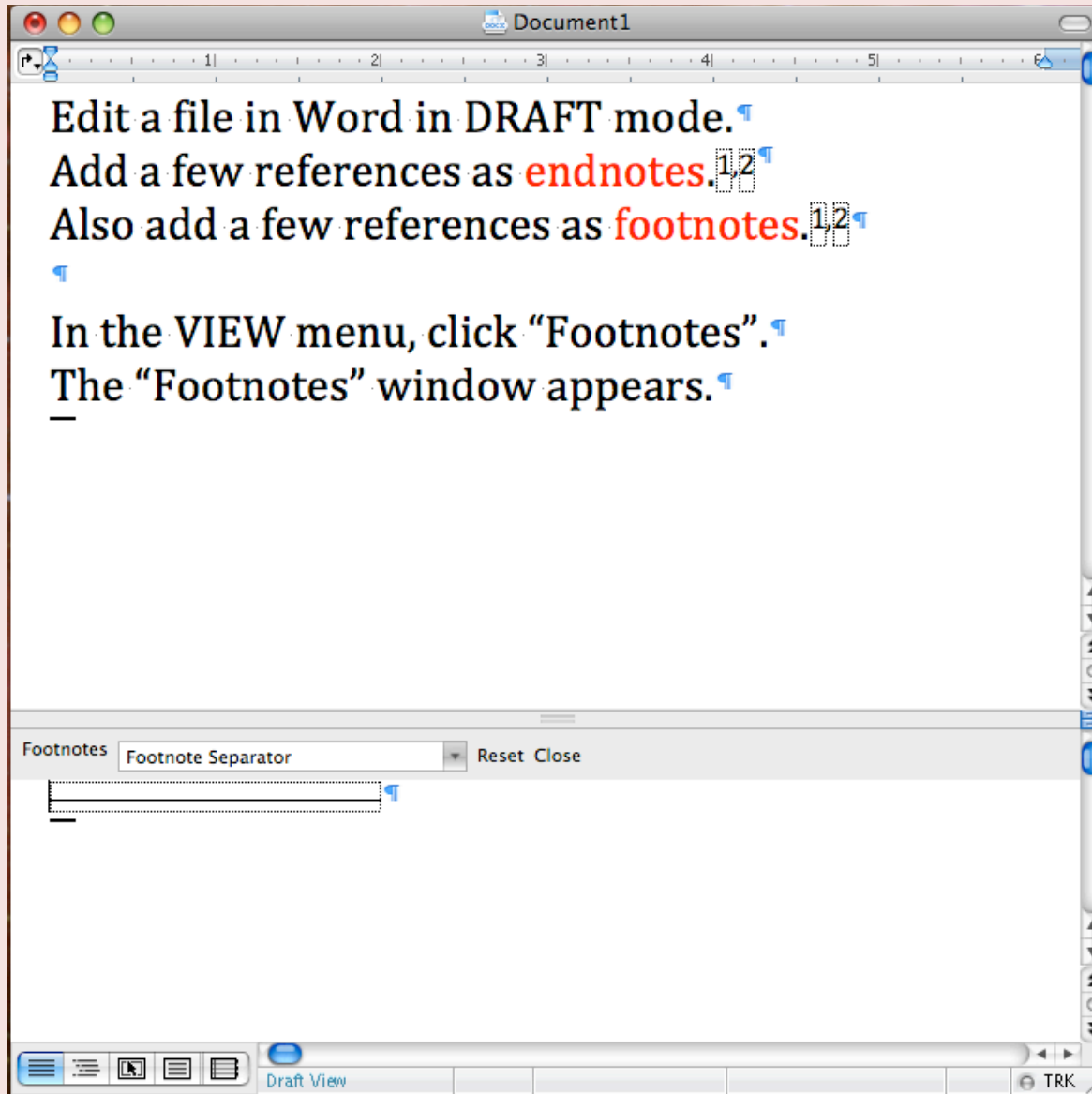
When “All Endnotes” is checked, then there will be menu lines for “Endnote Separator” etc.

Footnotes: All Footnotes Close

- ✓ All Footnotes
- All Endnotes
- Footnote Separator
- Footnote Continuation Separator
- Footnote Continuation Notice

Draft View Sec 1 Pages: 1 of 1 TRK

Formatting Reference Sections



Hanging References

Each **reference number** together with the **reference entry** is one paragraph.

Various formats for the reference number are common.

(21) 21. [21] 21 21)

The reference entry is **indented** and **hanging**.

Multiple Antioxidants and Parkinson's Disease

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Electronic Structures and Spin Topologies of γ -Picoliniumyl Radicals. A Study of the Homolysis of *N*-Methyl- γ -picolinium and of Benzo-, Dibenzo-, and Naphthoannulated Analogs

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Introduction

The redox reactions of quaternized nitrogen heterocycles, including both heterocyclic *N*-oxides and *N*-alkylated heterocycles, are chemically and biologically interesting. For example, the herbicide methyl viologen (paraquat) and the promising antitumor agent tirapazamine (Scheme 1) possess potent cytotoxic properties that stem from their propensity to undergo enzymatic one-electron reduction inside cells.^{1–6} Understanding the fate of the organic radicals resulting from one-electron reduction of these compounds is crucial for understanding their biological properties. In the case of paraquat, the radical reacts readily with molecular oxygen to regenerate paraquat and one equivalent of superoxide $O_2^{\cdot-}$.^{1–4} The repeated enzymatic reduction and back-oxidation by O_2 , i.e., the redox-cycling, can generate significant amounts of intracellular superoxide. Although cells contain enzyme systems that destroy $O_2^{\cdot-}$ and its decomposition product H_2O_2 , redox-cycling can overwhelm these protective mechanisms with deleterious results to the cell.⁷ Similarly, tirapazamine undergoes redox-cycling under aerobic conditions.^{5,6,8–11} Under low-oxygen (hypoxic) conditions, however, alternative reaction channels become available and the tirapazamine-derived radical can decompose either by homolytic N–O fragmentation and hydroxyl radical release or by way of dehydration to yield a benzotriazinyl radical.^{12,13} Regardless of

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Asymmetry in the *N*-Inversion of Heteroarene Imines: Pyrimidin-4(3*H*)-Imine, Pyridin-2(1*H*)-Imine, and 1*H*-Purine-6(9*H*)-Imine

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Computational Methods

Potential energy surface (PES) analyses¹⁸ were performed with second-order Møller–Plesset perturbation theory (MP2)^{19,20}

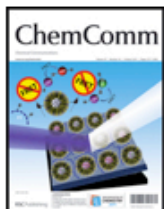
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estimated. Local harmonic analysis of the SOSP structure becomes altogether irrelevant in this situation because the molecular motion along the deformation vector associated with ν_2 is a vibration.

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KCN sensor: unique chromogenic and 'turn-on' fluorescent chemodosimeter: rapid response and high selectivity

Hyun Jung Kim, Kyoung Chul Ko, Jae Hong Lee, Jin Yong Lee and Jong Seung Kim

Chem. Commun., 2011, **47**, 2886-2888

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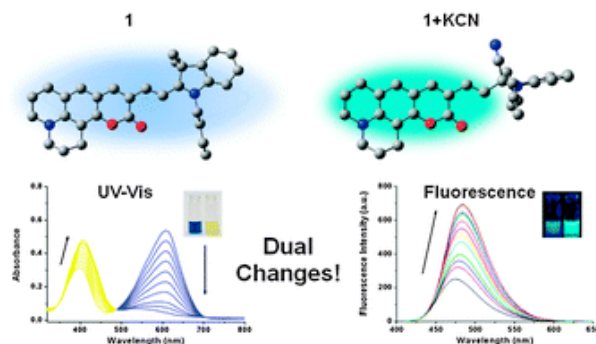
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Abstract

An indole conjugated coumarin **1** for KCN chemodosimeter has been prepared and displayed considerable dual changes in both absorption (blue-shift) and emission (turn-on) bands exclusively for KCN. DFT/TDDFT calculations support that the fluorescence enhancement of **1**-KCN is mainly due to blocking of the ICT process.



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COMMUNICATION

KCN sensor: unique chromogenic and ‘turn-on’ fluorescent chemodosimeter: rapid response and high selectivity†

Hyun Jung Kim,^{†a} Kyoung Chul Ko,^{‡b} Jae Hong Lee,^a Jin Yong Lee^{*b} and Jong Seung Kim^{*a}

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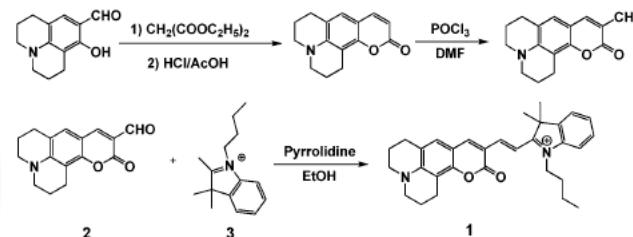
An indole conjugated coumarin 1 for KCN chemodosimeter has been prepared and displayed considerable dual changes in both absorption (blue-shift) and emission (turn-on) bands exclusively for KCN. DFT/TDDFT calculations support that the fluorescence enhancement of 1-KCN is mainly due to blocking of the ICT process.

usually used as a counter cation. However, since KCN is known to be very toxic and therefore limited to 0.8 mg L⁻¹

in drinking water by EPA standard, detection of KCN rather than that of (n-Bu)₄N⁺CN⁻ should be more meaningful in aspect of a practical application in CN⁻ detection. The corresponding response time for the CN⁻ detection has also remained problematic.

In light of these considerable drawbacks in CN⁻ sensing

from dark blue to yellow and a fluorescence change from weak



Scheme 1 Synthetic pathway of 1.

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† Electronic supplementary information (ESI) available: Experimental procedures and additional figures. See DOI: 10.1039/c0cc05018k

‡ Equally contributed to this work.

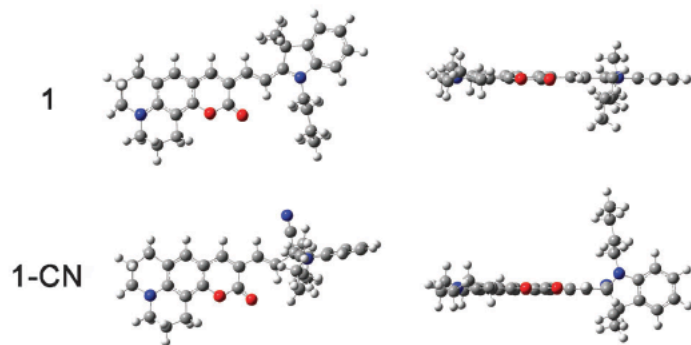


Fig. 3 The optimized structures of **1** and **1-CN**.

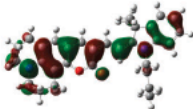
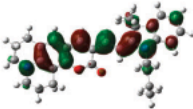
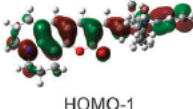
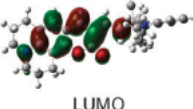
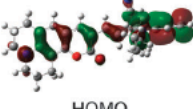
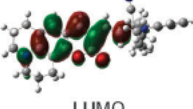
Molecular orbitals		Electronic contribution of transition
1		HOMO →LUMO 100 %
		
1-CN		HOMO-1 →LUMO 90.6 %
		
1-CN		HOMO →LUMO 9.4 %
		

Fig. 4 Molecular orbitals and electronic contributions of the relevant excitations for **1** and **1-CN**.

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