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# **Studies in Gas Phase Ion Chemistry**

A thesis presented for the degree of

**Doctor of Science**

in

**The Faculty of Science**

of

**The University of Adelaide**

by

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**B.Sc.(First Class Honours) 1986, Ph.D. (Adelaide) 1991**

**December 2004**



## Publications (B): Inorganic and Organometallic Gas Phase Ion Chemistry

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### **Publications (B): Inorganic and Organometallic Gas Phase Ion Chemistry**

- (B1) Damrauer, R.; Krempp, M.; O'Hair, R. A. J., "Gas-Phase Chemistry of  $\text{HSiS}^-$  and  $\text{HSiNH}^-$  : Ions Related to Silathioformaldehyde and the Silaazomethine of Formaldehyde", *J. Am. Chem. Soc.*, **1993**, *115*, 1998-2005. (O'Hair 30% Postdoctoral researcher; Krempp: Postdoctoral researcher; Damrauer: principal author and research supervisor)
- (B2) Shimizu, H.; Gordon, M. S.; Damrauer, R.; O'Hair, R. A. J., " Potential Energy Surface of the Reaction of the Silaformyl Anion and  $\text{CO}_2$ ", *Organometallics*, **1995**, *14*, 2664-2671. (O'Hair, 10% Postdoctoral researcher; Shimizu: Iowa State University collaborator; Gordon and Damrauer principal authors and research supervisors)
- (B3) O'Hair, R. A. J.; Krempp, M.; Damrauer, R.; DePuy, C. H., "Gas-Phase Ion Chemistry of  $\text{HP}_2^-$ ,  $\text{FP}_2^-$  and  $\text{HP}_2^+$  ", *Inorg. Chem.*, **1992**, *31*, 2092-2096. (O'Hair, 60% Postdoctoral researcher; Krempp: Postdoctoral researcher; Damrauer and DePuy principal authors and research supervisors)
- (B4) O'Hair, R. A. J.; DePuy, C. H.; Bierbaum, V. M., "Gas-Phase Chemistry and Thermochemistry of the Hydroxysulfide Anion,  $\text{HOS}^-$ ", *J. Phys. Chem.*, **1993**, *97*, 7955-7961. (O'Hair, 60% Postdoctoral researcher; DePuy: University of Colorado collaborator; Bierbaum: principal author and research supervisor)
- (B5) Downard, K. M.; Bowie, J. H.; O'Hair, R. A. J.; Krempp, M.; DePuy, C. H., "Gas Phase Reactions of the Methylsulfinyl and Methyldisulfide Anions", *Int. J. Mass Spectrom. Ion Proc.*, **1992**, *120*, 217-229. (O'Hair, 25% Postdoctoral researcher; Downard: University of Adelaide collaborator; Krempp: University of Colorado collaborator; Bowie and DePuy principal authors and research supervisors)
- (B6) Smith, J. D.; O'Hair, R. A. J., "Reactions of Phosphorus Trifluoride with Anionic Nucleophiles in the Gas Phase.", *Eur. Mass Spectrom.*, **1996**, *2*, 225-231. (O'Hair 80% principal author and research supervisor; Smith: MS student)
- (B7) Smith, J. D.; O'Hair, R. A. J., "Gas Phase Reactions of Dialkoxydisulfides, ROSSOR (R =  $\text{CH}_3$  and  $\text{CH}_3\text{CH}_2$ ), with Anionic Nucleophiles", *Phos. Sulf. Silicon Rel. Elements*, **1997**, *126*, 257-272. (O'Hair 80% principal author and research supervisor; Smith: MS student)

- (B8) Smith, J. D.; O'Hair, R. A. J.; Williams, T. D., "Gas Phase Chemistry of Sulfonate Anions: Basicities and Fragmentation Reactions.", *Phos. Sulf. Silicon Rel. Elements*, **1996**, *119*, 49-59. (O'Hair 80% principal author and research supervisor; Smith: MS student; Williams: University of Kansas collaborator)
- (B9) Styles, M. L.; O'Hair, R. A. J.; McFadyen, W.D.; Tannous, L.; Holmes, R.J.; Gable, R.W., "Formation and Gas Phase Fragmentation Reactions of Ligand Substitution Products of Platinum(II) Complexes via Electrospray Ionization Tandem Mass Spectrometry." *J. Chem. Soc., Dalton Trans.*, **2000**, 93-99. (O'Hair 50% principal author and joint research supervisor; Styles and Holmes: PhD students; Tannous: Honours student; McFadyen and Gable: School of Chemistry collaborators)
- (B10) Wee, S.; Grannas, M.J.; McFadyen, W.D.; O'Hair, R. A. J "Gas-Phase and Condensed-Phase Studies on the Reactivity of the Azido(2,2':6',2''-terpyridine)-platinum(II) Cation.", *Aust. J. Chem.*, **2001**, *54*, 245-252. (O'Hair 50% joint principal author and joint research supervisor; Wee: honours student; McFadyen: joint principal author and joint research supervisor; Grannas: School of Chemistry collaborator)
- (B11) Wee, S.; White, J.M.; McFadyen, W.D., O'Hair, R.A.J "Gas-phase studies on the reactivity of the azido(diethylenetriamine)platinum(II) cation and derived species." *Aust. J. Chem.*, **2003**, *56*, 1201-1207. (O'Hair 50% joint principal author and joint research supervisor; Wee: honours student; McFadyen: joint principal author and joint research supervisor; White: School of Chemistry collaborator)
- (B12) Wee, S.; O'Hair, R. A. J.; McFadyen, W.D., "Gas Phase Ligand Loss and Ligand Substitution Reactions of Platinum(II) Complexes of Tridentate Nitrogen Donor Ligands.", *Rapid Commun. Mass Spectrom.*, **2004**, *18*, 1221-1226. (O'Hair 50% joint principal author and joint research supervisor; Wee: honours student; McFadyen: joint principal author and joint research supervisor)
- (B13) Holmes, R.J.; O'Hair, R. A. J.; McFadyen W.D., "ESI/MS/MS Studies of Competitive Pyridine Loss From Platinum(II) Ethylenediamine Complexes by the Kinetic Method" *Rapid Commun. Mass Spectrom.*, **2000**, *14*, 2385-2392. (O'Hair 70% principal author; Holmes: PhD student; McFadyen: School of Chemistry collaborator and research supervisor)
- (B14) Liyanage, R.; Styles, M. L.; O'Hair, R. A. J.; Armentrout, P. B. "Sequential Bond Energies of  $\text{Pt}(\text{NH}_3)_x^+$  ( $x = 1 - 4$ ) Determined by Collision-induced Dissociation and Theory", *Int. J. Mass Spectrom.*, (invited contribution to Professor Dunbar Honour Issue), **2003**, *227*, 47 - 62. (O'Hair 10%; Liyanage: University of Utah collaborator; Styles: PhD student; Armentrout: principal author and University of Utah collaborator)

- (B15) Liyanage, R.; Styles, M. L.; O'Hair, R. A. J.; Armentrout, P. B. "Guided Ion Beam and Ab initio Studies of Platinum Chloride Cations", *J. Phys. Chem. A*, **2003**, *107*, 10303-10310. (O'Hair 10%; Liyanage: University of Utah collaborator; Styles: PhD student; Armentrout: principal author and University of Utah collaborator)
- (B16) Waters, T.; O'Hair, R. A. J.; Wedd, A. G. " Probing the Catalytic Oxidation of Alcohols via an Anionic Dimolybdate Centre Using Multistage Mass Spectrometry." *Chem. Comm.*, **2000**, 225-226. (O'Hair 60% principal author and joint research supervisor; Waters: PhD student; Wedd: principal author, joint research supervisor and School of Chemistry collaborator)
- (B17) Waters, T.; O'Hair, R. A. J.; Wedd, A. G. "Catalytic Gas Phase Oxidation of Methanol to Formaldehyde.", *J. Am. Chem. Soc.*, **2003**, *125*, 3384-3396. (O'Hair 60% principal author and joint research supervisor; Waters: PhD student; Wedd: principal author, joint research supervisor and School of Chemistry collaborator)
- (B18) Waters, T.; O'Hair, R. A. J.; Wedd, A. G. " Catalytic Gas Phase Dehydration of Acetic Acid to Ketene. ", *Int. J. Mass Spectrom.*, (invited contribution to Professor Schwarz Honour Issue), **2003**, *228*, 599 - 611. (O'Hair 60% principal author and joint research supervisor; Waters: PhD student; Wedd: joint research supervisor and School of Chemistry collaborator)
- (B19) Feyel, S.; Waters, T.; O'Hair, R. A. J.; Wedd, A.G., "Gas Phase Oxidation of Alkoxo Ligands in Bis(peroxo)  $[MO(O_2)_2(OR)]^-$  and Trisoxo  $[MO_3(OR)]^-$  Anions (M = Cr, Mo, W).", *Dalton Trans.*, **2004**, 4010 - 4016. (O'Hair 40% principal author and joint research supervisor; Feyel: visiting graduate student; Waters: PhD student; Wedd: principal author, joint research supervisor and School of Chemistry collaborator)
- (B20) Waters, T.; Wang, X.-B.; Yang, X.; Zhang, L.; O'Hair, R. A. J.; Wang, L.-S.; Wedd, A. G. " Photoelectron Spectroscopy of the Doubly-Charged Anions  $[M^{IV}O(mnt)_2]^{2-}$  (M = Mo, W;  $mnt = S_2C_2(CN)_2^{2-}$ ): Access to the Ground and Excited States of the  $[M^V O(mnt)_2]^-$  Anion.", *J. Am. Chem. Soc.*, **2004**, *126*, 5119-5129. (O'Hair 10%; Waters: PhD student; Wang, Yang, Zhang: PNNL collaborators.; Wang: joint principal author and PNNL collaborator; Wedd: joint principal author, joint research supervisor and School of Chemistry collaborator)
- (B21) Yang, X.; Waters, T.; Wang, X.-B.; O'Hair, R. A. J.; Wedd, A.G.; Dixon, D.A.; Li, J.; Wang, L.S.; "Photoelectron Spectroscopy of Free Polyoxoanions  $Mo_6O_{19}^{2-}$  and  $W_6O_{19}^{2-}$  in the Gas Phase.", *J. Phys. Chem. A*, **2004**, *108*, 10089-10093. (O'Hair 10%; Waters: PhD student; Yang, Wang, Dixon, Li: PNNL collaborators; Wedd: School of Chemistry collaborator; Wang: principal author and PNNL collaborator)

- (B22) O'Hair, R. A. J "Dimethylargenate is a stable species in the gas phase." *Chem. Comm.*, **2002**, 20 - 21. (O'Hair 100%)
- (B23) James, P. F.; O'Hair, R. A. J., "Dimethyl cuprate undergoes C-C bond coupling with methyl iodide in the gas phase but dimethyl argenate does not.", *Org. Lett.*, **2004**, *6*, 2761–2764. (O'Hair 70% principal author and research supervisor; James: undergraduate student)
- (B24) O'Hair, R. A. J.; Vrkic, A. K.; James, P. F., "Gas Phase Synthesis and Reactivity of the Organomagnesates [CH<sub>3</sub>MgL<sub>2</sub>] (L = Cl and = O<sub>2</sub>CCH<sub>3</sub>): From Ligand Effects to Catalysis.", *J. Am. Chem. Soc.*, **2004**, *126*, 12173-12183. (O'Hair 70% principal author and research supervisor; Vrkic: PhD student; James: undergraduate student)
- (B25) Khairallah, G.N.; O'Hair, R. A. J., " Gas Phase Synthesis of Ag<sub>4</sub>H<sup>+</sup> and its Mediation of C-C Bond Coupling of Allylbromide.", *Angew. Chem. Int. Ed.*, in press. (O'Hair 70% principal author and research supervisor; Khairallah: postdoctoral researcher)

## Publications (C): Organic Gas Phase Ion Chemistry

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### **Publications (C): Organic Gas Phase Ion Chemistry**

- (C1) Damrauer, R.; Krempp, M.; O'Hair, R. A. J.; Simon, R., "The Gas Phase Acidities of Hindered Amines and Some Reaction Chemistry of their Corresponding Amide Ions", *Int. J. Mass Spectrom. Ion Proc.*, **1992**, *117*, 199-211. (O'Hair, 25% Postdoctoral researcher; Krempp and Simon: University of Colorado collaborators; Damrauer principal author and research supervisor)
- (C2) O'Hair, R. A. J.; Davico, G. E.; Hacaloglu, J.; Dang, T. T.; DePuy, C. H.; Bierbaum, V. M., "Measurement of Solvent and Secondary Kinetic Isotope Effects for the Gas-Phase S<sub>N</sub>2 Reactions of Fluoride with Methyl Halides", *J. Am. Chem. Soc.*, **1994**, *116*, 3609-3610. (O'Hair, 40% Postdoctoral researcher; Davico, Hacaloglu, Dang, DePuy: University of Colorado collaborators; Bierbaum: principal author and research supervisor)
- (C3) O'Hair, R. A. J.; Androutsopoulos, N. K., "Can Transacylation Reactions Occur via S<sub>N</sub>2 Pathways in the Gas Phase? Insights via Ion-Molecule Reactions of N-Acylpyridinium ions and *Ab Initio* Calculations.", *Org. Lett.*, **2000**, *2*, 2567-2570. (O'Hair 90% principal author and research supervisor; Androutsopoulos: honours student)
- (C4) Vrkic, A. K.; O'Hair, R. A. J.; "Gas Phase Ion Chemistry of Para Substituted Benzene Diazonium Ions, Their Salt Clusters and Their Related Phenyl Cations.", *Int. J. Mass Spectrom.*, **2002**, *218*, 131-160. (O'Hair 70% principal author and research supervisor; Vrkic: PhD student)

- (C5) Sheldon, J. C.; O'Hair, R. A. J.; Downard, K. M.; Gronert, S.; Krempp, M.; DePuy, C.H.; Bowie, J. H., "A Potential Surface Map of the  $\text{H}^-/\text{N}_2\text{O}$  System. The Gas Phase Ion Chemistry of  $\text{HN}_2\text{O}^-$ ", *Aust. J. Chem.*, **1995**, *48*, 155-165. (O'Hair, 35% Postdoctoral researcher; Sheldon and Downard: University of Adelaide collaborators; Gronert and Krempp: University of Colorado collaborators; Bowie and DePuy principal authors and research supervisors)
- (C6) O'Hair, R. A. J.; Gronert, S.; DePuy, C. H., "New Insights into the Gas-Phase Anion Chemistry of Nitrous Oxide.", *Eur. Mass Spectrom.*, **1995**, *1*, 429-436. (O'Hair, 50% Postdoctoral researcher and principal author; Gronert and DePuy: University of Colorado collaborators)
- (C7) Sheldon, J. C.; Bowie, J. H.; Dua, S.; Smith, J. D.; O'Hair, R. A. J., "The Gas Phase Cannizzaro Disproportionation Reactions of Benzaldehyde and Pivaldehyde.", *J. Org. Chem.*, **1997**, *62*, 3931-3937. (O'Hair 15%; Sheldon and Dua: University of Adelaide collaborators; Bowie principal author; Smith: MS student)
- (C8) Waters, T.; Blanksby, S.J.; Zhang, L.; O'Hair, R. A. J.; "Formation of the Heterocumulene Anion  $\text{SCCCN}^-$  by a Cyano Migration from the Radical Anion of 1,2-dicyanoethylenedithiolate.", *Org. Bio. Chem.*, **2004**, *2*, 190-194. (O'Hair 50% joint principal author; Waters: PhD student; Blanksby: joint principal author and University of Wollongong collaborator; Zhang: School of Chemistry collaborator)

## Publications (D): International Patent

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### International Patent

**(D1) International Application No. PCT/US03/36739.** Filed with US Patent & Trademark Office: November 18, 2003. **Title of Invention:** Method for analysing amino acids, peptides and proteins; **Inventors:** Reid, G. E.; Simpson, R. J.; O,Hair, R. A. J. (all inventors:33%) **Awarded: 2004** (listed in Chemical Abstracts as CAN 140: 420 396).

## Publications (E-F)

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### Invited Reviews

(E1) O'Hair, R. A. J.; "Anion-Molecule Reactions of Organophosphorus and Organosulfur Species: Some Mechanistic Aspects", *Mass Spectrom. Rev.*, 1991, 10, 133-173. (O'Hair 100%)

(E2) O'Hair, R. A. J., "Designer Reactions: Biomolecules in the Gas Phase.", *Chemistry in Australia*, 1998, September Issue, 50-53. (O'Hair 100%)

(E3) O'Hair, R. A. J. "The Role of Nucleophile-Electrophile Interactions in the Unimolecular and Bimolecular Gas Phase Ion Chemistry of Peptides and Related Systems", *J. Mass Spectrom.*, 2000, 35, 1377 -1381. (O'Hair 100%)

- (E4) O'Hair, R. A. J., "Organic Gas Phase Ion Chemistry", *Annu. Rep. Prog. Chem., Sect. B*, Chapter 8, **2001**, 393-455. (O'Hair 100%)
- (E5) Waters, T.; O'Hair, R. A. J., "Organic Gas Phase Ion Chemistry", *Annu. Rep. Prog. Chem., Sect. B*, Chapter 9, **2002**, 433-501. (Waters 50%, O'Hair 50%)
- (E6) O'Hair, R. A. J.; Khairallah, G.N., "Gas Phase Ion Chemistry of Transition Metal Clusters: Production, Reactivity and Catalysis.", *J. Cluster Sc.*, **2004**, 3, 331-363. (O'Hair 50%, Khairallah 50%)

### Invited Book Chapters

- (F1) O'Hair, R. A. J., "Gas-Phase Positive and Negative Ion Chemistry of Organophosphorus Compounds via Mass Spectrometric Techniques", in "The Chemistry of Organophosphorus Compounds - Volume 4" (Hartley, F.R.; Ed.; ISBN: 0-471-95706-2), Wiley, New York, Chapter 8, **1996**, 731-765. (O'Hair 100%)
- (F2) O'Hair, R. A. J., "Ion Chemistry and Fragmentation", in "Mass Spectrometry in Drug Discovery" (Rossi, D.T.; Sinz, M.W.; Eds.; ISBN: 0-8247-0607-2), Marcel Dekker, New York, Chapter 4, **2002**, 85 - 124. (O'Hair 100%)
- (F3) Rossi, D.T.; O'Hair, R. A. J., "Future Prospects", in "Mass Spectrometry in Drug Discovery" (Rossi, D.T.; Sinz, M.W.; Eds.; ISBN: 0-8247-0607-2), Marcel Dekker, New York, Chapter 13, **2002**, 399 - 413. (Rossi 70%, O'Hair 30%)
- (F4) O'Hair, R. A. J., "Fragmentation mechanisms of protonated peptides in the gas phase." In: Simpson, R.J. "Proteins and Proteomics: A Laboratory Manual" (ISBN: 0-8247-0607-2), Cold Spring Harbor Laboratory Press, New York, Chapter 8, **2003**, 577 - 584. (O'Hair 100%)

### Invited Encyclopedia Contributions

- (G1) O'Hair, R. A. J., Contribution to "The Encyclopedia of Mass Spectrometry" (Gross, M.L. and Caprioli, R. Eds. in Chief), Volume 1: Theory and Ion Chemistry (Armentrout, P. Ed. ISBN: 0-08-043802-4), Elsevier, Amsterdam, Chapter 9: Organic Ion Chemistry (Positive), Topic: "S<sub>N</sub>2 and related reactions", **2003**, 604-619. (O'Hair 100%)
- (G2) Damrauer, R.; O'Hair, R. A. J., Contribution to "The Encyclopedia of Mass Spectrometry" (Gross, M.L. and Caprioli, R. Eds. in Chief), Volume 1: Theory and Ion Chemistry (Armentrout, P. Ed. ISBN: 0-08-043802-4), Elsevier, Amsterdam, Chapter 10: Organic Ion Chemistry (Negative), Topic: "Organo-aluminum, -silicon, -phosphorus, and -sulfur Chemistry", **2003**, 674-686. (Damrauer 50%, O'Hair 50%)
- (G3) Waters, T.; O'Hair, R. A. J., Contribution to "Encyclopedia of Mass Spectrometry", Volume 7. Fundamentals of and Applications to Organic (and Organometallic)

Compounds (Nibbering, N.M.M. Ed.), General Subject Area G. Metal Ion Complexes: Formation and Reactivity, Topic: "G14. Organometallic catalysis in the gas phase", 2004, in press. (Waters 50%, O'Hair 50%)

#### **Other Invited Scientific Publications**

- (H1) **Book Review:** O'Hair, R. A. J.; Derrick, P.J, *Eur. J. Mass Spectrom.*, **2002**, 8, 333-335, review of "Interpreting Protein Mass Spectra" by A Peter Snyder, Published by Oxford University Press Inc, New York, USA, Copyright 2000 ISBN 0-841-23571-6.
- (H2) **News and Views Announcement:** Green, A.; O'Hair, R. A. J.; "Professor John Bowie Festschrift." *Chemistry in Australia*, **2003**, 70(4, May Issue), 36.
- (H3) **Editorial and Biographical Sketch:** O'Hair, R. A. J.; "John Hamilton Bowie: An Appreciation" *Aust. J. Chem.*, **2003**, 56, 343-348.
- (H4) **Editorial and Historical Sketch:** O'Hair, R. A. J.; "The Australian and New Zealand Society for Mass Spectrometry Conference – A Tradition of Over Thirty Years." *Eur. J. Mass Spectrom.*, **2003**, 9, 525-529.

