CURRICULUM VITAE

LEO RADOM

CONTACT INFORMATION:

Address: School of Chemistry, University of Sydney, Sydney, NSW 2006, AUSTRALIA

Email: radom@chem.usyd.edu.au **TEL:** +61-2-9351 2733 **FAX:** +61-2-9351 3329

BORN: December 13, 1944 **NATIONALITY**: Australian

PRIMARY EDUCATION: Naremburn Primary School (1950–1954)
Artarmon Opportunity School (1955–1956)

SECONDARY EDUCATION: North Sydney Boys' High School (1957–1961)
Maximum pass in Leaving Certificate Examination
24th position in the State.

TERTIARY EDUCATION: University of Sydney (1962–1965)
Double major in Chemistry (3 x High Distinction) and Mathematics (2 x High Distinction, 1 x Distinction)
1st Class Honours, University Medal in Chemistry

DEGREES HELD:

B.Sc. (1st Class Honours) 1966	(University of Sydney)
M.Sc. 1967	(University of Sydney)
Ph.D. 1969	(University of Sydney)
D.Sc. 1982	(Australian National University)

GRADUATE RESEARCH: Physical Organic Chemistry. Professor R.J.W. LeFèvre and Professor S. Sternhell, School of Chemistry, University of Sydney (1965–1969)

POSTDOCTORAL RESEARCH: Computational Quantum Chemistry. Fulbright Fellow with Professor J.A. Pople, Dept of Chemistry, Carnegie-Mellon University (1969–1972)
Queen Elizabeth II Fellow, Research School of Chemistry, Australian National University (1972–1974)

PREVIOUS POSITIONS:
Fellow, Research School of Chemistry, Australian National University (1974–1979)
Senior Fellow, Research School of Chemistry, ANU (1979–1990)
Professorial Fellow, Research School of Chemistry, ANU (1990–1991)
Professor, Research School of Chemistry, ANU (1991–2003)

CURRENT POSITION:
Professor, School of Chemistry, University of Sydney (2003–)
CI, ARC Centre of Excellence for Free Radical Chemistry and Biotechnology (2005–2013)

NAMED LECTURESHIPS AND PROFESSORSHIPS:

Troisième Cycle Lectureship, Switzerland (1988)
Mulliken Lectureship (University of Georgia) (1995)
Marchon Lectureship (University of Newcastle-upon Tyne) (1997)
BBV Foundation Professorship (Autonoma University of Madrid) (1998)
Stranks Lectureship (University of Melbourne) (2001)
Dozor Lectureship (Ben Gurion University) (2003)
Lise-Meitner Lectureship (Hebrew University Jerusalem) (2003)
Raymond Lemieux Lectureship (University of Ottawa) (2005)
Halpern Lectureship (University of Wollongong) (2006)
Schleyer Lectureship (University of Georgia) (2008)
Dillon Steele Lectureship (University of Queensland) (2008)
Löwdin Lectureship (Uppsala University) (2009)
ACENet ICC Lecturer (Atlantic Canada Universities) (2012)
Almlöf-Gropen Lecturer (Universities of Oslo and Tromsø) (2014)

AWARDS and HONOURS:

G.S. Caird Scholarship (1964)
The Union Carbide (Aust.) Ltd. Major Scholarship for Chemistry (1965)
C.S.I.R.O. Junior Postgraduate Studentship (1965)
C.S.R. Chemicals Prize for Chemistry (1965)
University Medal in Chemistry (1965)
Royal Australian Chemical Institute Prize (1965)
C.S.I.R.O. Senior Postgraduate Studentship (1966–1969)
Fulbright Fellowship (1969–1972)
Queen Elizabeth II Fellowship (1972–1974)
Rennie Medal (RACI) (1977)
Fellowship of the Royal Australian Chemical Institute (FRACI) (1979)
Japan Society for Promotion of Science Visiting Fellowship (IMS, Okazaki) (1984)
Lady Davis Visiting Professorship (Hebrew University Jerusalem) (1987)
H.G. Smith Medal (RACI) (1988)
Maccoll Prize (BSMS) (1991)
Archibald Olle Prize (RACI) (1992)
Schrödinger Medal (WATOC) (1994)
Centenary Medal (Australian Government) (2003)
Radom Honour Symposium, PacifiChem (2005)
Fukui Medal (APATCC) (2006)
David Craig Medal (Australian Academy of Science) (2008)
Fellowship of the Royal Society of Chemistry (FRSC) (2008)
AMMA (Association of Molecular Modellers of Australasia) Medal (2010)
RACI Division of Physical Chemistry Medal (RACI) (2010)

ACADEMIES

Fellowship of the Australian Academy of Science (FAA) (1988)
Election to International Academy of Quantum Molecular Science (1989)

PROFESSIONAL SOCIETIES:

American Chemical Society
The Royal Society of Chemistry
Royal Australian Chemical Institute (President, Canberra Branch, 1985)
Sydney University Chemical Society (President, 2006)
World Association of Theoretical and Computational Chemists (WATOC) (President 2005–2011)
Asia Pacific Association of Theoretical and Computational Chemists (APATCC) (President 2012 –)

EDITORIAL BOARDS:

Journal of Computational Chemistry (1979–) (Foundation member)
Journal of Molecular Structure: Theochem (1980–2004) (Foundation member)
Rapid Communications in Mass Spectrometry (1986–1990) (Foundation member)
Advances in Quantum Chemistry (1987)
Structural Chemistry (1988–1993) (Foundation member)
Theoretica Chimica Acta (1989–1991)
Accounts of Chemical Research (1989–1994)
Current Topics in Ion Chemistry and Physics (1991) (Foundation member)
Journal of the Chemical Society, Perkin Transactions 2 (1992– 2002)
European Journal of Mass Spectrometry (1995–) (Foundation member)
Australian Journal of Chemistry (1995–2001)
International Journal of Mass Spectrometry and Ion Processes (1996–1999)
International Journal of Quantum Chemistry (1997–2005)
Journal of Physical Organic Chemistry (1999–2005)
Journal of Chemical Theory and Computation (2005–) (Foundation member)
Molecular Physics (2007–2012)
Chemical Physics Letters (2008–)
Wiley Interdisciplinary Reviews (WIREs): Computational Molecular Science (2008–)

PUBLICATIONS:

Approximately 500, see attached list

CITATIONS

Hirsch Index of 84, which is the highest of Australian chemists. Average citations per article 63.81. Publication 321 (1996) as at October 2013 had received 4718 citations.

VISITING APPOINTMENTS:

1977/1978	University of California, Irvine (3 months), Berkeley (4 months)
1983	Ben Gurion University of the Negev, Beer Sheva (1 month)
1984	Institute of Molecular Science, Okazaki (1 month)
1987/1988	Hebrew University, Jerusalem (5 weeks)
1994	National University of Singapore (2 weeks)
1997	University of Newcastle upon Tyne (1 week)
1998	Universidad Autonoma de Madrid (2 weeks)

PLENARY AND INVITED CONFERENCE LECTURES:

Approximately 100. Since 1998, these have included conferences dealing with physical organic chemistry, radicals, reactive intermediates, B_{12} chemistry, computational science, and theoretical chemistry in Miraflores (Spain, 1998), Mexico City (Mexico, 1998), Florianopolis (Brazil, 1998), Amelia Island (USA, 1999), Plymouth (USA, 1999), New Orleans (USA, 1999), Hong Kong (2000), Menton (France, 2000), Marburg (Germany, 2000), Honolulu (USA, 2000), Seattle (USA, 2001), York (England, 2002), Nottingham (England, 2002), Lugarno (Switzerland, 2002), Oslo (Norway, 2003), Singapore (2003), Gyeongju (Korea, 2004), Okazaki (Japan, 2004), Sydney (Australia, 2004), Philadelphia (USA, 2004), Canberra (Australia, 2004), Cape Town (South Africa, 2005), Bangkok (Thailand, 2005), Honolulu (USA, 2005), Okazaki (Japan, 2006), Canberra (Australia, 2006), Sydney (Australia, 2006), Maui (USA, 2007), Budapest (Hungary, 2007), Beijing (China, 2007), Ubonratchathani (Thailand, 2008), Santiago de Compostela (Spain, 2008), Heron Island (Australia, 2008), Tokyo (Japan, 2009), Halifax (Canada, 2009), Primosten (Croatia, 2009), Erlangen (Germany, 2009), Canberra (Australia, 2010), Berkeley (USA, 2010), Bologna (Italy, 2010), Melbourne (Australia, 2010), Honolulu (USA, 2010), Santiago de Compostela (Spain, 2011), Tokyo (Japan, 2010), Canberra (Australia, 2011), Wollongong (Australia, 2011), Rotorua (New Zealand, 2011), Ghent (Belgium, 2012), Philadelphia (USA, 2012), Gyeongju (South Korea, 2013).

CONFERENCE ORGANIZATION

Since 1987, these include conferences in Budapest (Hungary, 1987), Haifa (Israel, 1990), Toronto (Canada, 1990), Canberra (Australia, 1992), Honolulu (USA, 1995), Jerusalem (Israel, 1996), London (England, 1999), Honolulu (USA, 2000), San Diego (USA, 2002), Melbourne (Australia, 2003), Singapore (2003), Okazaki (Japan, 2004), Shanghai (China, 2004), Philadelphia (USA, 2004), San Diego (USA, 2005), Bangkok (Thailand, 2005), Warsaw (Poland, 2006), Santiago de Compostela (Spain, 2008), Sydney (Australia, 2008), Busan (Korea, 2010), Durham (England, 2012), Ottawa (Canada, 2014), Honolulu (USA, 2015) and Sydney (2016).

LIST OF PUBLICATIONS

Leo Radom

1. Molecular Polarisability. The Anistotropic Polarisabilities of Anthracene and Several Halogenated Anthracenes.
   R.J.W. Le Fèvre, L. Radom and G.L.D. Ritchie, *J. Chem. Soc., B*, 595-598 (1967).
2. Molecular Polarisability. The Conformations of Diphenyl Ketone, Dimesityl Ketone, and Mesityl Phenyl Ketone as Solutes.
   P.H. Gore, J.A. Hoskins, R.J.W. Le Fèvre, L. Radom and G.L.D. Ritchie, *J. Chem. Soc., B*, 741-743 (1967).
3. Molecular Polarisability. Carbon-Carbon Bond Polarisabilities in Relation to Bond Lengths.
   R.J.W. Le Fèvre and L. Radom, *J. Chem. Soc., B*, 1295-1298 (1967).
4. Molecular Polarisability. The Molar Kerr Constants of Aniline and of Three Substituted Anilines in a Variety of Non-Polar Media.
   M.J. Aroney, R.J.W. Le Fèvre, L. Radom and G.L.D. Ritchie, *J. Chem. Soc., B*, 507-512 (1968).
5. Molecular Polarisability. The Conformations of Some 9-Substituted Anthracenes as Solutes.
   R.J.W. Le Fèvre, L. Radom and G.L.D. Ritchie, *J. Chem. Soc., B*, 775-778 (1968).
6. Molecular Polarisability. The Conformations of Some Polynuclear Aromatic Hydrocarbons.
   E.D. Bergmann, M. Rabinovitz, M.J. Aroney, R.J.W. Le Fèvre, L. Radom and G.L.D. Ritchie, *J. Chem. Soc., B*, 1551-1554 (1968).
7. Proton Magnetic Resonance Spectra of Some Aromatic Amines and Derived Amides.
   R.F.C. Brown, L. Radom, S. Sternhell and I.D. Rae, *Can. J. Chem.*, **46,** 2577-2587 (1968).
8. Molecular Polarisability. The Conformation of 9-Benzoylanthracene.
   P.H. Gore, J.A. Hoskins, R.J.W. Le Fèvre, L. Radom and G.L.D. Ritchie, *J. Chem. Soc., B*, 227-230 (1969).
9. Molecular Polarisability. The Conformations of 1-Acetyl and 1,5-Diacetylnaphthalenes and -anthracenes.
   P.H. Gore, J.A. Hoskins, C.K. Thadani, R.J.W. Le Fèvre, L. Radom and G.L.D.Ritchie, *J. Chem. Soc., B*, 426-429 (1969).
10. Molecular Polarisability. The Dipole Moments and Molar Kerr Constants of 1,3- and 1,4-Diacetylbenzenes and their Polymethylated Derivatives.
    P.H. Gore, J.A. Hoskins, R.J.W. Le Fèvre, L. Radom and G.L.D.Ritchie, *J. Chem. Soc., B*, 485-488 (1969).
11. Polarity, Polarisability and Association in Methyl- and Chloro- anilines.
    R.J.W. Le Fèvre, L. Radom and G.L.D. Ritchie, *J. Chem. Soc., B*, 913-918 (1969).
12. Molecular Orbital Theory of Bond Separation.
    R. Ditchfield, W.J. Hehre, J.A. Pople and L. Radom, *Chem. Phys. Lett.*, **5**, 13-14

(1970).

13. Molecular Orbital Theory of the Electronic Structure of Organic Compounds. IV. Internal Rotation in Hydrocarbons Using a Minimal Slater-Type Basis.
L. Radom and J.A. Pople, *J. Am. Chem. Soc.*, **92**, 4786-4795 (1970).
14. Molecular Orbital Theory of the Electronic Structure of Organic Compounds. V. Molecular Theory of Bond Separation.
W.J. Hehre, R. Ditchfield, L. Radom and J.A. Pople, *J. Am. Chem. Soc.*, **92**, 4796-4801 (1970).
15. Rotational Barriers of Alkyl Cations.
L. Radom, J.A. Pople, V. Buss and P.v.R. Schleyer, *J. Am. Chem. Soc.*, **92**, 6380-6382 (1970).
16. Rotational Barriers in 1-Propyl Cations.
L. Radom, J.A. Pople, V. Buss and P.v.R. Schleyer, *J. Am. Chem. Soc.*, **92**, 6987-6988 (1970).
17. Molecular Polarisability. The Dipole Moments and Molar Kerr Constants of Benzaldehyde, Acetopheneone, 1,4-Diformylbenzene, and 1,4-Diacetyl- benzene.
P.H. Gore, P.A. Hopkins, R.J.W. Le Fèvre, L. Radom and G.L.D. Ritchie, *J. Chem. Soc., B*, 120-123 (1971).
18. Molecular Polarisability. Association of Some Aromatic Aldehydes and Ketones with Benzene.
P.A. Hopkins, R.J.W. Le Fèvre, L. Radom and G.L.D. Ritchie, *J. Chem. Soc., B*, 574-576 (1971).
19. Molecular Orbital Theory of the Electronic Structure of Organic Compounds. VII. A Systematic Study of Energies, Conformations, and Bond Interactions.
L. Radom, W.J. Hehre and J.A. Pople, *J. Am. Chem. Soc.,* **93**, 289-300 (1971).
20. Structures and Relative Stabilities of $C_3H_7^+$ Cations.
L. Radom, J.A. Pople, V. Buss and P.v.R. Schleyer, *J. Am. Chem. Soc.,* **93**, 1813-1815 (1971).
21. Molecular Orbital Theory of the Electronic Structure of Organic Compounds. VIII. Geometries and Energies of C_3 Hydrocarbons.
L. Radom, W.A. Lathan, W.J. Hehre and J.A. Pople, *J. Am. Chem. Soc.*, **93**, 5339-5342 (1971).
22. Conformations and Heats of Formation of Organic Molecules by Use of a Minimal Slater Type Basis.
L. Radom, W.J. Hehre and J.A. Pople, *J. Chem, Soc., A*, 2299-2303 (1971).
23. Molecular Polarisability. Conformations of Some Substituted Styrenes.
P.L. Britton, C.L. Cheng, R.J.W. Le Fèvre, L. Radom and G.L.D. Ritchie, *J. Chem. Soc., B*, 2100-2103 (1971).
24. Molecular Orbital Theory of the Electronic Structure of Organic Compounds. XI. Geometries and Energies of $C_3H_7^+$ Cations.
L. Radom, J.A. Pople, V. Buss and P.v.R. Schleyer, *J. Am. Chem. Soc.,* **94**, 311-321 (1972).
25. Molecular Orbital Theory of the Electronic Structure of Organic Compounds. XII. Conformations, Stabilities and Charge Distributions in Monosubstituted Benzenes.
W.J. Hehre, L. Radom and J.A. Pople, *J. Am. Chem. Soc.,* **94**, 1496-1504 (1972).
26. Molecular Orbital Theory of the Electronic Structure of Organic Compounds.

XIII. Fourier Component Analysis of Internal Rotation Potential Functions in Saturated Molecules.
L. Radom, W.J. Hehre and J. A. Pople, *J. Am. Chem. Soc.,* **94**, 2371-2381 (1972).

27. Distortion of the Double Bond in Ethylene.
L. Radom, J.A. Pople and W.L. Mock, *Tetrahedron Lett.*, 479-482 (1972).

28. Torsional Barriers in *para*-Substituted Phenols from *Ab Initio* Molecular Orbital Theory and Far Infrared Spectroscopy.
L. Radom, W.J. Hehre, J.A. Pople, G.L. Carlson and W.G. Fateley, *J. Chem. Soc., Chem. Commun.*, 308-309 (1972).

29. *Ab Initio* Molecular Orbital Theory of Organic Molecules.
L. Radom and J.A. Pople in *MTP International Review of Science (Theoretical Chemistry)*, W. Byers Brown, Ed., Butterworth, London, 1972, pp 71-112.

30. Molecular Orbital Theory of the Electronic Structure of Organic Compounds. XVI. Conformations and Stabilities of Substituted Ethyl, Propyl, and Butyl Cations.
L. Radom, J.A. Pople and P.v.R. Schleyer, *J. Am. Chem. Soc.,* **94**, 5935-5945 (1972).

31. Internal Rotation in Some Organic Molecules Containing Methyl, Amino, Hydroxyl and Formyl Groups.
L. Radom, W.A. Lathan, W.J. Hehre and J.A. Pople, *Aust. J. Chem.,* **25**, 1601-1612 (1972).

32. Inversion Barriers in *para*-Substituted Anilines from *Ab Initio* Molecular Orbital Theory.
W.J. Hehre, L. Radom and J. A. Pople, *J. Chem. Soc., Chem. Commun.*, 669-670 (1972).

33. The Application of *Ab Initio* Molecular Orbital Theory to the Anomeric Effect. A Comparison of Theoretical Predictions and Experimental Data on Conformations and Bond Lengths in Some Pyranoses and Methyl Pyranosides.
G.A. Jeffrey, J.A. Pople and L. Radom, *Carbohyd. Res.,* **25**, 117-131 (1972).

34. Strong Conformational Consequences of Hyperconjugation.
R. Hoffmann, L. Radom, J.A. Pople, P.v.R. Schleyer, W.J. Hehre and L. Salem, *J. Am. Chem. Soc.,* **94**, 6221-6223 (1972).

35. Internal Rotation Potentials in Biological Molecules.
J. A. Pople and L.Radom, in *Jerusalem Symposia on Quantum Aspects of Chemistry and Biochemistry*, **V**, B. Pullman and E.D. Bergmann, Eds., pp 747-759, Academic Press, New York (1973).

36. Molecular Orbital Theory of the Electronic Structure of Organic Compounds. XVII. Internal Rotation in 1,2-Disubstituted Ethanes.
L. Radom, W.A. Lathan, W.J. Hehre and J.A. Pople, *J. Am. Chem. Soc.,* **95**, 693-698 (1973).

37. Molecular Orbital Theory of the Electronic Structure of Organic Compounds. XVIII. Conformations and Stabilities of Trisubstituted Methanes.
W.A. Lathan, L. Radom, W.J. Hehre and J.A. Pople, *J. Am. Chem. Soc.,* **95**, 699-703 (1973).

38. Structures and Stabilities of Three-Membered Rings from *Ab Initio* Molecular Orbital Theory.
W. A. Lathan, L. Radom, P.C. Hariharan, W.J. Hehre and J.A. Pople, *Fortsch.*

Chem. Forsch., **40**, 1-45 (1973).

39. Molecular Orbital Theory of the Electronic Structure of Organic Compounds. XIX. Geometries and Energies of $C_3H_5^+$ Cations.
L. Radom, P.C. Hariharan, J.A. Pople and P.v.R. Schleyer, *J. Am. Chem. Soc.,* **95**, 6531-6544 (1973).

40. Effects of Substituents on the Mechanism of Stereomutation of Allyl Cations.
L. Radom, J.A. Pople and P.v.R. Schleyer, *J. Am. Chem. Soc.,* **95**, 8193-8195 (1973).

41. Facilitation of Intramolecular 1,2-Shifts in Radicals by Protonation, and the Mechanism of Reactions Catalysed by 5'-Deoxyadenosylcobalamin.
B.T. Golding and L. Radom, *J. Chem. Soc., Chem. Commun.*, 939-941 (1973).

42. Molecular Orbital Theory of the Electronic Structure of Organic Compounds. XX. $C_3H_7^+$ Cations with a Polarized Basis Set.
P.C. Hariharan, L. Radom, J.A. Pople and P.v.R. Schleyer, *J. Am. Chem. Soc.,* **96**, 599-601 (1974).

43. Rotational Barriers in Substituted Ethyl Radicals.
L. Radom, J. Paviot, J.A. Pople and P.v.R. Schleyer, *J. Chem. Soc., Chem. Commun.*, 58-60 (1974).

44. *Ab Initio* Molecular Orbital Calculations on Acetyl Cations. Relative Hyperconjugative Abilities of C-X Bonds.
L. Radom, *Aust. J. Chem.*, **27**, 231-239 (1974).

45. An Additivity Scheme for Conformational Energies in Substituted Ethanes.
L. Radom and P.J. Stiles, *J. Chem. Soc., Chem. Commun.*, 190-192 (1974).

46. The Photoelectron Spectrum of Butatriene.
F. Brogli, E. Heilbronner, E. Kloster-Jensen, A. Schmelzer, A.S. Manocha, J.A. Pople and L. Radom, *Chem. Phys.,* **4**, 107-119 (1974).

47. *Ab Initio* Molecular Orbital Calculations on Anions. Determination of Gas Phase Acidities.
L. Radom, *J. Chem. Soc., Chem. Commun.*, 403-404 (1974).

48. The Application of *Ab Initio* Molecular Orbital Theory to Structural Moieties of Carbohydrates.
G.A. Jeffrey, J.A. Pople and L. Radom, *Carbohyd. Res.,* **38**, 81-95 (1974).

49. On the Interaction of Geminal Fluorines and Geminal Cyano Groups. "Anomalous" Ordering of Rotational Barriers in Fluoroethanes.
L. Radom and P.J. Stiles, *Tetrahedron Lett.*, 789-792 (1975).

50. Effects of Alkyl Groups on Acidities and Basicities in the Gas Phase. An *Ab Initio* Molecular Orbital Study.
L. Radom, *Aust. J. Chem.,* **28**, 1-6 (1975).

51. A Pairwise Additivity Scheme for Conformational Energies of Substituted Ethanes.
D.P. Craig, L. Radom and P.J. Stiles, *Proc. Roy. Soc.,* **343A**, 1-10 (1975).

52. Intramolecular Chiral Discrimination between Meso and *d,l* Isomers.
D.P. Craig, L. Radom and P.J. Stiles, *Proc. Roy. Soc.,* **343A**, 11-16 (1975).

53. An *Ab Initio* Molecular Orbital Study of Ethylenedione (O=C=C=O).
R.C. Haddon, D. Poppinger and L. Radom, *J. Am. Chem. Soc.,* **97**, 1645-1649 (1975).

54. Theoretical Predictions of the Molecular Structure of Sulphur Tetrafluoride.

L. Radom and H.F. Schaefer, *Aust. J. Chem.,* **28**, 2069-2072 (1975).

55. Molecular Orbital Theory of the Electronic Structure of Organic Compounds. XXII. Structures and Stabilities of $C_3H_3^+$ and C_3H^+ Cations.
L. Radom, P.C. Hariharan, J.A. Pople and P.v.R. Schleyer, *J. Am. Chem. Soc.,* **98**, 10-14 (1976).

56. Conformations of Vinyl Formate and Vinyl Acetate.
M.J. Aroney, E.A.W. Bruce, I.G. John, L.Radom and G.L.D. Ritchie, *Aust. J. Chem.,* **29**, 581-587 (1976).

57. Molecular Orbital Theory of the Electronic Structure of Molecules. 29. The Interaction of H_2 with Simple Lewis Acids.
J.B. Collins, P.v.R. Schleyer, J.S. Binkley, J.A. Pople and L. Radom, *J. Am. Chem. Soc.,* **98**, 3436-3441 (1976).

58. 1-Aza-4-boratricylco[2.2.2.$0^{1,4}$] octane and 1-Aza-4-borabicyclo{2.2.2]-octane: Stable Bond-Stretch Isomers? An *Ab Initio* Study.
M.N. Paddon-Row, L. Radom, and A.R. Gregory, *J. Chem. Soc., Chem. Commun.,* 427-429 (1976).

59. Structures of Simple Anions from *Ab Initio* Molecular Orbital Calculations.
L. Radom, *Aust. J. Chem.,* **29**, 1635-1640 (1976).

60. Molecular Orbital Theory of the Electronic Structure of Organic Compounds. 28. Geometries and Energies of Singlet and Triplet States of C_3H_2 Hydrocarbons.
W.J. Hehre, J.A. Pople, W.A. Lathan, L. Radom, E. Wasserman and Z.R. Wasserman, *J. Am. Chem. Soc.,* **98**, 4378-4383 (1976).

61. On the Mechanism of Action of Adenosylcobalamin.
B.T. Golding and L. Radom, *J. Am. Chem. Soc.,* **98**, 6331-6338 (1976).

62. Molecular Orbital Theory of Carbocations.
L. Radom, D. Poppinger and R.C. Haddon, in *Carbonium Ions*, Vol. 5, Chapter 38, G.A. Olah and P.v.R. Schleyer, Eds., Interscience, New York, pp 2303-2426 (1976).

63. Molecular Conformations of Methyl Formate and Methyl Vinyl Ether from *Ab Initio* Molecular Orbital Calculations.
I.G. John and L. Radom, *J. Mol. Struct.,* **36**, 133-147 (1977).

64. Molecular Anions.
L. Radom, in *Modern Theoretical Chemistry*, H.F. Schaefer, Ed., Plenum Press, New York, pp 333-356 (1977).

65. Bond-Stretch Isomerism in [2.2.2] Propellanes.
A.R. Gregory, M.N. Paddon-Row, L.Radom and W.D. Stohrer, *Aust. J. Chem.,* **30**, 473-485 (1977).

66. The Molecular Structure of Ammonia Oxide (NH_3O). An *Ab Initio* Study.
L. Radom, J.S. Binkley and J.A. Pople, *Aust. J. Chem.,* **30**, 699-703 (1977).

67. Molecular Conformations of Formic Anhydride and Divinyl Ether. An *Ab Initio* Molecular Orbital Study.
I.G. John and L.Radom, *J. Mol. Struct.,* **39**, 281-293 (1977).

68. On the Jahn-Teller Distortion in the Cyclopropenyl Radical.
D. Poppinger, L. Radom and M.A. Vincent, *Chem. Phys.,* **23**, 437-442 (1977).

69. Conformations of Furan-, Pyrrole-, and Pyridine-carbaldehydes: An *Ab Initio* Molecular Orbital Study.
I.G. John, G.L.D. Ritchie and L. Radom, *J. Chem. Soc., Perkin Trans.* **2**, 1601-

1607 (1977).

70. Vinyl Alcohol: A Stable Molecule.
W.J. Bouma, D. Poppinger and L. Radom, *J. Am. Chem. Soc.,* **99**, 6443-6444 (1977).

71. On the Limits of Stability of Multiply Charged Monocyclic Aromatic Cations: $C_3H_3^+$, $C_4H_4^{2+}$, $C_5H_5^{3+}$, $C_6H_6^{4+}$, $C_7H_7^+$, $C_8H_8^{2+}$, $C_9H_9^{3+}$.
L. Radom and H.F. Schaefer, *J. Am. Chem. Soc.,* **99**, 7522-7526 (1977).

72. A. Theoretical Study of the CHNO Isomers.
D. Poppinger, L. Radom and J.A. Pople, *J. Am. Chem. Soc.,* **99**, 7806-7816 (1977).

73. An *Ab Initio* Molecular Orbital Study of Structures and Energies of Spiro Compounds: Spiropentane, Spiropentene, Spiropentadiene, Spiro[2,4]hepta-4,6-diene, Spiro[2,4]heptatriene, and Spiro[4,4]-nonatetraene.
J. Kao and L. Radom, *J. Am. Chem. Soc.,* **100**, 760-767 (1978).

74. An *Ab Initio* Molecular Orbital Study of the Structure and Properties of Propadienone (Methyleneketene).
L. Radom, *Aust. J. Chem.,* **31**, 1-9 (1978).

75. Multiply Charged Aromatic Cations: The Heptalenium Dication.
D.P. Craig, L. Radom and H.F. Schaefer, *Aust. J. Chem.,* **31**, 261-266 (1978).

76. Molecular Structures and Potential Function for the Deformation of Cyclopropane, Cyclopropene, Cyclobutane and Cyclopentadiene.
J. Kao and L. Radom, *J. Am. Chem. Soc.,* **100**, 379-385 (1978).

77. The Structure of Vinyl Alcohol.
W.J. Bouma and L. Radom, *J. Mol. Struct.,* **43**, 267-271 (1978).

78. *Ab Initio* Study of the Benzene Radical Anion.
A.L. Hinde, D. Poppinger and L. Radom, *J. Am. Chem. Soc.,* **100**, 4681-4685 (1978).

79. A Theoretical Study of Substituted CHNO Isomers.
D. Poppinger and L. Radom., *J. Am. Chem Soc.,* **100**, 3674-3685 (1978).

80. Pronounced Conformational Preferences in 1,4-Disubstituted But-2-ynes.
L. Radom, P.J. Stiles and M.A. Vincent, *J. Mol. Struct.,* **48**, 259-270 (1978).

81. Conformations, Stabilities, and Charge Distributions in 2- and 3- Monosubstituted Furans: An *Ab Initio* Molecular Orbital Study.
I.G. John and L. Radom, *J. Am. Chem. Soc.,* **100**, 3981-3991 (1978).

82. Prototypes for Aliphatic and Aromatic Diazonium Ions. An *Ab Initio* Study of the Methane- and Benzene- Diazonium Ions.
M.A. Vincent and L. Radom, *J. Am. Chem. Soc.,* **100**, 3306-3312 (1978).

83. Keto-Enol Tautomerism. Relative Stabilization of Enol Isomers.
W.J. Bouma and L. Radom, *Aust. J. Chem.,* **31**, 1167-1176 (1978).

84. A Prototype 1,2-Disubstituted Ethane with *Cis* and *Trans* Rotational Isomers: 1-Fluoro-2-lithioethane.
L. Radom, P.J. Stiles and M.A. Vincent, *Nouv. J. Chim.,* **2**, 115-116 (1978).

85. Structural and Energetic Predictions for Anions from a Modified Hartree-Fock Procedure.
D. Poppinger and L. Radom, *Chem. Phys.,* **30**, 415-422 (1978).

86. An *Ab Initio* Molecular Orbital Study of Structures and Energies of Spiro-Compounds: Spiro[3.3]heptane and Spiro[3.3]hepta-1,5-diene.

J. Kao and L. Radom, *Tetrahedron,* **34**, 2515-2521 (1978).

87. Fluorine Peroxide (FOOF): A Problem Molecule for Theoretical Structural Predictions.
R.R. Lucchese, H.F. Schaefer, W.R. Rodwell and L. Radom, *J. Phys. Chem.*, **68**, 2507-2508 (1978).

88. Theoretical Studies of the Effect of Electron Correlation on the Geometry and Barriers to Internal Rotation in Hydrogen Peroxide.
W.R. Rodwell, N.R. Carlsen and L. Radom, *Chem. Phys.*, **31**, 177-186 (1978).

89. An *Ab Initio* Approach to Creating a Simple Stable Enol.
W. J. Bouma and L. Radom, *Aust. J. Chem.*, **31**, 1649-1660 (1978).

90. Theoretical Characterization of an Unusual Isomer of $C_2H_4O^{+\bullet}$: An Open Ethylene Oxide Cation.
W.J. Bouma, J.K. MacLeod and L. Radom, *Nouv. J. Chim.,* **2**, 439-440 (1978).

91. Influence of Substituent Electronegatives on Conformational Preferences in 1,2-Disubstituted Ethanes.
L. Radom, P.J. Stiles and M.A. Vincent, *J. Mol. Struct.,* **48**, 431-440 (1978).

92. Experimental Proof of the Existence of a Fourth Stable Gas Phase $C_2H_4O^{+\bullet}$ Isomer: The Open Ethylene Oxide Ion.
W.J. Bouma, J.K. MacLeod and L. Radom, *J. Chem. Soc., Chem. Commun.*, 724-725 (1978).

93. Does a Methyl Substituent Stabilize or Destabilize Anions?
A. Pross and L. Radom, *J. Am. Chem. Soc.*, **100**, 6572-6575 (1978).

94. Nitrosyl Cyanide and Related Aspects of the ONCN Potential Surface.
B.G. Gowenlock and L. Radom, *Aust. J. Chem.,* **31**, 2349-2353 (1978).

95. *Ab Initio* Molecular Orbital Studies of Sigmatropic Rearrangements.
W. J. Bouma, M.A.Vincent and L. Radom, *Int. J. Quantum Chem.,* **14**, 767-777 (1978).

96. Conformations, Stabilities and Charge Distributions in 2- and 3- Monosubstituted Thiophenes: An *Ab Initio* Molecular Orbital Study.
J. Kao and L. Radom, *J. Am. Chem. Soc.*, **101**, 311-318 (1979).

97. A Model Theoretical Study for Alkylation in Benzimidazoles: *Ab Initio* Electrostatic Potentials.
A.L. Hinde, L. Radom and M. Rasmussen, *Aust. J. Chem.,* **32**, 11-20 (1979).

98. Is Formamide Planar or Non-Planar?
N.R. Carlsen, L. Radom, N.V. Riggs and W.R. Rodwell, *J. Am. Chem. Soc.,* **101**, 2233-2234 (1979).

99. Nitrosoacetaldehyde and its Enol and Oxime Isomers. A Theoretical Investigation of an Asymmetric 1,5-Sigmatropic Hydrogen Shift.
W. J. Bouma and L. Radom, *J. Am. Chem. Soc.,* **101**, 3487-3490 (1979).

100. Is the Carboxylic Acid-Fluoride Bond Really the Strongest Type of Hydrogen Bond?
W.J. Bouma and L. Radom, *Chem. Phys. Lett.,* **64**, 216-218 (1979).

101. Conformations, Stabilities and Charge Distributions in 2- and 3- Monosubstituted Pyrroles: An *Ab Initio* Molecular Orbital Study.
J. Kao, A. L. Hinde and L. Radom, *Nouv. J. Chim.,* **3**, 473-485 (1979).

102. Creation of a Simple Stable Enol. The Stabilizing Properties of the Diazonium Substituent.

M.J. Ballard, W.J. Bouma, L. Radom and M.A. Vincent, *Aust. J. Chem..,* **32**, 1401-1406 (1979).

103. An *Ab Initio* Molecular Orbital Study of the Structures and Stabilities of the $C_2H_4O^{+\bullet}$ Isomers.
W.J. Bouma, J.K. MacLeod and L. Radom, *J. Am. Chem. Soc.,* **101**, 5540-5545 (1979).

104. Intramolecular Interactions through Triple Bonds. Internal Rotation in Aminoborylpolyynes, $NH_2(C{\equiv}C)_nBH_2$.
L. Radom and M.A. Vincent, *Israel J. Chem.*, **19**, 305-308 (1980).

105. The Hartree-Fock Geometry of Ammonia.
W.R. Rodwell and L. Radom, *J. Chem. Phys.,* **72**, 2205-2206 (1980).

106. An *Ab Initio* Molecular Orbital Study of the $CH_2O^{+\bullet}$ Isomers: The Stability of the Hydroxymethylene Molecular Cation.
W. J. Bouma, J.K. MacLeod and L. Radom, *Int. J. Mass Spectrom. Ion Phys.,* **33**, 87-93 (1980).

107. A Theoretical Approach to Substituent Effects. Stabilities and Rotational Barriers of β-Substituted Ethyl Anions.
A. Pross and L. Radom, *Aust. J. Chem.,* **33**, 241-248 (1980).

108. Saddle-Point Geometries and Barriers to Internal Rotation of Formamide: An *Ab Initio* Study.
L. Radom and N.V. Riggs, *Aust. J. Chem.,* **33**, 249-255 (1980).

109. Structures and Stabilities of $C_3H_6O^{+\bullet}$ Isomers. An *Ab Initio* Molecular Orbital Study.
W.J. Bouma, J.K. MacLeod and L. Radom, *J. Am. Chem. Soc.,* **102**, 2246-2252 (1980).

110. Theoretical Approach to Substituent Effects. Phenols and Phenoxide Ions.
A. Pross, L. Radom and R.W. Taft, *J. Org. Chem.,* **45**, 818-826 (1980).

111. A Theoretical Approach to Substituent Effects. Structural Consequences of Methyl Hyperconjugation. Methyl Tilt Angles and C-H Bond Lengths.
A. Pross, L. Radom and N.V. Riggs, *J. Am. Chem. Soc.,* **102**, 2253-2259 (1980).

112. A Theoretical Approach to the Birch Reduction. Structures and Stabilities of the Radical Anions of Substituted Benzenes.
A.J. Birch, A.L. Hinde and L. Radom, *J. Am. Chem. Soc.,* **102**, 3370-3376 (1980).

113. A Theoretical Approach to Substituent Effects. Interaction Between Directly Bonded Groups in the Isoelectronic Series XNH_3^+, XCH_3 and XBH_3^-.
A. Pross and L. Radom, *Tetrahedron,* **36,** 673-676 (1980).

114. A Theoretical Approach to Substituent Effects. Stabilities and Conformational Preferences in β-Substituted Ethyl Radicals.
A. Pross and L. Radom, *Tetrahedron,* **36**, 1999-2003 (1980).

115. Nitrosomethane and its Nitrone and Oxime Isomers. A Theoretical Study of 1,2- and 1,3-Intramolecular Hydrogen Shifts.
P. D. Adeney, W.J. Bouma, L. Radom and W.R. Rodwell, *J. Am. Chem. Soc.,* **102**, 4069-4074 (1980).

116. A Theoretical Approach to Substituent Effects. Interaction Between Directly Bonded Goups in the Neutrals X-NH_2, X-OH and X-F, and the Anions X-NH^- and X-O^-.

A.L. Hinde, A. Pross and L. Radom, *J. Comput. Chem.,* **1**, 118-128 (1980).

117. A Theoretical Approach to the Birch Reduction. Structures and Stabilities of Cyclohexadienyl Radicals.
A.J. Birch, A.L. Hinde and L. Radom, *J. Am. Chem. Soc.,* **102**, 4074-4080 (1980).

118. A Theoretical Approach to Substituent Effects. Examination of Phenoxides and Anilides as Models for Benzyl Anions.
G. Kemister, A. Pross, L. Radom and R.W. Taft, *J. Org. Chem.,* **45**, 1056-1060 (1980).

119. The C_7H_6 Isomers: Cyclopheptatrienylidene and Phenylcarbene.
L. Radom, H.F. Schaefer and M.A. Vincent, *Nouv. J. Chim.,* **4**, 411-415 (1980).

120. *Ab Initio* Studies of 1,3-Sigmatropic Rearrangements: Effects of Basis Set and Electron Correlation.
W.R. Rodwell, W.J. Bouma and L. Radom. *Int. J. Quantum Chem.,* **18**, 107-116 (1980).

121. Structures and Thermodynamic Stabilities of the C_2H_4O Isomers: Acetaldehyde, Vinyl Alcohol and Ethylene Oxide.
W.J. Bouma, L. Radom and W.R. Rodwell, *Theor. Chim. Acta,* **56**, 149-155 (1980).

122. *Ab Initio* Studies of Reaction Mechanisms.
L. Radom, in *Proceedings of the Summer Seminar/Workshop in Molecular Physics and Quantum Chemistry*, Lecture 1.2, pp 1-28, Wollongong University Press, 1980.

123. A Theoretical Approach to Substituent Effects. Structural Consequences of Electrostatic and Orbital Interactions in Model Mono- and Di-Substituted Methanes.
A. Pross and L. Radom, *J. Comput. Chem.,* **1**, 295-300 (1980).

124. *Ab Initio* Studies on Amides: Conformational Preferences of Formimide and Barriers to Interconverstion of the Conformers.
L. Radom and N.V. Riggs, *Aust. J. Chem.*, **33**, 1635-1642 (1980).

125. A Theoretical Approach to the Birch Reduction. Structures and Stabilities of Cyclohexadienyl Anions.
A.J. Birch, A.L. Hinde and L. Radom, *J. Am. Chem. Soc.,* **102,** 6430-6437 (1980).

126. Influence of Basis Set and Electron Correlation on Calculated Barriers to 1,2-Hydrogen Shifts. The Oxoniomethylene Cation: A New CH_3O^+ Isomer?
R.H. Nobes, L. Radom and W.R. Rodwell, *Chem. Phys. Lett.,* **74**, 269-272 (1980).

127. Selective Ion/Molecule Reactions of the Stable $C_2H_4O^{+\bullet}$ Isomers.
W.J. Bouma, J.K. MacLeod and L. Radom, *Adv. Mass Spectrom.,* 178-185 (1980).

128. *Ab Initio* Studies on Amides: Conformational Preferences of Diacetamide and Barriers to Interconversion of the Conformers.
L. Radom and N.V. Riggs, *Aust. J. Chem.,* **33**, 2337-2342 (1980).

129. Experimental Proof for the Gas-Phase Existence of the C...C Ring-Opened Trimethylene Oxide Cation: A New Stable $C_3H_6O^{+\bullet}$ Isomer.
B.C. Baumann, J.K. MacLeod and L. Radom, *J. Am. Chem. Soc.,* **102**, 7927-7928

(1980).

130. A Theoretical Approach to Substituent Interactions in Substituted Benzenes.
A. Pross and L. Radom, *Prog. Phys. Org. Chem.,* **13**, 1-61 (1981).

131 The Geometric and Electronic Structures of Oxocarbons. An *Ab Initio* Molecular Orbital Study.
L. Farnell, L. Radom and M.A. Vincent, *J. Mol Struct., Theochem,* **76**, 1-10 (1981).

132. A Theoretical Approach to the Birch Reduction. Structures and Stabilities of Substituted Cyclohexadienes.
A.J. Birch, A.L. Hinde and L. Radom, *J. Am. Chem. Soc.,* **103**, 284-289 (1981).

133. An Analysis of the Acidities of 3- and 4- Substituted Pyridinium and Anilinium Ions.
M. Taagepera, K.D. Summerhays, W.J. Hehre, R.D. Topsom, A. Pross, L. Radom and R.W. Taft, *J. Org. Chem.,* **46**, 891-903 (1981).

134. *Ab Initio* Studies on Amides: Triformamide.
L. Radom and N.V. Riggs, *Aust. J. Chem.,* **34**, 7-11 (1981).

135. A Theoretical Approach to Substituent Effects. Structures and Stabilities of Carbanions XCH_2^-.
A. Pross, D.J. DeFrees, B.A. Levi, S.K. Pollack, L. Radom and W.J. Hehre, *J. Org. Chem.,* **46**, 1693-1699 (1981).

136. A Theoretical Study of Propadienone and its Isomers Propynal and Cyclopropenone.
A. Komornicki, C.E. Dykstra, M.A. Vincent and L. Radom, *J. Am. Chem. Soc.,* **103**, 1652-1656 (1981).

137. The Oxygen Analogue of the Protonated Cyclopropane Problem. A Theoretical Study of the $C_2H_5O^+$ Potential Surface.
R.H. Nobes, W.R. Rodwell, W.J. Bouma and L. Radom, *J. Am. Chem. Soc.,* **103**, 1913-1922 (1981).

138. The Geometric and Electronic Structure of $C_6O_6^{4-}$. Spin Multiplicity of the Ground State.
L. Farnell and L. Radom, *J. Mol. Struct., Theochem,* **76**, 251-257 (1981).

139. Structures and Stabilities of Isomeric [10]Annulenes.
L. Farnell, J. Kao, L. Radom and H.F. Schaefer, *J. Am. Chem. Soc.,* **103**, 2147-2151 (1981).

140. Definitive Theoretical Evidence for the Non-Planarity of the Hydronium Ion (H_3O^+).
W.R. Rodwell and L. Radom, *J. Am. Chem. Soc.,* **103**, 2865 (1981).

141. HOC^+: An Observable Interstellar Species? A Comparision With the Isomeric and Isoelectronic HCO^+, HCN and HNC.
R.H. Nobes and L. Radom, *Chem. Phys.*, **60**, 1-10 (1981).

142. Equilibrium Conformations of Higher-Energy Rotational Isomers of Vinyl Alcohol and Methyl Vinyl Ether.
R.H. Nobes, L. Radom and N.L. Allinger, *J. Mol. Struct., Theochem,* **85**, 185-194 (1981).

143. A Theoretical Approach to Substituent Effects. A Comparison of the Isoelectronic BH_3^- CH_3 and NH_3^+ Groups and their Interaction with Substituents in Disubstituted Benzenes.

G. Kemister, A. Pross, L. Radom and R.W. Taft, *J. Comput. Chem.,* **2**, 470-477 (1981).

144. A Revised Mechanism for the Structure-Specific Gas Phase Enol Cation-Cyclobutanol Reaction.
W.J. Bouma, J.K. MacLeod and L. Radom, *Org. Mass Spectrom.,* **16**, 301-302 (1981).

145. Effect of Substituents on the Structure of Reaction Complexes.
A. Pross and L. Radom, *J. Am. Chem. Soc.*, **103**, 6049-6053 (1981).

146. The Methylenoxonium Radical Cation ($CH_2OH_2^{+\bullet}$): A Surprisingly Stable Isomer of the Methanol Radical Cation.
W.J. Bouma, R.H. Nobes and L. Radom, *J. Am. Chem. Soc.,* **104**, 2929-2930 (1982).

147. Experimental Evidence for the Existence of a Stable Isomer of $CH_3OH^{+\bullet}$: The Methylenoxonium Radical Cation, $CH_2OH_2^{+\bullet}$.
W.J. Bouma, J.K. MacLeod and L. Radom, *J. Am. Chem. Soc.,* **104**, 2930-2931 (1982).

148. A Theoretical Consideration of the Quasi-bent Nature of the HCNO Molecule.
L. Farnell, R.H. Nobes and L. Radom, *J. Mol. Spectrosc.*, **93**, 271-280 (1982).

149. On the Existence of Stable Structural Isomers of Ketene. A Theoretical Study of the C_2H_2O Potential Energy Surface.
W.J. Bouma, R.H. Nobes, L. Radom and C.E. Woodward, *J. Org. Chem.,* **47**, 1869-1875 (1982).

150. On the Nature of the 'Methoxy' Cation.
W.J. Bouma, R.H. Nobes and L. Radom, *Org. Mass Spectrom.,* **17**, 315-317 (1982).

151. The Structure and Dissociation Pathways of Protonated Methanol: An *Ab Initio* Molecular Orbital Study.
R.H. Nobes and L. Radom, *Org. Mass Spectrom.,* **17**, 340-344 (1982).

152. Structural Consequences of Hyperconjugation.
L. Radom, *Prog. Theor. Org. Chem.,* **3**, 1-64 (1982).

153. The Structure of Vinylamine.
S. Saebo and L. Radom, *J. Mol. Struct., Theochem.,* **89**, 227-233 (1982).

154. *Ab Initio* Studies on Amides: Acetamide, *N*-Methylformamide and *N*-Methylacetamide.
L. Radom and N.V. Riggs, *Aust. J. Chem.,* **35**, 1071-1077 (1982).

155. The Additivity of Polarization Function and Electron Correlation Effects in *Ab Initio* Molecular-Orbital Calculations.
R.H. Nobes, W.J. Bouma and L. Radom, *Chem. Phys. Lett.*, **89**, 497-500 (1982).

156. The Structure of Propadienone (CH_2=C=C=O).
L. Farnell and L. Radom, *Chem. Phys. Lett.,* **91**, 373-377 (1982).

157. The 6-31G^{++} Basis Set: An Economical Basis Set for Correlated Wavefunctions.
R.H. Nobes, W.R. Rodwell and L. Radom, *J. Comput. Chem.,* **3**, 561-564 (1982).

158. On the Structures and Relative Energies of $CH_3F^{+\bullet}$ Isomers.
W.J. Bouma, B.F. Yates and L. Radom, *Chem. Phys. Lett.,* **92**, 620-625 (1982).

159. Structures and Stabilities of 1,6-Methano[10]annulene and its Derivatives.
L. Farnell and L. Radom, *J. Am. Chem. Soc.,* **104**, 7650-7654 (1982).

160. The Methylamine Radical Cation $[CH_3NH_2]^{+\bullet}$ and its Stable Isomer, the Methylenammonium Radical Cation $[CH_2NH_3]^{+\bullet}$.
W.J. Bouma, J.M. Dawes and L. Radom, *Org. Mass. Spectrom.,* **18**, 12-15 (1983).

161. A Theoretical Study of the Condensation Reactions of Methyl Cation with Ammonia, Water, Hydrogen Fluoride and Hydrogen Sulphide.
R.H. Nobes and L. Radom, *Chem. Phys.,* **74**, 163-169 (1983).

162. Structures and Stabilities of Gas-Phase $C_2H_3O^+$ Ions: An Ab Initio Molecular Orbital Study.
R.H. Nobes, W.J. Bouma and L. Radom, *J. Am. Chem. Soc.,* **105**, 309-314 (1983).

163. Unusual Low-Energy Isomers of the Ethanol and Dimethyl Ether Radical Cations.
W.J. Bouma, R.H. Nobes and L. Radom, *J. Am. Chem. Soc.,* **105**, 1743-1746 (1983).

164. Structural Predictions for Open-Shell Systems: A Comparative Assessment of Ab Initio Procedures.
L. Farnell, J.A. Pople and L. Radom, *J. Phys. Chem.,* **87**, 79-82 (1983).

165. The Weakly Exothermic Rearrangement of Methoxy Radical ($CH_3O^{\bullet}$) to Hydroxymethyl Radical ($CH_2OH^{\bullet}$).
S. Saebo, L. Radom and H.F. Schaefer, *J. Chem. Phys.*, **78**, 845-853 (1983).

166. Unusual Gas-Phase Isomers of Simple Organic Radical Cations.
W.J. Bouma, J.K. MacLeod, R.H. Nobes and L. Radom, *Int. J. Mass Spectrom. Ion Phys.,* **46**, 235-238 (1983).

167. Vibrational Frequencies of the HCCN Molecule. A Near Degeneracy Between Bent Cyanocarbene and Linear Allene-Related Geometries.
K.S. Kim, H.F. Schaefer, L. Radom, J.A. Pople and J.S. Binkley, *J. Am. Chem. Soc.,* **105**, 4148-4154 (1983).

168. Unusual Low-Energy Isomers for Simple Radical Cations.
M.J. Frisch, K. Raghavachari, J.A. Pople, W.J. Bouma and L. Radom, *Chem. Phys.,* **75**, 323-329 (1983).

169. The Structure of the Cyclobutane Radical Cation.
W.J. Bouma, D. Poppinger and L. Radom, *J. Mol. Struct., Theochem,* **12**, 209-218 (1983).

170. The Structure of Aminopropenenitrile (CH_2=C(NH_2)CN).
S. Saebo and L. Radom, *J. Mol. Struct., Theochem,* **105**, 119-128 (1983).

171. The Ionization of Alkanes.
W.J. Bouma, D. Poppinger and L. Radom, *Israel J. Chem.,* **23**, 21-36 (1983).

172. The Methyleneoxonium and Hydroxymethylene Dications: Dicationic Analogues of Ethylene and Acetylene.
W.J. Bouma and L. Radom, *J. Am. Chem. Soc.,* **105**, 5484-5486 (1983).

173. The Vinyloxonium Cation ($CH_2CHOH_2^+$).
R.H. Nobes and L. Radom, *Chem. Phys. Lett.,* **99**, 107-111 (1983).

174. The Structure of Butatrienone (CH_2=C=C=C=O).
L. Farnell and L. Radom, *J. Am. Chem. Soc.,* **106**, 25-28 (1984).

175. The Structure of 1,4-Dithiin.
S. Saebo, L. Radom and G.L.D. Ritchie, *J. Mol. Struct., Theochem,* **108**, 59-63

(1984).

176. The Nature of the C...C Ring-Opened Form of the Ethylene Oxide Radical Cation.
W.J. Bouma, D. Poppinger, S. Saebo, J.K. MacLeod and L. Radom, *Chem. Phys. Lett.,* **104**, 198-202 (1984).

177. Rearrangement and Fragmentation Processes in the Methanethiol and Dimethyl Sulfide Radical Cations.
R.H. Nobes, W.J. Bouma and L. Radom, *J. Am. Chem. Soc.,* **106**, 2774-2781 (1984).

178. Structures and Relative Energies of Gas-Phase $C_3H_7O^+$ Ions.
R.H. Nobes and L. Radom, *Org. Mass Spectrom.,* **19**, 385-393 (1984).

179. The Molecular Structure, Rotational Constants and Vibrational Frequencies for Ethynamine (NH_2-C≡CH): A Possible Interstellar Molecule.
S. Saebo, L. Farnell, N.V. Riggs and L. Radom, *J. Am. Chem. Soc.,* **106**, 5047-5051 (1984).

180. The Mechanism of 1,2-Migration in β-Acyloxyalkyl Radicals.
S. Saebo, A.L.J. Beckwith and L. Radom, *J. Am. Chem. Soc.,* **106**, 5119-5122 (1984).

181. The Detection of the Prototype Phosphonium (CH_2PH_3), Sulfonium (CH_2SH_2), and Chloronium (CH_2ClH) Ylides by Neutralization-Reionization Mass Spectrometry: A Theoretical Prediction.
B.F. Yates, W.J. Bouma and L. Radom, *J. Am. Chem. Soc.,* **106**, 5805-5808 (1984).

182. The Potential Energy Surface for the $[C_2H_2O]^{+\bullet}$ System: The Ketene Radical Cation $[CH_2{=}C{=}O]^{+\bullet}$ and Other Stable $[C_2H_2O]^{+\bullet}$ Isomers.
W.J. Bouma, P.M.W. Gill and L. Radom, *Org. Mass Spectrom.,* **19**, 610-615 (1984).

183. A Theoretical Approach to Gas-Phase Ion Chemistry.
L. Radom, W.J. Bouma, R.H. Nobes and B.F. Yates, *Pure Appl. Chem.,* **56**, 1831-1842 (1984).

184. A Theoretical Approach to Molecular Conformational Analysis.
L. Radom, J. Baker, P.M.W. Gill, R.H. Nobes and N.V. Riggs, *J. Mol. Struct.,* **126**, 271-290 (1985).

185. The Hydrazinium Radical Cation ($NH_3NH_3^{+\bullet}$) and Dication ($NH_3NH_3^{2+}$): Prototypes for the Ionized Forms of Medium-Ring Bicyclic Compounds.
W.J. Bouma and L. Radom, *J. Am. Chem. Soc.,* **107**, 345-348 (1985).

186. Ab Initio Studies on Amides: Cyanamide, Dicyanamide and Tricyanamide.
N.V. Riggs and L. Radom, *Aust. J. Chem.,* **38**, 835-840 (1985).

187. The Isomerization of Cyclopropylidene to Allene.
A. Rauk, W.J. Bouma and L. Radom, *J. Am. Chem. Soc.,* **107**, 3780-3786 (1985).

188. The Methyleneammonium Radical Cation.
B.F. Yates, R.H. Nobes and L. Radom, *Chem. Phys. Lett.,* **116**, 474-477 (1985).

189. A Planar Hydrazine: Bi(1,2,3-azadiboririn-1-yl).
N.V. Riggs and L. Radom, *J. Chem. Soc., Chem. Commun.,* 1193-1194 (1985).

190. Is the Methylenemethonium Radical Cation ($CH_2{}^{\bullet}CH_4^+$) a Stable Species?
J. Baker, E.E. Kingston, W.J. Bouma, A.G. Brenton and L. Radom, *J. Chem. Soc., Chem. Commun.,* 1625-1626 (1985).

191. Benzyne and Related Systems: An *Ab Initio* Molecular Orbital Approach.
L. Radom, R.H. Nobes, D.J. Underwood and W.K. Li, *Pure Appl. Chem.,* **58**, 75-88 (1986).

192. The Equilibrium Geometry of F_2^+ in its Ground Electronic State. A Simple Example of the Effects of Symmetry Breaking on an Observable Molecular Property.
R. Murphy, H.F. Schaefer, R.H. Nobes, L. Radom and R.M. Pitzer, *Int. Rev. Phys. Chem.,* **5**, 229-237 (1986).

193. A Rationalization of Scrambling Processes Among $[C_2H_3O]^+$ Ions.
R.H. Nobes and L. Radom, *Org. Mass Spectrom.,* **21**, 407-409 (1986).

194. Rearrangement and Dissociative Processes in the $[H_2,C,O]^{+\bullet}$ Potential Energy Surface: An Example of Non-Ergodic Behaviour?
W.J. Bouma, P.C. Burgers, J.L. Holmes and L. Radom, *J. Am. Chem. Soc.,* **108**, 1767-1770 (1986).

195. The Evaluation of Molecular Electron Affinities.
J. Baker, R.H. Nobes and L. Radom, *J. Comput. Chem.,* **7**, 349-358 (1986).

196. Rearrangement of the Fulminate Anion (CNO^-) to the Cyanate Anion (OCN^-): Possible Intermediacy of the Oxazirinyl Anion.
W.K. Li, J. Baker and L. Radom, *Aust. J. Chem.,* **39**, 913-921 (1986).

197. Deceptive Convergence in Møller-Plesset Perturbation Energies.
P.M.W. Gill and L. Radom, *Chem. Phys. Lett.,* **132**, 16-22 (1986).

198. Distonic Radical Cations: Guidelines for the Assessment of their Stability.
B.F. Yates, W.J. Bouma and L. Radom, *Tetrahedron,* **42**, 6225-6234 (1986).

199. Ylide Dications: An Examination of First- and Second-Row Systems.
B.F. Yates, W.J. Bouma and L. Radom, *J. Am. Chem. Soc.,* **108**, 6545-6554 (1986).

200. Ab Initio Molecular Orbital Theory.
W.J. Hehre, L. Radom, P.v.R. Schleyer and J.A. Pople, Wiley, New York, pp 1-548 (1986).

201. An *Ab Initio* Investigation of the Equilibrium Structures of Hydrazine and of the Transition Structures Connecting Them.
N.V. Riggs and L. Radom, *Aust. J. Chem.,* **39**, 1917-1928 (1986).

202. Structures and Rearrangement Processes for the Prototype Alkyl, Alkenyl and Alkynyl Anions: A Theoretical Study of the Ethyl, Ethenyl and Ethynyl Anions.
W.K. Li, R.H. Nobes and L. Radom, *J. Mol. Struct., Theochem,* **149**, 67-79 (1987).

203. Is the $PhCH_2(N_2O)^+$ Cation Likely to be a Reaction Intermediate? A Theoretical Study.
P.M.W. Gill, H. Maskill, D. Poppinger and L. Radom, *J. Chem. Research (S),* 54-55 (1987).

204. Spontaneous Intramolecular Hydrogen Migration in Ionized Ethane-1,2-diol.
B.F. Yates, W.J. Bouma, J.K. MacLeod and L. Radom, *J. Chem. Soc., Chem. Commun.,* 204-205 (1987).

205. The 3-21G(N^*) Basis Set: An Economical Polarized Basis Set for *Ab Initio* Studies on Nitrogen-Containing Molecules.
N.V. Riggs and L. Radom, *Int. J. Quantum Chem.,* **31**, 393-403 (1987).

206. The Ionization of Ethylene Oxide.

R.H. Nobes, W.J. Bouma, J.K. MacLeod and L. Radom, *Chem. Phys. Lett.,* **135**, 78-83 (1987).

207. The Ethyl Dication ($CH_3CH_2^{2+\bullet}$): Classical (Open) or Non-Classical (Bridged)?
M.W. Wong, J. Baker, R.H. Nobes and L. Radom, *J. Am. Chem. Soc.,* **109**, 2245-2250 (1987).

208. Ylides and Ylidions: A Comparative Study of Unusual Gas-Phase Structures.
B.F. Yates, W.J. Bouma and L. Radom, *J. Am. Chem. Soc.,* **109**, 2250-2263 (1987).

209. Intramolecular Hydrogen Migration in Ionized Amines: A Theoretical Study of the Gas-Phase Analogues of the Hofmann-Löffler and Related Rearrangements.
B.F. Yates and L. Radom, *J. Am. Chem. Soc.,* **109**, 2910-2915 (1987).

210. Remarkably Stable Trications and Tetracations: The Triheliomethyl Trication ($CHe_3^{3+\bullet}$). and Tetraheliomethane Tetracation (CHe_4^{4+}).
M.W. Wong, R.H. Nobes and L. Radom, *J. Chem. Soc., Chem. Commun.,* 233-234 (1987).

211. Structures and Relative Energies of Gas-Phase $[C_2H_7N]^{+\bullet}$ Radical Cations.
B.F. Yates and L. Radom, *Org. Mass Spectrom.,* **22**, 430-436 (1987).

212. Substituted Methylene Dications (HCX^{2+}): Some Remarkably Short Bonds to Carbon.
M.W. Wong, B.F. Yates, R.H. Nobes, and L. Radom, *J. Am. Chem. Soc.,* **109**, 3181-3187 (1987).

213. Multiply-Charged Helium-Containing Cations: $HeCO^{2+}$, $HeCF^{3+}$ and $HeCNe^{4+}$.
M.W. Wong, R.H. Nobes and L. Radom, *Rapid Commun. Mass Spectrom.,* **1**, 3-5 (1987).

214. A Rationalization of Unusually Late Transition Structures for Dication Fragmentations.
P.M.W. Gill and L. Radom, *Chem. Phys. Lett.,* **136**, 294-298 (1987).

215. The Structure of the $C_2H_4^{2+}$ Dication.
R.H. Nobes, M.W. Wong and L. Radom, *Chem. Phys. Lett.,* **136**, 299-302 (1987).

216. Slow Convergence of the Møller-Plesset Perturbation Series: The Dissociation Energy of Hydrogen Cyanide and the Electron Affinity of the Cyano Radical.
R.H. Nobes, J.A. Pople, L. Radom, N.C. Handy and P.J. Knowles, *Chem. Phys. Lett.,* **138**, 481-485 (1987).

217. Ab Initio Studies of Hydrazines: The Structures of Equilibrium Species of 1,1-Dimethylhydrazine and of Transition Structures Connecting Them.
N.V. Riggs and L. Radom, *Aust. J. Chem.,* **40**, 1783-1793 (1987).

218. Molecular Orbital Theory of Carbanions.
R.H. Nobes, D. Poppinger, W.K. Li and L. Radom, in *Comprehensive Carbanion Chemistry*, Part C, Chapter 1, pp 1-92, E. Buncel and T. Durst, Eds., Elsevier, Amsterdam (1987).

219. The $[HCS]^+$ and $[H_2CS]^{2+}$ Potential Energy Surfaces: Predictions of Bridged Equilibrium Structures.
M.W. Wong, R.H. Nobes and L. Radom, *J. Mol. Struct., Theochem*, **163**, 151-161 (1988).

220. Multiply-Charged Cations: Remarkable Structures and Stabilities.
L. Radom, P.M.W. Gill, M.W. Wong and R.H. Nobes, *Pure Appl. Chem.,* **60**, 183-188 (1988).

221. A Simple Model for the Mean and Difference of NH-Stretching Frequencies for NH_2 Groups, and Its Application to Results of Some Ab Initio Vibrational Frequency Calculations.
N.V. Riggs and L. Radom, *Aust. J. Chem.,* **41**, 387-396 (1988).

222. Remarkable Stabilities of the Diatomic Multiply-Charged Cations $SiHe^{\bullet 3+}$ and $SiHe^{4+}$.
M.W. Wong and L. Radom, *J. Am. Chem. Soc.,* **110**, 2375-2378 (1988).

223. Structures and Stabilities of Singly-Charged Three-Electron Hemi-Bonded Systems and their Hydrogen-Bonded Isomers.
P.M.W. Gill and L. Radom, *J. Am. Chem. Soc.,* **110**, 4931-4941 (1988).

224. How Does a Dication Lose a Proton?
P.M.W. Gill and L. Radom, *J. Am. Chem. Soc.,* **110**, 5311-5314 (1988).

225. 6-311G(MC)(d,p): A Second-Row Analogue of the 6-311G(d,p) Basis Set. Calculated Heats of Formation for Second-Row Hydrides.
M.W. Wong, P.M.W. Gill, R.H. Nobes and L. Radom, *J. Phys. Chem.,* **92**, 4875-4880 (1988).

226. Ab Initio Studies on Hydrazines: 1H-Pyrrol-1-amine (N-Aminopyrrole).
N.V. Riggs and L. Radom, *Aust. J. Chem.,* **41**, 397-403 (1988).

227. Molecular Structure and Spectroscopic Properties of Carbodiimide (HN=C=NH).
M.T. Nguyen, N.V. Riggs, L. Radom, M. Winnewisser, B.P. Winnewisser and M. Birk, *Chem. Phys.,* **122**, 305-315 (1988).

228. The ACDCP Model for Estimating the Kinetic Energy Release and Transition Structure Bond Length in the Fragmentation of a Diatomic Dication.
P.M.W. Gill and L. Radom, *Chem. Phys. Lett.,* **147**, 213-218 (1988).

229. Why Does Unrestricted Møller-Plesset Perturbation Theory Converge So Slowly for Spin-Contaminated Wavefunctions?
P.M.W. Gill, J.A. Pople, L. Radom and R.H. Nobes, *J. Chem. Phys.,* **89**, 7307-7314 (1988).

230. The Vinyl Dication ($CH_2CH^{\bullet 2+}$): Classical or Bridged?
M.W. Wong and L. Radom, *Int. J. Mass. Spectrom. Ion. Processes,* **86**, 319-327 (1988).

231. Simple Models for Describing the Fragmentation Behaviour of Multiply-Charged Cations.
L. Radom, P.M.W. Gill and M.W. Wong, *Int. J. Quantum Chem., Symp.,* **22**, 567-573 (1988).

232. How Well Can RMP4 Theory Treat Homolytic Fragmentations?
P.M.W. Gill, M.W. Wong, R.H. Nobes and L. Radom, *Chem. Phys. Lett.*, **148**, 541-549 (1988).

233. Fragmentation Mechanisms for Multiply-Charged Cations.
L. Radom, P.M.W. Gill and M.W. Wong, in *The Structure of Small Molecules and Ions*, R. Naaman and Z. Vager, Eds., pp 219-225, Plenum, New York (1988).

234. Structural and Energetic Consequences of Single and Double Ionization.
L. Radom, M.W. Wong and P.M.W. Gill, *Adv. Mass Spectrom.*, 702-712 (1989).

235. Methane Dication: Planar but not Square.
M.W. Wong and L. Radom, *J. Am. Chem. Soc.*, **111**, 1155-1156 (1989).

236. The Hemi-Bonded Dimer Radical Cation of Thiirane.
P.M.W. Gill, P. Weatherall and L. Radom, *J. Am. Chem. Soc.*, **111**, 2782-2785

(1989).

237. Isoelectronic Analogues of Molecular Nitrogen: Tightly-Bound Multiply-Charged Species
M.W. Wong, R.H. Nobes, W.J. Bouma and L. Radom, *J. Chem. Phys.*, **91**, 2971-2979 (1989).

238. Structures and Stabilites of the Dimer Dications of First- and Second-Row Hydrides.
P.M.W. Gill and L. Radom, *J. Am. Chem. Soc.,* **111**, 4613-4622 (1989).

239. A Theoretical Study of the $C_3H_4^{2+}$ Potential Energy Surface.
M.W. Wong and L. Radom, *J. Mol. Struct.*, **198**, 391-402 (1989).

240. Multiply-Bonded Argon-Containing Ions: The Structures and Stabilities of XAr^{n+} Cations (X = B, C and N, with n = 1-3).
M.W. Wong and L. Radom, *J. Phys. Chem.*, **93**, 6303 (1989).

241. The $HCNArF^+$ Cation: Prediction of a Stable Argon-Nitrogen Bonded Species.
M.W. Wong and L. Radom, *J. Chem. Soc., Chem. Commun.*, 719-721 (1989).

242. Structures and Stabilites of $C_3H_2^{\bullet+}$ and $C_3H_2^{2+}$ Ions.
M.W. Wong and L. Radom, *Org. Mass Spectrom.*, **24**, 539-545 (1989).

243. Neutralization-Reionization of $CH_4^{+\bullet}$: At Which Stage Does the Fragmentation Occur?
C.E.C.A. Hop, J.L. Holmes, M.W. Wong and L. Radom, *Chem. Phys. Lett.,* **159**, 580-586 (1989).

244. Multiply-Charged Isoelectronic Analogues of $C_3H_3^+$: Cyclic or Open-Chain?
M.W. Wong and L. Radom, *J. Am. Chem. Soc.*, **111**, 6976-6983 (1989).

245. Ethynol: Remarkably High Gas-Phase Acidity.
B.J. Smith, L. Radom and A.J. Kresge, *J. Am. Chem. Soc.*, **111**, 8297-8299 (1989).

246. Heat of Formation for the Hydroxymethylene ($HCOH^{\bullet+}$) Radical Cation. The Importance of Reverse Activation Energy.
N.L. Ma, B.J. Smith, M.A. Collins, J.A Pople and L. Radom, *J. Phys. Chem.*, **93**, 7759-7760 (1989).

247. Isoelectronic Analogues of PN: Remarkably Stable Multiply-Charged Cations.
M.W. Wong and L. Radom, *J. Phys. Chem.*, **94**, 638-644 (1990).

248. Transition Structures for the Interchange of Hydrogen Atoms Within the Water Dimer.
B.J. Smith, D.J. Swanton, J.A. Pople, H.F. Schaefer and L. Radom, *J. Chem. Phys.*, **92**, 1240-1247 (1990).

249. Structure and Stability of the Tetrahydridoselenonium Dication, SeH_4^{2+}.
M.W. Wong and L. Radom, *Struct. Chem.*, **1**, 13-18 (1990).

250. John A. Pople: Early Ab Initio Days.
L. Radom, *J. Phys. Chem.*, **94**, 5439-5444 (1990).

251. The Structure of Vinyl Alcohol: A Resolution of the Discrepancy Between Theory and Experiment.
B.J. Smith and L. Radom, *J. Am. Chem. Soc.*, **112**, 7525-7528 (1990).

252. The Heat of Formation of the Acetyl Cation: A Theoretical Evaluation.
B.J. Smith and L. Radom, *Int. J. Mass Spectrom. Ion Proc.*, **101**, 209-217 (1990).

253. Neutralization-Reionization and Ab Initio Study of the CH_2=CHSOH $\Leftrightarrow$ CH_3CH=S=O Rearrangement.

F. Turecek, F.W. McLafferty, B.J. Smith and L. Radom, *Int. J. Mass Spectrom. Ion Proc.*, **101**, 283-300 (1990).

254. Extension of Gaussian-1 (G1) Theory to Bromine-Containing Molecules.
M.P. McGrath and L. Radom, *J. Chem. Phys.*, **94**, 511-516 (1991).

255. The Formamidine-Formic Acid Dimer: A Theoretical Examination of its Equilibrium Structure and of the Double-Proton-Transfer Process.
I. Agranat, N.V. Riggs and L. Radom, *J. Chem. Soc., Chem. Commun.*, 80-81 (1991).

256. A Theoretical Study of the Structure and Unimolecular Decomposition Pathways of Ethyloxonium, $[CH_3CH_2OH_2]^+$.
D.J. Swanton, D.C.J. Marsden and L. Radom, *Organic Mass Spectrom.*, **26**, 227-234 (1991).

257. Chemistry by Computer: A Theoretical Approach to Gas-Phase Ion Chemistry.
L. Radom, *Organic Mass Spectrom.*, **26**, 359-373 (1991).

258. Unimolecular Rearrangements Connecting Hydroxyethylidene (CH_3-C-OH), Acetaldehyde (CH_3-CH=O) and Vinyl Alcohol (CH_2=CH-OH).
B.J. Smith, M.T. Nguyen and L. Radom, *J. Am. Chem. Soc.*, **113**, 6452-6458 (1991).

259. Characterization of the Bifurcated Structure of the Water Dimer.
C.J. Marsden, B.J. Smith, J.A. Pople, H.F. Schaefer and L. Radom, *J. Chem. Phys.*, **95**, 1825-1828 (1991).

260. Rearrangement and Dissociative Reactions of the Methanol Radical Cation ($CH_3OH^{\bullet+}$): A Comparison of Theory and Experiment.
N.L. Ma, B.J. Smith, J.A. Pople and L. Radom, *J. Am. Chem. Soc.*, **113**, 7903-7912 (1991).

261. The Structure and Stability of the O_2^{2+} Dication: A Dramatic Failure of Møller-Plesset Perturbation Theory.
R.H. Nobes, D. Moncrieff, M.W. Wong, L. Radom, P.M.W. Gill and J.A. Pople, *Chem. Phys. Lett.*, **182**, 216-224 (1991).

262. The Evaluation of Accurate Gas-Phase Acidities.
B.J. Smith and L. Radom, *J. Phys. Chem.*, **95**, 10549-10551 (1991).

263. Ethynamine: The Remarkable Acid-Strengthening and Base-Weakening Effect of the Acetylenic Linkage. A Comparison with Ethenamine and Methylamine.
B.J. Smith and L. Radom, *J. Am. Chem. Soc.*, **114**, 36-41 (1992).

264. The Heat of Formation of Formaldimine.
B.J. Smith, J.A. Pople, L.A. Curtiss and L. Radom, *Aust. J. Chem.*, **45**, 285-288 (1992).

265. Classical Trajectory Study of the Decomposition of $HCOH^{\bullet+}$ on a Symmetry-Invariant Potential Energy Surface.
N. L. Ma, L. Radom and M. A. Collins, *J. Chem. Phys.*, **96**, 1093-1104 (1992); **97**, 1612-1613 (1992).

266. Ionized Methyl Formate ($CH_3OCHO^{\bullet+}$) and its Distonic Isomer ($\dot{C}H_2O\overset{+}{C}HOH$).
B.J. Smith, M.T. Nguyen and L. Radom, *J. Am. Chem. Soc.*, **114**, 1151-1156 (1992).

267. *Closo*-silaboranes and *closo*-Carboranes: Contrasting Relative Stabilities and Breakdown of the Rule of Topological Charge Stabilization.
E.D. Jemmis, G. Subramanian and L. Radom, *J. Am. Chem. Soc.*, **114**, 1481-1483

(1992).

268. The Vinylidene-Acetylene Rearrangement. A Phantom Minimum on the MP2 Potential Energy Surface.
B.J. Smith, R. Smernik and L. Radom, *Chem. Phys. Lett.*, **188**, 589-594 (1992).

269. The Thermochemistry of the Mercaptomethyl (CH_2SH^+) and Thiomethoxy (CH_3S^+) Cations: A Comparison of G2 Theory and Experiment.
R.H. Nobes and L. Radom, *Chem. Phys. Lett.*, **189**, 554-559 (1992).

270. Structure, Infrared and Raman Spectra, and Thermochemistry of Trithia[1.1.1]propellane.
N.V. Riggs, U. Zoller, M.T. Nguyen and L. Radom, *J. Am. Chem. Soc.*, **114**, 4354-4356 (1992).

271. Helides of Carbon and Silicon: An Ab Initio Study of Their Geometric and Electronic Structures.
E.D. Jemmis, M.W. Wong, H.B. Bürgi and L. Radom, *J. Mol. Struct., Theochem*, **261**, 385-401 (1992).

272. The Chemistry of Gas-Phase Ions: A Theoretical Approach.
L. Radom, *Int. J. Mass Spectrom. Ion Processes*, **118/119**, 339-368 (1992); *Adv. Mass Spectrom.*, **12**, 339-368 (1992).

273. Bowlane: Towards Planar Tetracoordinate Carbon.
M.P. McGrath, L. Radom and H.F. Schaefer, *J. Org. Chem.*, **57**, 4847-4850 (1992).

274. Refined Thermochemistry for the Methanol Radical Cation ($CH_3OH^{\bullet+}$) and its Distonic Isomer ($CH_2OH_2^{\bullet+}$).
N.L. Ma, B.J. Smith and L. Radom, *J. Phys. Chem.*, **96**, 5804-5807 (1992).

275. Potential Energy Surfaces Describing Ion Complexes Containing Molecular Hydrogen.
J. Ischtwan, B.J. Smith, M.A. Collins and L. Radom, *J. Chem. Phys.*, **97**, 1191-1210 (1992).

276. The Energy Difference Between Formaldehyde and Hydroxymethylene Radical Cations: Failure of Unrestricted (UMP2) and Restricted (RMP2) Møller-Plesset Procedures.
N.L. Ma, B.J. Smith and L. Radom, *Chem. Phys. Lett.*, **193**, 386-394 (1992).

277. Refined Calculations of the Structures and Stabilities of the Formyl (HCO^+) and Isoformyl (COH^+) Cations.
N.L. Ma, B.J. Smith and L. Radom, *Chem. Phys. Lett.*, **197**, 573-580 (1992).

278. Theoretical and Experimental Structures of Vinyl Fluoride and Vinyl Alcohol.
B.J. Smith, D. Coffey and L. Radom, *J. Chem. Phys.*, **97**, 6113-6120 (1992).

279. Theoretical Study of the Organosulfur Systems CSH_n (n = 0–4) and CSH_n^+ (n = 0–5): Dissociation Energies, Ionization Energies and Enthalpies of Formation.
L.A. Curtiss, R.H. Nobes, J.A. Pople and L. Radom, *J. Chem. Phys.*, **97**, 6766-6773 (1992).

280. Cyclopentadienylideneketene: Theoretical Confirmation of a Key Infrared Band.
A.P. Scott and L. Radom, *Chem. Phys. Lett.*, **200**, 15-20 (1992).

281. Thermochemistry and Ion–Molecule Reactions of Isomeric $C_3H_2^{\bullet+}$ Cations.
M.W. Wong and L. Radom, *J. Am. Chem. Soc.*, **115**, 1507-1514 (1993).

282. Theoretical and Experimental Structures of Vinyl Chloride and Vinyl Bromide.
D. Coffey, B.J. Smith and L. Radom, *J. Chem. Phys.*, **98**, 3952-3959 (1993).

283. Alkaplanes: A Class of Neutral Hydrocarbons Containing a Potentially Planar Tetracoordinate Carbon Atom.
M.P. McGrath and L. Radom, *J. Am. Chem. Soc.*, **115**, 3320-3321 (1993).

284. Assigning Absolute Values to Proton Affinities: A Differentiation Between Competing Scales.
B.J. Smith and L. Radom, *J. Am. Chem. Soc.*, **115**, 4885-4888 (1993).

285. The Possible Role of ClO_3 Isomers in Relation to Stratospheric Ozone.
A. Rauk, E. Tschuikow-Roux, Y. Chen, M.P. McGrath and L. Radom, *J. Phys. Chem.*, **97**, 7947–7954 (1993).

286. Reply to Comment on Cyclopentadienylideneketene: Theoretical Confirmation of a Key Infrared Band.
A.P. Scott and L. Radom, *Chem. Phys. Lett.*, **212**, 705–707 (1993).

287. Scaling Factors for Obtaining Fundamental Vibrational Frequencies and Zero-Point Energies from HF/6-31G* and MP2/6-31G* Harmonic Frequencies.
J.A. Pople, A.P. Scott, M.W. Wong and L. Radom, *Israel J. Chem.*, **33**, 345-350 (1993)

288. Are Polar Interactions Important in the Addition of Methyl Radical to Alkenes?
M.W. Wong, A. Pross and L. Radom, *J. Am. Chem. Soc.*, **115**, 11050-11051 (1993).

289. Addition of Methyl Radical to Alkenes: A Theoretical Study of the Reaction Mechanism.
M.W. Wong, A. Pross and L. Radom, *Israel J. Chem.*, **33**, 415–425 (1993).

290. Structures and Stabilities of $C_3H_4O^{+\bullet}$ Isomers: A G2 Theoretical Study.
M.L. McKee and L. Radom, *Org. Mass Spectrom.*, **28**, 1238-1244 (1993).

291. A Reappraisal of the Structures and Stabilities of Prototype Distonic Radical Cations and their Conventional Isomers.
J.W. Gauld and L. Radom, *J. Phys. Chem.*, **98**, 777–784 (1994).

292. Comparison of the Addition of $CH_3^{\bullet}$, $CH_2OH^{\bullet}$ and $CH_2CN^{\bullet}$ Radicals to Alkenes: A Theoretical Study of the Reaction Mechanism.
M.W. Wong, A. Pross and L. Radom, *J. Am. Chem. Soc.*, **116**, 6284–6292 (1994).

293. A Simple Failing of G2 Theory: Heats of Combustion.
A. Nicolaides and L. Radom, *J. Phys. Chem.*, **98**, 3092–3093 (1994).

294. Oxirene: To Be or Not to Be?
G. Vacek, J.M. Galbraith, Y. Yamaguchi, H.F. Schaefer, R.H. Nobes, A.P. Scott and L. Radom, *J. Phys. Chem.*, **98**, 8660–8665 (1994).

295. Octaplane: A Saturated Hydrocarbon with a Remarkably Low Ionization Energy Leading to a Cation with a Planar Tetracoordinate Carbon Atom.
J.E. Lyons, D.R. Rasmussen, M.P. McGrath, R.H. Nobes and L. Radom, *Angew. Chem. Int. Ed. Engl.*, **33**, 1667–1668 (1994).

296. Is S_N2 Substitution with Inversion of Configuration at Vinylic Carbon Feasible?
M.N. Glukhovtsev, A. Pross and L. Radom, *J. Am. Chem. Soc.*, **116**, 5961–5962 (1994).

297. The Wolff Rearrangement: The Relevant Portion of the Oxirene–Ketene Potential Energy Hypersurface.
A.P. Scott, R.H. Nobes, H.F. Schaefer and L. Radom, *J. Am. Chem. Soc.*, **116**, 10159–10164 (1994).

298. Addition of *tert*-Butyl Radical to Alkenes: A Theoretical Study of the Reaction Mechanism.
M.W. Wong, A. Pross and L. Radom, *J. Am. Chem. Soc.*, **116**, 11938–11944 (1994).

299. Seven-Membered Ring or Phenyl Substituted Cation? Relative Stabilities of the Tropylium and Benzyl Cations and their Silicon Analogues.
A. Nicolaides and L. Radom, *J. Am. Chem. Soc.*, **116**, 9769–9770 (1994).

300. An Evaluation of the Performance of Density Functional Theory, MP2, MP4, F4, G2(MP2) and G2 Procedures in Predicting Gas-Phase Proton Affinities.
B.J. Smith and L. Radom, *Chem. Phys. Letters*, **231**, 345–351 (1994).

301. New Theoretical and Experimental Proton Affinities for Methyl Halides and Diazomethane: A Revision of the Methyl Cation Affinity Scale.
M.N. Glukhovtsev, J.E. Szulejko, T.B. McMahon, J.W. Gauld, A.P. Scott, B.J. Smith, A. Pross and L. Radom, *J. Phys. Chem.*, **98**, 13099–13101 (1994).

302. Chemistry by Computer: A Theoretical Approach to Structure and Mechanism.
L. Radom, in *Organic Reactivity: Physical and Biological Aspects*, B T Golding, R J Griffin, and H Maskill, Eds., pp 278–300, Royal Society of Chemistry, Cambridge (1995).

303. *Ab Initio* Calculations of the Gas-Phase Acidities of Diazirine and Diazomethane.
A.J. Russell, A.P. Scott and L. Radom, *Aust. J. Chem.*, **48**, 401–405 (1995).

304. Gas-Phase Identity S_N2 Reactions of Halide Anions with Methyl Halides: A High Level Computational Study
M.N. Glukhovtsev, A. Pross and L. Radom, *J. Am. Chem. Soc.*, **117**, 2024–2032 (1995).

305. Calculation of Proton Affinities using the G2(MP2,SVP) Procedure.
B.J. Smith and L. Radom, *J. Phys. Chem.*, **99**, 6468–6471 (1995).

306. Extension of Gaussian-2 (G2) Theory to Bromine- and Iodine-Containing Molecules: Use of Effective Core Potentials.
M.N. Glukhovtsev, A. Pross, M.P. McGrath and L. Radom, *J. Chem. Phys.*, **103**, 1878 (1995).

307. Radical Addition to Alkenes: An Assessment of Theoretical Procedures.
M.W. Wong and L. Radom, *J. Phys. Chem.*, **99**, 8582–8588 (1995).

308. Determination of the Chirality of Enantiomeric [^{16}O, ^{17}O, ^{18}O] Sulfate Esters By Infrared Spectroscopy: An *Ab Initio* Evaluation.
A. Nicolaides and L. Radom, *J. Chem. Soc., Chem. Commun.*, 701–702 (1995)

309. Gas-Phase S_N2 Reactions of Halide Anions at Neutral Nitrogen: A High Level Computational Study.
M.N. Glukhovtsev, A. Pross and L. Radom, *J. Am. Chem. Soc.*, **117**, 9012–9018 (1995).

310. Extension of Gaussian-2 Theory to Molecules Containing Third-Row Atoms Ga–Kr.
L.A. Curtiss, M.P. McGrath, J.P. Blaudeau, N.E. Davis, R.C. Binning and L. Radom, *J. Chem. Phys.*, **103**, 6104–6113 (1995).

311. A Priori Prediction of Propagation Rate Coefficients in Free Radical Polymerizations: Propagation of Ethylene.
J.P.A. Heuts, R.G. Gilbert and L. Radom, *Macromolecules*, **28**, 8771–8781 (1995).

312. Gas-Phase Acidities: A Comparison of Density Functional, MP2, MP4, F4, G2(MP2,SVP), G2(MP2) and G2 Procedures.
B.J. Smith and L. Radom, *Chem. Phys. Letters*, **245**, 123–128 (1995).

313. Is the Most Stable Gas-Phase Isomer of the Benzenium Cation a Face-Protonated p-Complex?
M.N. Glukhovtsev, A. Pross, A. Nicolaides and L. Radom, *J. Chem. Soc., Chem. Commun.*, 2347–2348 (1995).

314. A Comparison of High-Quality *Ab Initio* Basis Sets: The Inversion Barrier in Ammonia
A.L.L. East and L. Radom, *J. Mol. Struct.*, **376**, 437–447 (1996).

315. Acidities, Proton Affinities and Other Thermochemical Properties of Hypohalous Acids, HOX (X = F – I): A High Level Computational Study.
M.N. Glukhovtsev, A. Pross and L. Radom, *J. Phys. Chem.*, **100**, 3498–3503 (1996).

316. Gas-Phase Non-Identity S_N2 Reactions of Halide Anions with Methyl Halides: A High Level Computational Study.
M.N. Glukhovtsev, A. Pross and L. Radom, *J. Am. Chem. Soc.*, **118**, 6273–6284 (1996).

317. Gaussian-2 Theory: Reduced Basis Set Requirements.
L.A. Curtiss, P.C. Redfern, B.J. Smith and L. Radom, *J. Chem. Phys.*, **104**, 5148–5152 (1996).

318. An Evaluation of the Performance of G2, G2(MP2) and G2(MP2,SVP) Theories for Heats of Formation and Heats of Reaction in the Case of "Large" Hydrocarbons.
A. Nicolaides and L. Radom, *Mol. Phys.*, **88**, 759–765 (1996).

319. Water-Catalyzed Interconversion of Conventional and Distonic Radical Cations: Methanol and Methyleneoxonium Radical Cations.
J.W. Gauld, H. Audier, J. Fossey and L. Radom, *J. Am. Chem. Soc.*, **118**, 6299–6300 (1996).

320. The Performance of B3–LYP Density Functional Theory in Describing S_N2 Reactions at Saturated Carbon.
M.N. Glukhovtsev, R.D. Bach, A. Pross and L. Radom, *Chem. Phys. Letters*, **260**, 558–564 (1996).

321. Harmonic Vibrational Frequencies: An Evaluation of Hartree-Fock, Møller-Plesset, Quadratic Configuration Interaction, Density Functional Theory and Semiempirical Scale Factors.
A.P. Scott and L. Radom, *J. Phys. Chem.*, **100**, 16502–16513 (1996).

322. Heats of Formation from G2, G2(MP2) and G2(MP2,SVP) Total Energies.
A. Nicolaides, A. Rauk, M.N. Glukhovtsev and L. Radom, *J. Phys. Chem.*, **100**, 17460–17464 (1996).

323. The Structure of the Methanol Radical Cation: An Artificially Short C--O Bond with MP2 Theory.
J.W. Gauld, M.N. Glukhovtsev and L. Radom, *Chem. Phys. Letters*, **262**, 187–193 (1996).

324. A Theoretical Study of Chlorine Atom and Methyl Radical Addition to Nitrogen Bases: Why Do Cl Atoms Form Two-Center–Three-Electron Bonds Whereas CH_3 Radicals Form Two-Center–Two-Electron Bonds?

M.L. McKee, A. Nicolaides and L. Radom, *J. Am. Chem. Soc.*, **118**, 10571–10576 (1996).

325. Hydrogen Transfer Between Ethyl Radical and Ethylene: An Example Where Kinetics Does Not Follow Thermodynamics.
J. P.A. Heuts, A. Pross and L. Radom, *J. Phys. Chem.*, **100**, 17087–17089 (1996).

326. Relative Stabilities and Hydride Affinities of Silatropylium and Silabenzyl Cations and Their Isomers. Comparison with the Carbon Analogues Tropylium and Benzyl Cations.
A. Nicolaides and L. Radom, *J. Am. Chem. Soc.*, **118**, 10561–10570 (1996).

327. Determination of Arrhenius Parameters for Propagation in Free-Radical Polymerizations: An Assessment of Ab Initio Procedures.
J. P.A. Heuts, R. G. Gilbert and L. Radom, *J. Phys. Chem.*, **100**, 18997–19006 (1996).

328. Gas-Phase Identity S_N2 Reactions of Halide Anions and Methyl Halides with Retention of Configuration.
M.N. Glukhovtsev, A. Pross, H.B. Schlegel, R.D. Bach and L. Radom, *J. Am. Chem. Soc.*, **118**, 11258–11264 (1996).

329. Ketene and Ketene Radical Cation: The Unusual Effect of Methyl and Dimethyl Substitution.
A.P. Scott and L. Radom, *Int. J. Mass Spectrom. Ion Proc.*, **160**, 73–81 (1997).

330. *Ab Initio* Statistical Thermodynamical Models for the Computation of Third-Law Entropies.
A.L.L. East and L. Radom, *J. Chem. Phys.*, **106**, 6655–6674 (1997).

331. An Evaluation of Additivity Schemes for the Estimation of Heats of Formation of Distonic Radical Cations.
J.W. Gauld, J.L. Holmes and L. Radom, *Acta Chem. Scand.*, **51**, 641–645 (1997).

332. Fulvalenes, Fulvenes and Related Molecules: An Ab Initio Study.
A.P. Scott, I. Agranat, P.U. Biedermann, N.V. Riggs and L. Radom, *J. Org. Chem.*, **62**, 2026–2038 (1997).

333. Catastrophes, Bifurcations and Hysteretic Loops in Torsional Potentials of Internal Rotations in Molecules.
J. Cioslowski, A.P. Scott and L. Radom, *Mol. Phys.*, **91**, 413–420 (1997).

334. An Assessment of Procedures for Calculating Radical Hyperfine Structures.
J.W. Gauld, L.A. Eriksson and L. Radom, *J. Phys. Chem. A*, **101**, 1352–1359 (1997).

335. Proton-Transport Catalysis: A Systematic Study of the Rearrangement of the Isoformyl Cation to the Formyl Cation.
A.J. Chalk and L. Radom, *J. Am. Chem. Soc.*, **119**, 7573–7578 (1997).

336. The Heats of Formation, Gas-Phase Acidities, and Related Thermochemical Properties of the Third-Row Hydrides GeH_4, AsH_3, SeH_2 and HBr from G2 *Ab Initio* Calculations.
P.M. Mayer, J.F. Gal and L. Radom, *Int. J. Mass Spectrom. Ion Proc.*, **167/168**, 689–696 (1997).

337. Phenyl Radical, Cation and Anion. The Triplet-Singlet Gap and Higher Excited States of the Phenyl Cation.
A. Nicolaides, D.M. Smith, F. Jensen and L Radom, *J. Am. Chem. Soc.*, **119**, 8083–8088 (1997).

338. Entropies and Free Energies of Protonation and Proton-Transfer Reactions.
A.L.L. East, B.J. Smith and L Radom, *J. Am. Chem. Soc.*, **119**, 9014–9020 (1997).

339. Extension of Gaussian-2 (G2) Theory to Molecules Containing Third-Row Atoms K and Ca.
J.P. Blaudeau, M.P. McGrath, L.A. Curtiss and L. Radom, *J. Chem. Phys.*, **107**, 5016–5021 (1997).

340. Accurate Theoretical Structures of Radical Cations Containing Unusually Long Bonds: The Structures of $CH_3CH_2OH^{\bullet+}$, $CH_3\overset{\bullet}{C}H\overset{+}{O}H_2$ and $\overset{\bullet}{C}H_2CH_2\overset{+}{O}H_2$.
J.W. Gauld and L. Radom, *Chem. Phys. Letters*, **275**, 28–34 (1997).

341. Effects of Neutral Bases on the Isomerization of Conventional Radical Cations $CH_3X^{\bullet+}$ to Their Distonic Isomers $\overset{\bullet}{C}H_2\overset{+}{X}H$ (X = F, OH, NH_2): Proton-Transport Catalysis and Other Mechanisms.
J.W. Gauld and L Radom, *J. Am. Chem. Soc.*, **119**, 9831–9839 (1997).

342. Dimethylcarbene. Its Radical Cation and Dication.
C. Aubry, M.J. Polce, J.L. Holmes, P.M. Mayer and L. Radom, *J. Am. Chem. Soc.*, **119**, 9039–9041 (1997).

343. Classical and Non-Classical Isomers of Tropylium, Silatropylium and Germatropylium Cations. Descending the Periodic Table Increases the Preference for Non-Classical Structures.
A. Nicolaides and L. Radom, *J. Am. Chem. Soc.*, **119**, 11933–11937 (1997).

344. An Ab Initio Study Concerning the Experimental Observability of $C_3H_6^{2+}$ Isomers.
P.M. Mayer and L. Radom, *Chem. Phys. Lett.*, **280**, 244–250 (1997).

345. The Effects of Protonation on the Structure, Stability and Thermochemistry of Carbon-Centered Organic Radicals
P.M. Mayer, M.N. Glukhovtsev, J.W. Gauld and L. Radom, *J. Am. Chem. Soc.*, **119**, 12889–12895 (1997).

346. An Assessment of Theoretical Procedures for the Calculation of Reliable Free Radical Thermochemistry. A Recommended New Procedure
P.M. Mayer, C.J. Parkinson, D.M. Smith and L. Radom, *J. Chem. Phys.*, **108**, 604–615 (1998).

347. Radical Additions to Alkenes: A Theoretical Perspective.
L. Radom, M.W. Wong and A. Pross, in *Controlled Radical Polymerization*, ACS Symposium Series 685, K. Matyjaszewski, Editor, pp 31–49, American Chemical Society, Washington, DC, 1998.

348. Radical Addition to Alkenes: Further Assessment of Theoretical Procedures
M.W. Wong and L. Radom, *J. Phys. Chem. A*, **102**, 2237–2245 (1998).

349. Deprotonating Molecules and Free Radicals to Form Carbon-Centered Anions: A G2 Ab Initio Study of Molecular and Free Radical Acidity
P.M. Mayer and L. Radom, *J. Phys. Chem. A*, **102**, 4918–4924 (1998).

350. An Ab Initio Study of Ionised Cyclobutanone and Cyclopentanone. Comparison of the Thermodynamic and Kinetic Stabilities of the Distonic Isomers $\overset{\bullet}{C}H_2(CH_2)_n\overset{+}{C}=O$
M. L. McKee, P. M. Mayer and L Radom, *Eur. Mass Spectrom.*, **4**, 23–30 (1998).

351. The Importance of Ion-Neutral Complexes in Gas-Phase Ionic Reactions: Fragmentation of $[CH_3CH_2OCH_2]^+$ as a Prototypical Case

A.J. Chalk and L. Radom, *J. Am. Chem. Soc.*, **120**, 8430-8437 (1998).

352 Thermochemistry of CH_3CN, CH_3NC and Their Cyclic Isomers, and Related Radicals, Cations and Anions: Some Curious Discrepancies Between Theory and Experiment.
P.M. Mayer, M.S. Taylor, M.W. Wong and L. Radom, *J. Phys. Chem. A*, **102**, 7074–7080 (1998).

353. Novel Pi-Ligand Exchange and Insertion Reactions Involving Three-Membered Phosphorus Heterocycles: An Ab Initio Investigation
T.I. Sølling, M.A. McDonald, S.B. Wild and L. Radom, *J. Am. Chem. Soc.*, **120**, 7063–7068 (1998).

354. Ring Opening of the Cyclopropylcarbinyl Radical and its *N*- and *O*-Substituted Analogues: A Theoretical Examination of Very Fast Unimolecular Reactions
D.M. Smith, A. Nicolaides, B.T. Golding and L. Radom, *J. Am. Chem. Soc.*, **120**, 10223–10233 (1998).

355. Gaussian-2 (G2) Theory for Third-Row Elements: A Systematic Study of the Effect of the 3d Orbitals
B.J. Duke and L. Radom, *J. Chem. Phys.*, **109**, 3352–3359 (1998).

356. Remarkable Cleavage of Molecular Hydrogen Without the Use of Metallic Catalysts
A.P. Scott, B.T. Golding and L. Radom, *New J. Chem.*, **22**, 1171–1173 (1998).

357. The Planar Carbon Story
L. Radom and D.R. Rasmussen, *Pure Appl. Chem.*, **70**, 1977–1984 (1998).

358. The Heat of Formation of *tert*-Butyl Radical
B.J. Smith and L. Radom, *J. Phys. Chem. A*, **102**, 10787-10790 (1998).

359. Cyanovinyl Radical: An Illustration of Poor Performance of Unrestricted Perturbation Theory and Density Functional Theory Procedures in Calculating Radical Stabilization Energies
C.J. Parkinson, P.M. Mayer and L. Radom, *Theor. Chem. Acc.*, **102**, 92–96 (1999).

360. Exchange Reactions of Chloriranium Ions and Chlorirenium Ions: A G2 Investigation
T.I. Sølling and L. Radom, *Int. J. Mass Spectrom.*, **185/186/187**, 263–270 (1999).

361. The Effect of Remote Substituents in Free Radical Addition Reactions: New Evidence for the Penultimate Unit Effect
M. L. Coote, T. P. Davis and L. Radom, *J. Mol. Struct., Theochem*, **461-462**, 91–96 (1999).

362. On the Mechanism of Action of Vitamin B_{12}: Theoretical Studies of the 2-Methyleneglutarate-Mutase-Catalyzed Rearrangement
D.M. Smith, B.T. Golding and L. Radom, *J. Am. Chem. Soc.*, **121**, 1037–1044 (1999).

363. Are Pi-Ligand Exchange Reactions of Thiirenium and Thiiranium Ions Feasible? An Ab Initio Investigation
T.I. Sølling, S.B. Wild and L. Radom, *Chem. Eur. J.*, **5**, 509–514 (1999).

364. Facilitation of Enzyme-Catalyzed Reactions by Partial Proton Transfer: Application to Coenzyme B_{12}-Dependent Methylmalonyl-CoA Mutase
D.M. Smith, B.T. Golding and L. Radom, *J. Am. Chem. Soc.*, **121**, 1383–1384 (1999).

365. Ion-Transport Catalysis: Catalyzed Isomerizations of NNH^+ and $NNCH_3^+$
A.J. Chalk and L. Radom, *J. Am. Chem. Soc.*, **121**, 1574–1581 (1999).

366. Exchange and Insertion Reactions Involving Borane Adducts of Phosphirane and Phosphirene: A G2(MP2) Ab Initio Investigation
T.I. Sølling, S.B. Wild and L. Radom, *J. Organomet. Chem.*, **580**, 320–327 (1999).

367. Effect of the Penultimate Unit on Radical Stability and Reactivity in Free-Radical Polymerization
M. L. Coote, T. P. Davis and L. Radom, *Macromolecules*, **32**, 2935–2940 (1999).

368. The Conformational Dependence of the Penultimate Unit Effect in Free-Radical Copolymerization
M.L. Coote, T.P. Davis and L. Radom, *Macromolecules*, **32**, 5270–5276 (1999).

369. Towards a Consistent Mechanism for Diol-Dehydratase-Catalyzed Reactions: An Application of the Partial-Proton-Transfer Concept
D. M. Smith, B. T. Golding and L. Radom, *J. Am. Chem. Soc.,* **121**, 5700–5704 (1999).

370. Planar Tetracoordinate Carbon in a Neutral Saturated Hydrocarbon: Theoretical Design and Characterization
D.R. Rasmussen and L. Radom, *Angew. Chem. Int. Ed. Engl.*, **38**, 2876–2878 (1999).

371. Magnesium- and Calcium- Containing Molecular Dications: A High Level Theoretical Study
S. Petrie and L. Radom, *Int. J. Mass Spectrom.,* **192**, 173–183 (1999).

372. Heats of Formation of Alkali and Alkaline Earth Oxides and Hydroxides: Some Dramatic Failures of the G2 Method
A. Schulz, B.J. Smith and L. Radom, *J. Phys. Chem. A*, **103**, 7522–7527 (1999).

373. Understanding the Mechanism of B_{12}-Dependent Methylmalonyl-CoA Mutase: Partial Proton-Transfer in Action
D.M. Smith, B.T. Golding and L. Radom, *J. Am. Chem. Soc.*, **121**, 9388–9399 (1999).

374. An Assessment of Theoretical Procedures for the Calculation of Reliable Radical Stabilization Energies
C.J. Parkinson, P.M. Mayer and L. Radom, *J. Chem. Soc., Perkin Trans. 2*, 2305–2314 (1999).

375. A G2 Ab Initio Investigation of Ligand-Exchange Reactions Involving Mono- and Bis–Adducts of the Phosphenium Ion
T.I. Sølling, S.B. Wild and L. Radom, *Inorg. Chem.*, **38**, 6049–6054 (1999).

376. Rearrangement and Fragmentation Pathways of $[C_3H_7Z]^+$ Ions (Z = NH and S): Are Ion-Neutral Complexes Important?
A.J. Chalk, P.M. Mayer and L. Radom, *Int. J. Mass Spectrom.*, **194**, 181–186 (2000).

377. Models for Free-Radical Copolymerization Propagation Kinetics.
M.L. Coote, T.P. Davis and L. Radom, in *Controlled/Living Radical Polymerization*, ACS Symposium Series 768, K. Matyjaszewski, Editor, pp 82–92, American Chemical Society, Washington, DC, 2000.

378. The Acetylene-Ammonia Dimer as a Prototypical C—H•••N Hydrogen-Bonded System: An Assessment of Theoretical Procedures

M. Hartmann and L. Radom, *J. Phys. Chem. A.,* **104**, 968–973 (2000).

379. Zeolites as Transition-Metal-Free Hydrogenation Catalysts: A Theoretical Mechanistic Study
S. Senger and L. Radom, *J. Am. Chem. Soc*., **122**, 2613–2620 (2000)

380. The Involvement of Ion-Neutral Complexes in Ethylene Loss From $[PhC(CH_3)_2]^+$ and its Isomers
A.J. Chalk and L. Radom, *Int. J. Mass Spectrom*., **199**, 29–40 (2000).

381. Formation of Three-Membered Phosphorus Heterocycles via Ligand-Exchange Reactions in Mono-Adducts of the Phosphenium Ion: An Ab Initio Investigation
T.I. Sølling, S.B. Wild and L. Radom, *Int. J. Mass Spectrom.,* **201**, 205–213 (2000).

382. Are Cumulenones Kinked? A Systematic High-Level Ab Initio Study of H_2CCCO, H_2CCCCO and $H_2CCCCCO$
A.P. Scott and L. Radom, *J. Mol. Struct.,* **556**, 253–261 (2000).

383. Proton-transport catalysis and proton-abstraction reactions: An *ab initio* dynamical study of $X + HOC^+$ and $XH^+ + CO$ (X = Ne, Ar and Kr)
M.A. Collins, S. Petrie, A.J. Chalk and L. Radom, *J. Chem. Phys.,* **112**, 6625–6634 (2000).

384. Hemispiroalkaplanes: Hydrocarbon Cage Systems with a Pyramidal-Tetracoordinate Carbon Atom and Remarkable Basicity
D.R. Rasmussen and L. Radom, *Chem. Eur. J.,* **6**, 2470–2483 (2000).

385. Are the Approach Directions of σ and π Nucleophiles to the Sulfur Atom of Thiiranium and Thiirenium Ions Different?
T.I. Sølling, S.B. Wild and L. Radom, *Chem. Eur. J*., **6**, 590–591 (2000).

386. Towards a Low-Barrier Transition-Metal-Free Catalysis of Hydrogenation Reactions: A Theoretical Mechanistic Study of $HAlX_4$-Catalyzed Hydrogenations of Ethene (X = F, Cl and Br)
S. Senger and L. Radom, *J. Phys. Chem.,* **104**, 7375–7385 (2000).

387. Exchange of Cl^+ Between Lone-Pair Donors and π-Donors: A Computational Study
T.I. Sølling and L. Radom, *Eur. Mass Spectrom.,* **6**, 153–160 (2000).

388. How B_6 Helps B_{12}: The Roles of B_6, B_{12} and the Enzymes in Aminomutase-Catalyzed Reactions
S.D. Wetmore, D.M. Smith and L. Radom, *J. Am. Chem. Soc.,* **122**, 10208–10209 (2000).

389. Understanding the Mechanism of B_{12}-Dependent Diol Dehydratase: A Synergistic Push-Pull Proposal
D.M. Smith, B.T. Golding and L. Radom, *J. Am. Chem. Soc*., **123**, 1664-1675 (2001).

390. C–H•••X Hydrogen Bonds of Acetylene, Ethylene and Ethane with First- and Second-Row Hydrides
M. Hartmann, S.D. Wetmore and L. Radom, *J. Phys. Chem. A.,* **105**, 4470–4479 (2001).

391. Theoretical Studies of Coenzyme B_{12}-Dependent Carbon-Skeleton Rearrangements
D.M. Smith, S.D. Wetmore and L. Radom, in *Theoretical Biochemistry - Processes and Properties of Biological Systems*, L. Eriksson Editor, pp. 183–214,

Elsevier, Amsterdam, (2001).

392. A G2 Study of SH^+ Exchange Reactions Involving Lone-Pair Donors and Unsaturated Hydrocarbons
T.I. Sølling and L. Radom, *Chem. Eur. J.,* **7**, 1516–1524 (2001).

393. Factors Controlling the Addition of Carbon-Centered Radicals to Alkenes – An Experimental and Theoretical Perspective
H. Fischer and L. Radom, *Angew. Chem. Int. Ed. Engl.,* **40**, 1340–1371 (2001).

394. Interconversion of (*S*)-Glutamate and (2*S*,3*S*)-3-Methylaspartate: A Distinctive B_{12}-Dependent Carbon-Skeleton Rearrangement
S.D. Wetmore, D.M. Smith, B.T. Golding and L. Radom, *J. Am. Chem. Soc.,* **123**, 7963–7972 (2001).

395. A High-Level Ab Initio Investigation of Identity and Non-Identity Gas-Phase S_N2 Reactions of Halide Ions with Halophosphines
T.I. Sølling, A. Pross and L. Radom, *Int. J. Mass Spectrom.,* **210/211**, 1–11 (2001).

396. Bond Dissociation Energies and Radical Stabilization Energies Associated With Substituted Methyl Radicals
D.J. Henry, C.J. Parkinson, P.M. Mayer and L. Radom, *J. Phys. Chem.* **105**, 6750–6756 (2001).

397. Enzyme Catalysis of 1,2-Amino Shifts: The Cooperative Action of B_6, B_{12} and Aminomutases
S.D. Wetmore, D.M. Smith and L. Radom, *J. Am. Chem. Soc.,* **123**, 8678–8689 (2001).

398. Singlet-Triplet Splittings and Barriers to Wolff Rearrangement for Carbonyl Carbenes
A.P. Scott, M.S. Platz and L. Radom, *J. Am. Chem. Soc.,* **123**, 6069–6076 (2001).

399. A Theoretical Investigation of the Effects of Electronegative Substitution on the Strength of C–H•••N Hydrogen Bonds
S.D. Wetmore, D.M Smith, R. Schofield and L. Radom, *J. Phys. Chem. A,* **105**, 8718–8726 (2001).

400. Theoretical Thermochemistry of Radicals,
D.J. Henry and L. Radom, in *Theoretical Thermochemistry*, J. Cioslowski, editor, pp 161–197, Kluwer, Dordrecht (2001).

401. Towards Multi-Reference Equivalents of the G2 and G3 Methods
T.I. Sølling, D.M. Smith, L. Radom, M.A. Freitag and M.S. Gordon, *J. Chem. Phys.,* **115**, 8758–8772 (2001).

402. Catalysis by Mutants of Methylmalonyl-CoA Mutase: A Theoretical Rationalization for a Change in the Rate-Determining Step
S.D. Wetmore, D.M. Smith and L. Radom, *ChemBioChem,* **2**, 919–922 (2001).

403. Factors Controlling the Addition of Carbon-Centered Radicals to Alkenes
H. Fischer and L. Radom, in *Macromolecular Symposia*, **182**, 1–14 (2002).

404. An Assessment of the Performance of High-level Theoretical Procedures in the Computation of the Heats of Formation of Small Open-Shell Molecules
D.J. Henry, C.J. Parkinson and L. Radom, *J Phys. Chem. A*, **106**, 7927–7936 (2002).

405. Substituent Effects in Isoxazoles: Identification of 4-Substituted Isoxazoles as Michael Acceptors

C.K.Y. Lee, C.J. Easton, M. Gebara-Coghlan, L. Radom, A.P. Scott, G.W. Simpson and A.C. Willis, *J. Chem. Soc. Perkin Trans. 2*, 2031–2038 (2002).

406. Understanding the Mechanism of Action of B_{12}-Dependent Ethanolamine Ammonia Lyase: Synergistic Interactions at Play
S.D. Wetmore, D.M. Smith, J.T. Bennett, and L. Radom, *J. Am. Chem. Soc.*, **124**, 14054–14065 (2002).

407. Methyl Radical Addition to C=S Double Bonds: Kinetic Versus Thermodynamic Preferences
M.L. Coote, G.P.F. Wood and L. Radom, *J. Phys. Chem. A*, **106**, 12124–12138 (2002).

408. Ab Initio Evidence for Slow Fragmentation in RAFT Polymerization
M.L. Coote and L. Radom, *J. Am. Chem. Soc.*, **125**, 1490–1491 (2003).

409. G3-RAD and G3X-RAD: Modified Gaussian-3 (G3) and Gaussian-3X (G3X) Procedures for Radical Thermochemistry
D.J. Henry, M.B. Sullivan and L. Radom, *J. Chem. Phys.* **118**, 4849–4860 (2003).

410. Alkoxy Radicals in the Gaseous Phase: β-Scission Reactions and Formation by Radical Addition to Carbonyl Compounds
A. Rauk, R.J. Boyd, S.L. Boyd, D.J. Henry, and L. Radom, *Can. J. Chem.* **81**, 431–442 (2003).

411. Calculation of Accurate Imaginary Frequencies and Tunnelling Coefficients for Hydrogen Abstraction Reactions using IRCmax
M.L. Coote, M.A. Collins and L. Radom, *Mol. Phys.* **101**, 1329–1338 (2003).

412. Proton-Transport Catalysis, Proton Abstraction and Proton Exchange in HF + HOC^+ and H_2O + HOC^+ and Analogous Deuterated Reactions
M.A. Collins and L. Radom, *J. Chem. Phys.* **118**, 6222–6229 (2003).

413. Design of Radical-Resistant Amino Acid Residues: A Combined Theoretical and Experimental Investigation
A.K. Croft, C.J. Easton and L. Radom, *J. Am. Chem. Soc.* **125**, 4119–4124 (2003).

414. Homo-Anomeric Effect in the 1,2-Dimethoxyethyl Radical
D.J. Henry, A.L.J. Beckwith and L. Radom, *Aust. J.Chem.* **56**, 429–436 (2003).

415. Heats of Formation of Alkali Metal and Alkaline Earth Metal Oxides and Hydroxides: Surprisingly Demanding Targets for High-Level Ab Initio Procedures
M.B. Sullivan, M.A. Iron, P.C. Redfern, J.M.L. Martin, L.A. Curtiss and L. Radom, *J. Phys. Chem. A,* **107**, 5617–5630 (2003).

416. The Reversible Addition-Fragmentation Chain Transfer Process and the Strength and Limitations of Modeling: Comment on "The Magnitude of the Fragmentation Rate Coefficient"
C. Barner-Kowollik, M.L. Coote, T.P. Davis, L. Radom and P. Vana, *J. Polym. Sci., Part A,* **41**, 2828–2832 (2003).

417. What is the Origin of the Contrathermodynamic Behavior in Methyl Radical Addition to Alkynes versus Alkenes?
R. Gómez-Balderas, M.L. Coote, D.J. Henry, H. Fischer and L. Radom, *J. Phys. Chem. A* **107**, 6082–6090 (2003).

418. Strategic Use of Amino Acid *N*-Substituents to Limit α-Carbon-Centered Radical Formation and Consequent Loss of Stereochemical Integrity

A.K. Croft, C.J. Easton, K. Kociuba and L. Radom, *Tetrahedron Asymmetry*, **14**, 2919–2926 (2003).

419. Performance of the RB3-LYP, RMP2 and UCCSD(T) Procedures in Calculating Radical Stabilization Energies for •NHX Radicals
G.P.F. Wood, D.J. Henry, and L. Radom, *J. Phys. Chem. A*, **107**, 7985–7990 (2003).

420. Interactions Between Neutral Molecules and Ca^{2+}: An Assessment of Theoretical Procedures
I. Corral, O. Mó, M. Yáñez, A.P. Scott, and L. Radom. *J. Phys. Chem. A*, **107**, 10456–10461 (2003).

421. Variable Trends in R–X Bond Dissociation Energies (R = Me, Et, iso-Pr, tert-Bu)
M.L. Coote, A. Pross, and L. Radom, *Org. Lett.*, 5, 4689–4692 (2003).

422. Comparison of the Kinetics and Thermodynamics for Methyl Radical Addition to C=C, C=O, and C=S Double Bonds
D.J. Henry, M.L. Coote, R. Gómez-Balderas, and L. Radom, *J. Am. Chem. Soc.*, **126**, 1732–1740 (2004).

423. Reliable Theoretical Procedures for Calculating the Rate of Methyl Radical Addition to Carbon-Carbon Double and Triple Bonds
R. Gómez-Balderas, M.L. Coote, D.J. Henry and L. Radom, *J. Phys. Chem. A,* **108**, 2874–2883 (2004).

424 Substituent Effects in Xanthate-Mediated Polymerization of Vinyl Acetate: Ab Initio Evidence for an Alternative Fragmentation Pathway
M.L. Coote and L. Radom, *Macromolecules*, **37**, 590–596 (2004).

425. Understanding Alkyl Substituent Effects in R-O Bond Dissociation Reactions in Open- and Closed-Shell Systems
M.L. Coote, A. Pross, and L. Radom, In "Fundamental World of Quantum Chemistry: A Tribute to the Memory of Per-Olov Löwdin", Volume 3, Edited by E.J. Brändas and E.S. Kryachko, Kluwer-Springer, Dordrecht, pp 581–595, 2004.

426. Understanding Metal-Free Catalytic Hydrogenation: A Systematic Theoretical Study of the Hydrogenation of Ethene
B. Chan and L. Radom, *Aust. J. Chem.*, **57**, 659–663 (2004).

427. The Unusual Bifunctional Catalysis of Epimerization and Desaturation by Carbapenem Synthase
M. Topf, G.M. Sandala, D.M. Smith, C.J. Schofield, C.J. Easton and L. Radom, *J. Am. Chem. Soc.,* **126**, 9932–9933 (2004).

428. Suicide Inactivation of Dioldehydratase by Glycolaldehyde and Chloroacetaldehyde: An Examination of the Reaction Mechanism
G.M. Sandala, D.M. Smith, M.L. Coote and L. Radom, *J. Am. Chem. Soc.*, **126**, 12206–12207 (2004).

429. Inhibition of Peptidylglycine α-Amidating Monooxygenase by Exploitation of Factors Affecting the Stability and Ease of Formation of Glycyl Radicals
B.J.W. Barratt, C.J. Easton, D.J. Henry, I.H.W. Li, L. Radom and J.S. Simpson, *J. Am. Chem. Soc.* **126**, 13306–13311 (2004).

430. Gas-Phase Reactions Between Urea and Ca^{2+}: The Importance of Coulomb Explosions
I. Corral, O. Mó, M. Yáñez, J.-Y. Salpin, J. Tortajada and L. Radom, *J. Phys. Chem. A,* **108**, 10080–10088 (2004).

431. Base-Catalyzed Hydrogenation: Rationalizing the Effects of Catalyst and Substrate Structures, and Solvation
B. Chan and L. Radom, *J. Am. Chem. Soc.*, *127*, 2443–2454 (2005).

432. Why are the Ca^{2+} and K^+ Binding Energies of Formaldehyde and Ammonia Reversed With Respect to Their Proton Affinities?
I. Corral, O. Mó, M. Yáñez and L. Radom, *J. Phys. Chem. A*, **109**, 6735–6742 (2005).

433. On the Relationship Between the Preferred Site of Hydrogen Bonding and Protonation
B. Chan, J.E. Del Bene, J. Elguero and L. Radom, *J. Phys. Chem. A*, **109**, 5509–5517 (2005).

434. Divergent Mechanisms of Suicide Inactivation for Ethanolamine Ammonia-Lyase
G.M. Sandala, D.M. Smith and L. Radom, *J. Am. Chem. Soc.,* **127**, 8856–8864 (2005).

435. Bond Dissociation Energies and Radical Stabilization Energies Associated with Model Peptide-Backbone Radicals
G.P.F. Wood, D. Moran, R. Jacob and L. Radom, *J. Phys. Chem. A*, **109**, 6318–6325 (2005).

436. Trends in R–X Bond Dissociation Energies (R = Me, Et, *i*-Pr, *t*-Bu; X = H, CH_3, OCH_3, OH, F): A Surprising Shortcoming of Density Functional Theory
E.I. Izgorodina, M.L. Coote, and L. Radom, *J. Phys. Chem. A*, **109**, 7558–7566 (2005).

437. Structures and Thermochemistry of Calcium-Containing Molecules
N.L. Haworth, M.B. Sullivan, A.K. Wilson, J.M.L. Martin, and L. Radom, *J. Phys. Chem. A,* **109**, 9156–9168 (2005).

438. Modelling β-Scission Reactions of Peptide Backbone Alkoxy Radicals: Backbone C–C Bond Fission
G.P.F. Wood, A. Rauk and L. Radom, *J. Chem. Theor. Comput.,* **1**, 889–899 (2005).

439. Transfer Hydrogenation Between Ethane and Ethene: A Critical Assessment of Theoretical Procedures
D.J. Miller, D.M. Smith, B. Chan and L. Radom, *Mol. Phys.,* 104, 777–794 (2006).
[Special issue in honour of Professor Michael A. Robb]

440. An Experimental and Theoretical Investigation of Gas-Phase Reactions of Ca^{2+} With Glycine
I. Corral, O. Mó, M. Yáñez, J.-Y. Salpin, J. Tortajada, D. Moran and L. Radom, *Chem. Eur. J.* **12**, 6787–6796 (2006).

441. Metal-Mediated Formation of Gas-Phase Amino Acid Radical Cations
C.K. Barlow, D. Moran, L. Radom, W.D. McFadyen and R.A.J. O'Hair, *J. Phys. Chem. A,* **110**, 8304–8315 (2006).

442. Insights into the Hydrogen-Abstraction Reactions of Diol Dehydratase: Relevance to the Catalytic Mechanism and Suicide Inactivation
G.M. Sandala, D.M. Smith, M.L. Coote, B.T. Golding and L. Radom, *J. Am. Chem. Soc.,* **128**, 3433–3444 (2006).
[Highlighted in *Chem. Aust.*, **73** (4), 32 (2006)]

443. Design of Effective Zeolite Catalysts for the Complete Hydrogenation of CO_2

B. Chan and L. Radom, *J. Am. Chem. Soc.*, **128**, 5322–5323 (2006).
[Highlighted in *Chem. Aust.*, **73** (6), 32 (2006)]

444. An Assessment of Theoretical Procedures for Predicting the Thermochemistry and Kinetics of Hydrogen Abstraction by Methyl Radical from Benzene
K. Hemelsoet, D. Moran, V. Van Speybroeck, M. Waroquier and L. Radom, *J. Phys. Chem. A*, **110**, 8942–8951 (2006).

445. Rearrangements in Model Peptide-Type Radicals via Intramolecular Hydrogen-Atom Transfer
D. Moran, R. Jacob, G.P.F. Wood, M.L. Coote, M.J. Davies, R.A.J. O'Hair, C.J. Easton, and L. Radom, *Helv. Chim. Acta*, **89**, 2254–2272 (2006).

446. Suicide Inactivation in the Coenzyme B_{12}-Dependent Enzyme Diol Dehydratase
G.M. Sandala, D.M. Smith, M.L. Coote and L. Radom, In "Modelling Molecular Structure and Reactivity in Biological Systems", Edited by K.J. Naidoo, M. Hann, J. Gao, M. Field, and J. Brady, Royal Society of Chemistry, pp 174–180, 2006.

447. A Restricted-Open-Shell Complete-Basis-Set Model Chemistry
G.P.F. Wood, L. Radom, G.A. Petersson, E.C. Barnes, M.J. Frisch and J.A. Montgomery, Jr., *J. Chem. Phys.*, **125**, 094106-1–094106-16 (2006).

448. Effect of Side Chains on Competing Pathways for β-Scission Reactions of Peptide-Backbone Alkoxyl Radicals
G.P.F. Wood, C.J. Easton, A. Rauk, M.J. Davies and L. Radom, *J. Phys. Chem. A*, **110**, 10316–10323 (2006).

449. Thermochemistry and Kinetics of Hydrogen Abstraction by Methyl Radical from Polycyclic Aromatic Hydrocarbons
K. Hemelsoet, V. Van Speybroeck, D. Moran, G. B. Marin, L. Radom and M. Waroquier, *J. Phys. Chem. A*, **110**, 13624–13631 (2006).

450. Gas-phase Regiocontrolled Generation of Charged Amino Acid and Peptide Radicals
S. Wee, A. Mortimer, D. Moran, A. Wright, C.K. Barlow, R.A.J. O'Hair, L. Radom and C.J. Easton, *Chem. Comm.*, 4233–4235 (2006).

451. In Search of Radical Intermediates in the Reactions Catalyzed by Lysine 2,3-Aminomutase and Lysine 5,6-Aminomutase
G.M. Sandala, D.M. Smith and L. Radom, *J. Am. Chem. Soc.*, **128**, 16004–16005 (2006).
[Highlighted in *Chem. Aust.*, **74** (3), 29–30 (2007)]

452. Hydrogenation of Simple Aromatic Molecules: A Computational Study of the Mechanism
G. Zhong, B. Chan and L. Radom, *J. Am. Chem. Soc.*, **129**, 924-933 (2007).
[Highlighted in *Chem. Aust.*, **74** (4), 31–32 (2007)]

453. Toward an Improved Understanding of the Glutamate Mutase System
G.M. Sandala, D.M. Smith, E.N.G. Marsh and L. Radom, *J. Am. Chem. Soc.*, **129**, 1623–1633 (2007).
[Highlighted in *Chem. Aust.*, **74** (5), 32 (2007)]

454. Uncatalyzed 1,4-Hydrogenation of Polycyclic Aromatic Hydrocarbons: A Computational Study
G. Zhong, B. Chan and L. Radom, *Theochem, 811*, 13–17 (2007).

455. Uncatalyzed Transfer Hydrogenation of Quinones and Related Systems: A Theoretical Mechanistic Study

B. Chan and L. Radom, *J Phys. Chem. A*, **111**, 6456–6467 (2007).

456. Proton-Bound Homodimers: How Are the Binding Energies Related to Proton Affinities?
B. Chan, J.E. Del Bene and L. Radom, *J. Am. Chem. Soc.,* **129**, 12197–12199 (2007).

457. An Evaluation of Harmonic Vibrational Frequency Scale Factors
J.P. Merrick, D. Moran and L. Radom, *J. Phys. Chem. A*, **111**, 11683–11700 (2007).

458. Bond Dissociation Energies and Radical Stabilization Energies: An Assessment of Contemporary Theoretical Procedures
A.S. Menon, G.P.F. Wood, D. Moran and L. Radom, *J. Phys. Chem. A*, **111**, 13638–13644 (2007).

459. Lithium Monoxide Anion: A Ground-State Triplet with the Strongest Base to Date
Z. Tian, B. Chan, M.B. Sullivan, L. Radom, and S.R. Kass, *Proc. Nat. Acad. Sci.*, **105**, 7647–7651 (2008).
[Highlighted in *Chem. Aust.*, **75** (9), 38 (2008)]

460. Zeolite-Catalyzed Hydrogenation of Carbon Dioxide and Ethene
B. Chan and L. Radom, *J. Am. Chem. Soc.*, **130**, 9790–9799 (2008).
[Highlighted in *Chem. Aust.*, **75** (10), 32 (2008)]

461. The Carbon-Skeleton Rearrangement in Tropane Alkaloid Biosynthesis
G.M. Sandala, D.M. Smith and L. Radom, *J. Am. Chem. Soc.,* **130**, 10684–10690 (2008).
[Highlighted in *Chem. Aust.*, **75** (11), 32–33 (2008)]

462. The Nature of Glycine and its α-Carbon Radical in Aqueous Solution: A Theoretical Investigation
G.P.F. Wood, M.S. Gordon, L. Radom and D.M. Smith, *J. Chem. Theory Comput.*, **4**, 1788–1794 (2008).

463. Consequences of Spin Contamination in Unrestricted Calculations on Open-Shell Species: Effect of Hartree–Fock and Møller–Plesset Contributions in Hybrid and Double-Hybrid Density Functional Theory Approaches
A.S. Menon and L. Radom, *J. Phys. Chem. A*, **112**, 13225–13230 (2008).
[Special issue in honour of Professor Sason Shaik]

464. What Factors Determine Whether a Proton-Bound Homodimer Has a Symmetric or an Asymmetric Hydrogen Bond?
B. Chan, J.E. Del Bene and L. Radom, *Mol. Phys.* **107**, 1095–1105 (2009).
[Special issue in honour of Professor H.F. Schaefer III]

465. Low Barrier Hydrogenolysis of the Carbon–Heteroatom Bond as Catalyzed by $HAlF_4$
G. Zhong, B. Chan and L. Radom, *Org. Lett.*, **11**, 749–751 (2009).

466. Ab Initio Investigation of the Fragmentation of 5,5-Diamino-Substituted 1,4,2-Oxathiazoles
R.J. O'Reilly and L. Radom, *Org. Lett.*,**11**, 1325–1328 (2009).

467. On the Reaction of Glycerol Dehydratase and But-3-ene-1,2-diol
G.M. Sandala, B. Kovačević, D. Barić, D.M. Smith and L. Radom, *Chem. Eur. J.,* **15**, 4865–4873 (2009).

468. Hydrogen Abstraction by Chlorine Atom from Small Organic Molecules Containing Amino Acid Functionalities: An Assessment of Theoretical Procedures
M.S. Taylor, S.A. Ivanic, G.P.F. Wood, C.J. Easton, G.B. Bacskay and L. Radom, *J. Phys. Chem. A*, **113**, 11817–11832 (2009).
[Special issue in honour of Professor Walter Thiel]

469. On the Importance of Ribose Orientation in the Substrate Activation of the Coenzyme B_{12}-Dependent Mutases
B. Durbeej, G.M. Sandala, D. Bucher, D. M. Smith and L. Radom, *Chem. Eur. J.* **15**, 8578–8585 (2009).
[Special issue in honour of Professor Itzhak Apeloig]

470. Structures and Thermochemistry of the Alkali Metal Monoxide Anions (MO^-), Monoxide Radicals ($MO^\bullet$) and Hydroxides (MOH)
B. Mintz, B. Chan, M.B. Sullivan, T. Buesgen, A.P. Scott, S.R. Kass, L. Radom and A.K. Wilson, *J. Phys. Chem. A*, **113**, 9501–9510 (2009).

471. Optimization and Basis-Set Dependence of a Restricted Open-Shell Form of B2–PLYP Double-Hybrid Density Functional Theory
D.C. Graham, A.S. Menon, L. Goerigk, S. Grimme and L. Radom, *J. Phys. Chem. A*, **113**, 9861–9873 (2009).
[Cover article for the September 10, 2009 issue of the *Journal of Physical Chemistry A*]

472. Modeling the Reactions Catalyzed by Coenzyme B_{12}-Dependent Enzymes
G.M. Sandala, D.M. Smith and L. Radom, *Accounts Chem. Res.*, **43**, 642–651 (2010).

473. A Computational Study of Methanol-To-Hydrocarbon Conversion: Towards the Design of a Low-Barrier Process
B. Chan and L. Radom, *Can. J. Chem.*, **88**, 866–876 (2010).
[Special issue in honour of Professor Russell Boyd]

474. Gas-Phase Synthesis and Reactivity of Lithium Acetylide Anion, $Li–C{\equiv}C^-$
M.M. Meyer, B. Chan, L. Radom and S.R. Kass, *Angew. Chem. Int. Ed. Engl.*, **49**, 5161–5164 (2010).

475. G4-SP, G4(MP2)-SP, G4-sc and G4(MP2)-sc: Modifications to G4 and G4(MP2) for the Treatment of Medium-Sized Radicals
B. Chan, M.L. Coote and L. Radom, *J. Chem. Theory Comput.*, **6**, 2647–2653 (2010).

476. One-Electron Reduction of N-Chlorinated and N-Brominated Species is a Potential Source of Radicals and Bromine Atom Formation in Inflammatory Diseases
D.I. Pattison, R.J. O'Reilly, O. Skaff, L. Radom, R.F. Anderson, and M.J. Davies, *Chem. Res. Toxicol.*, **24**, 371–382 (2011).

477. G4(MP2)-6X: A Cost-Effective Improvement to G4(MP2)
B. Chan, J. Deng and L. Radom, *J. Chem. Theory Comput.*, **7**, 112–120 (2011).

478. O–H Bond Dissociation Energies
B. Chan, M. Morris, and L. Radom, *Aust. J. Chem.*, **64**, 394–402 (2011).
[Special issue in memory of Professor Athel Beckwith]

479. Model for the Exceptional Reactivity of Peroxiredoxins 2 and 3 with Hydrogen Peroxide: A Kinetic and Computational Study

P. Nagy, A. Karton, A. Betz, A.V. Peskin, P. Pace, R. O'Reilly, M.B. Hampton, L. Radom, and C.C. Winterbourn, *J. Biol. Chem.,* **286**, 18048–18055 (2011).

480. Effect of Substituents on the Stabilities of Multiply-Substituted Carbon-Centered Radicals
A. S. Menon, D. J. Henry, T. Bally and L. Radom, *Org. Biomol. Chem.*, **9**, 3636–3657 (2011).
[Cover Article, also selected as an OBC Hot Article]

481. Effect of Substituents on the Strength of N–X (X = H, F and Cl) Bond Dissociation Energies: A High-Level Quantum Chemical Study
R.J. O'Reilly, A. Karton and L. Radom, *J. Phys. Chem. A*, **115**, 5496–5504 (2011).

482. The Spectroscopy and Thermochemistry of Phenylallyl Radical Chromophores
T.P. Troy, N. Chalyavi, A.S. Menon, G.D. O'Connor, B. Fückel, K. Nauta, L. Radom and T.W. Schmidt, *Chem. Science*, **2**, 1755–1765 (2011).

483. Obtaining Good Performance With Triple-Zeta-Type Basis Sets in Double-Hybrid Density Functional Theory Procedures
B. Chan and L. Radom, *J. Chem. Theory Comput.,* **7**, 2852–2863 (2011).

484. Hydrogen Abstraction by Chlorine Atom from Amino Acids: The Remarkable Influence of Polar Effects on Regioselectivity
R.J. O'Reilly, B. Chan, M.S. Taylor, S. Ivanic, G.B. Bacskay, C.J. Easton, and L. Radom, *J. Am. Chem. Soc.*, **133**, 16553–16559 (2011).
[Highlighted in *Chem. Aust.*, **79** (2), 10 (2012)]

485. Spectroscopy and Thermochemistry of a Jet-Cooled Open-Shell Polyene: 1,4-Pentadienyl Radical
N. Chalyavi, G. B. Bacskay, A. S. Menon, T. P. Troy, N. J. L. K. Davis, L. Radom, S. A. Reid, and T. W. Schmidt, *J. Chem. Phys.*, **135**, 124306-1–124306-7 (2011).

486. Assessment of Theoretical Procedures for Hydrogen-Atom Abstraction by Chlorine, and Related Reactions
B. Chan and L. Radom, *Theor. Chem. Acc.*, **130**, 251–260 (2011).
[Special issue in honour of Professor Shigeru Nagase]

487. Theoretical Studies on Radical Enzymes
G.M. Sandala, D.M Smith and L. Radom, in *Encyclopedia of Radicals in Chemistry, Biology and Materials*, C. Chatgilialoglu and A. Studer, editors, pp 1547–1576, John Wiley & Sons, Chichester, UK (2012).

488. N–H and N–Cl Homolytic Bond Dissociation Energies and Radical Stabilization Energies: An Assessment of Theoretical Procedures Through Comparison With Benchmark-Quality W2w Data
R.J. O'Reilly, A. Karton and L. Radom, *Int. J. Quantum Chem.*, **112**, 1862–1878 (2012).
(Special issue on radicals)

489. Proton-Bound Homodimers Involving Second-Row Atoms
B. Chan, J.E. Del Bene and L. Radom, *Theor. Chem. Acc.*, **131**, 1088–1096 (2012).
[Special issue in honour of Professor E.D. Jemmis]

490. The Elusive 5'-Deoxyadenosyl Radical in Coenzyme-B_{12}-Mediated Reactions

D. Bucher, G.M. Sandala, B. Durbeej, L. Radom and D.M. Smith, *J. Am. Chem. Soc.*, **134**, 1591–1599 (2012).
[Highlighted in *Chem. Aust.*, **79** (3), 12 (2012)]

491. Approaches for Obtaining Accurate Rate Constants for Hydrogen Abstraction by Chlorine Atom
B. Chan and L. Radom, *J. Phys. Chem. A*, **116**, 3745–3752 (2012).

492. Assessment of Theoretical Procedures for Calculating Barrier Heights for a Diverse Set of Water-Catalyzed Proton-Transfer Reactions
A. Karton, R.J. O'Reilly and L. Radom, *J. Phys. Chem. A*, **116**, 4211–4221 (2012).

493. BDE261: A Comprehensive Set of High-Level Theoretical Bond Dissociation Energies
B. Chan and L. Radom, *J. Phys. Chem. A*, **116**, 4975–4986 (2012).

494. Determination of Barrier Heights for Proton Exchange in Small Water Clusters with G4(MP2)-Type, MP*n*, and SCS-MP*n* Procedures—A Caveat
A. Karton, R.J. O'Reilly, B. Chan and L. Radom, *J. Chem. Theory Comput.,* **8**, 3128–3136 (2012).

495. Heats of Formation for CrO, CrO_2 and CrO_3: An Extreme Challenge for Black-Box Composite Procedures
B. Chan, A. Karton, K. Raghavachari and L. Radom, *J. Chem. Theory Comput.*, **8**, 3159–3166 (2012).

496. Comment on the Ionization Energy of B_2F_4,
B. Chan, A.J. Trevitt, S.J. Blanksby and L. Radom, *J. Phys. Chem. A*, **116**, 9214–9215 (2012).

497. Influence of Connector Groups on the Interactions of Substituents with Carbon-Centered Radicals
A.S. Menon, T. Bally and L. Radom, *J. Phys. Chem. A*, **116**, 10203–10208 (2012).

498. W1X-1 and W1X-2: W1-Quality Accuracy With an Order Of Magnitude Reduction in Computational Cost
B. Chan and L. Radom, *J. Chem. Theory Comput.*, **8**, 4259–4269 (2012).

499. On the Reactivities of Amino Acid Derivatives Towards Hydrogen Abstraction by Cl• and OH•
B. Chan, R.J. O'Reilly, C.J. Easton, and L. Radom, *J. Org. Chem.*, **77**, 9807–9812 (2012).

500. Computational Design of Effective, Bioinspired HOCl Antioxidants: The Role of Intramolecular Cl^+ and H^+ Shifts
A. Karton, R.J. O'Reilly, D.I. Pattison, M.J. Davies, and L. Radom, *J. Am. Chem. Soc.*, **134**, 19240–19245 (2012).
[Highlighted in *Nature Chemistry*, **5**, 5 (2013)]
[Highlighted in *Chem. Aust.*, **80** (2), 9 (2013)]

501. Performance of Gradient-Corrected and Hybrid Density Functional Theory: Role of the Underlying Local Density Approximation and the Gradient Correction
B. Chan, P.M.W. Gill and L. Radom, *J. Chem. Theory Comput.*, **8**, 4899–4906 (2012).
[Special issue in honour of Professor H. Bernhard Schlegel]

502. On the Heteroatomic Deprotonation of Substituted Methanes and Methyl Radicals: Theoretical Insights into Structure, Stability, and Thermochemistry
M. Morris, B. Chan and L. Radom, *J. Phys. Chem. A*, **116**, 12381–12387 (2012).

503. Effect of Substituents on the Preferred Modes of One-Electron Reductive Cleavage of N–Cl and N–Br Bonds
R.J. O'Reilly, A. Karton and L. Radom, *J. Phys. Chem. A*, **117**, 460–472 (2013).

504. Evaluation of the Heats of Formation of Corannulene and C_{60} by Means of High-Level Theoretical Procedures
A. Karton, B. Chan, K. Raghavachari and L. Radom, *J. Phys. Chem. A,* **117**, 1834–1842 (2013).
[Cover article, February 28, 2013]

505. Accurate Quantum Chemical Energies for Tetrapeptide Conformations: Why MP2 Data With an Insufficient Basis Set Should be Handled With Caution
L. Goerigk, A. Karton, J. Martin and L. Radom, *Phys. Chem. Chem. Phys.*, **15**, 7028–7031 (2013).
[Cover article, May 21, 2013]

506. A Hierarchy of Relative Bond Dissociation Enthalpies and Their Use to Efficiently Compute Accurate Absolute Bond Dissociation Enthalpies for C–H, C–C and C–F Bonds
B. Chan and L. Radom, *J. Phys. Chem. A*, **117**, 3666–3675 (2013).

507. Gas-Phase Infrared Spectrum and Acidity of the Radical Cation of 9-Methylguanine
L. Feketeová, G.N. Khairallah, B. Chan, V. Steinmetz, P. Maître, L. Radom and R.A.J. O'Hair, *Chem. Comm.*, **49**, 7343–7345 (2013).

508. Chemoselective Peptide Ligation–Desulfurization Chemistry at Aspartate
R.E. Thompson, B. Chan, L. Radom, K.A. Jolliffe and R.J. Payne, *Angew. Chem. Int. Ed.*, in press.

CONFERENCE LECTURES

1. *Geometries and Energies of $C_3H_n^+$ Cations*
   XXIII International Congress of Pure and Applied Chemistry
   Boston, Massachusetts, U.S.A., July 1971
2. *Reversal of Substituent Effects in the Gas Phase: Common Text Book Errors*
   Royal Australian Chemical Institute, Division of Organic Chemistry
   2nd National Conference
   Cowes, Victoria, February 1974
3. *The Intramolecular Fulminic Acid-Isocyanic Acid Rearrangement*
   Royal Australian Chemical Institute, Division of Organic Chemistry
   3rd National Conference
   Brisbane, Queensland, August 1975
4. *Theoretical Approaches to Aromatic Polycations: The Heptalenium Dication*
   Royal Australian Chemical Institute, Division of Organic Chemistry
   4th National Conference
   Richmond, N.S.W., May 1977
5. *Potential Energy Surfaces for Unimolecular Reactions*
   American Conference on Theoretical Chemistry
   Boulder, Colorado, U.S.A., June 1978
   (Invited Lecture)
6. *Molecular Orbitals and Organic Chemistry: A Theoretical Approach to Hyperconjugation*
   Royal Australian Chemical Institute, Division of Organic Chemistry
   5th National Conference
   Hobart, Tasmania, January 1979
   (Plenary Lecture)
7. *Ab Initio Studies of Reaction Mechanism*
   Summer Seminar/Workshop in Molecular Physics and Quantum Chemistry
   Wollongong, N.S.W., February 1980
   (Invited Lecture)
8. *Structural Consequences of Hyperconjugation: A Theoretical Approach*
   Eighth Austin Symposium of Molecular Structure
   Austin, Texas, U.S.A., March 1980
   (Invited Lecture)
9. *The Oxygen Analogue of the Protonated Cyclopropane Problem: A Theoretical Approach*
   Royal Australian Chemical Institute, Division of Organic Chemistry
   6th National Conference
   Melbourne, Victoria, August 1980
10. *A Theoretical Approach to Gas-Phase Ion Chemistry*
    Second Conference on Atomic and Molecular Reactions and Structure
    Adelaide, South Australia, February 1982
    (Invited Lecture)
11. *Adventures in Gas-Phase Ion Chemistry*.
    Symposium on Electron Correlation.
    183rd National Meeting of the American Chemical Society,

Las Vegas, U.S.A., March 1982
(Invited Lecture)

12. *A Theoretical Approach to the Elucidation of Gas-Phase Ion Structure*
Third Asilomar Conference on Mass Spectrometry
Pacific Grove, California, U.S.A., September 1983
(Plenary Lecture)

13. *Structure and Mechanism in Gas-Phase Ion Chemistry*
18th Okazaki Conference on Theories of Chemical Reaction Mechanisms
Okazaki, Japan, January 1984
(Invited Lecture)

14. *A Theoretical Approach to Gas-Phase Ion Chemistry*
Seventh IUPAC Conference on Physical Organic Chemistry
Auckland, New Zealand, August 1984
(Plenary Lecture)

15. *A Theoretical Approach to Structure and Mechanism in Gas-Phase Ion Chemistry*
9th Conference of the Australian and New Zealand Society for Mass Spectrometry
Canberra, August 1984
(Plenary Lecture)

16. *An Ab Initio Approach to Molecular Conformational Analysis*
Oji International Seminar on Rotational Isomerism
Tokyo, Japan, September 1984
(Invited Lecture)

17. *Ylides, Ylidions and Ylide Dications*
Symposium on Applied Quantum Chemistry
Second International Chemical Congress of Pacific Basin Societies
Honolulu, U.S.A., December 1984
(Invited Lecture)

18. *Benzyne and Related Systems: An Ab Initio Molecular Orbital Approach*
5th International Symposium on Novel Aromatic Compounds
St Andrews, Scotland, July 1985
(Plenary Lecture)

19. *A Theoretical Approach to Carbanion Chemistry*
Molecular Structure and Chemical Reactivity
Satellite Symposium of the 5th International Congress on Quantum Chemistry
Toronto, Canada, August 1985
(Invited Lecture)

20. *A Theoretical Approach to Gas-Phase Ion Chemistry*
Structure and Reactivity of Gas Phase Ions
Sixth Annual Congress of the Royal Society of Chemistry
Warwick, England, April 1986
(Invited Lecture)

21. *Distonic Radical Cations: Structures, Stabilities and Unimolecular Reactions*
Gordon Research Conference on Radical Ions
Plymouth, New Hampshire, U.S.A., June 1986
(Invited Lecture)

22. *Multiply Charged Cations: Remarkable Structures and Stabilities*

World Association of Theoretical Organic Chemists
First World Congress
Budapest, Hungary, August 1987
(Plenary Lecture)

23. *Structures and Stabilities of Small Multiply-Charged Ions: An Ab Initio Approach*
International Workshop on the Structure of Small Molecules and Ions
Jerusalem, Israel, December 1987
(Invited Lecture)

24. *Gas-Phase Ion Chemistry*
The Twenty-Eighth Sanibel Symposium
Gainesville, Florida, U.S.A., March 1988
(Plenary Lecture)

25. *A Molecular Orbital Approach to Gas-Phase Ion Chemistry*
Eleventh International Mass Spectrometry Conference
Bordeaux, France, August 1988
(Keynote Lecture)

26. *A Theoretical Approach to Gas-Phase Ion Chemistry*
37th Conference of the American Society for Mass Spectrometry
Miami, Florida, U.S.A., May 1989
(Plenary Lecture)

27. *Chemistry by Computer: A Theoretical Approach to Structure and Reactivity*
H.G. Smith Lecture
Royal Australian Chemical Institute Organic Division, Eleventh National Conference Division of Organic Chemistry
Townsville, Queensland, July 1989
(Plenary Lecture)

28. *John A. Pople: Early Ab Initio Days*
Forty Years of Quantum Chemistry: An International Conference in Honor of Professor John A. Pople
Athens, Georgia, U.S.A., October 1989
(Plenary Lecture)

29. *A Theoretical Approach to Ion-Cluster Chemistry*
Symposium on Advances in Computational Chemistry
1989 International Chemical Congress of Pacific Basin Societies
Honolulu, Hawaii, U.S.A., December 1989
(Invited Lecture)

30. *The Remarkable Structures and Stabilities of Multiply-Charged Cations*
Symposium on Quantum Chemistry: Rethinking Conventional Chemical Concepts in the Light of Modern Theoretical Results
1989 International Chemical Congress of Pacific Basin Societies
Honolulu, Hawaii, U.S.A., December 1989
(Invited Lecture)

31. *Chemistry by Computer: A Theoretical Approach to Structure and Reactivity*
H.G. Smith Lecture
Sixth Australian Conference on Atomic and Molecular Physics and Quantum Chemistry

Perth, W.A., February 1990
(Invited Lecture)

32. *A Theoretical Approach to the Chemistry of Ion Dimers*
World Association of Theoretical Organic Chemists
Second World Congress
Toronto, Canada, July 1990
(Invited Lecture)

33. *Ionization and Neutralization Processes in Organic Mass Spectrometry: A Theoretical Approach*
First Chemical Institute of Canada Congress
Halifax, Nova Scotia, July 1990
(Invited Lecture)

34. *Chemistry by Computer: A Theoretical Approach to Gas-Phase Ion Chemistry*
Allan Maccoll Lecture
Silver Jubilee Meeting of the British Mass Spectrometry Society
London, England, September 1990
(Plenary Lecture)

35. *Structures and Stabilities of Ion Dimers*
23rd Quantum Theory Conference
Oxford, England, September 1990

36. *Structures and Stabilities of Ion Dimers: A Theoretical Approach*
Eighth Asilomar Conference on Mass Spectrometry
Pacific Grove, California, U.S.A., September 1990
(Invited Lecture)

37. *Rearrangement and Fragmentation Reactions of Simple Organic Molecules and Ions*
Seventh International Congress of Quantum Chemistry
Menton, France, July 1991
(Invited Lecture)

38. *Ab Initio Studies of Reactive Intermediates*
International Symposium/Workshop on Reactive Intermediates
Heron Island, Queensland, July 1991
(Invited Lecture)

39. *A Theoretical Approach to Gas-Phase Ion Chemistry*
12th International Mass Spectrometry Conference
Amsterdam, The Netherlands, August 1991
(Plenary Lecture)

40. *A Theoretical Approach to the Chemistry of Ion Dimers*
17th Australian Spectroscopy Conference
Canberra, Australia, October 1991
(Invited Lecture)

41. *Chemistry by Computer: A Theoretical Approach to Structure and Mechanism*
Wolf Symposium in Honour of John A. Pople
Beer Sheva, Israel, May 1992.
(Plenary Lecture)

42. *Theoretical Studies of Strained-Ring Systems*
Toronto International Conference on Organic Reactive Intermediates

Toronto, Canada, July 1992
(Plenary Lecture)

43. *Theoretical Studies of Ion Thermochemistry*
Gordon Conference on Structures, Energetics and Reaction Dynamics of Gaseous Ions
Ventura, California, U.S.A., March 1993
(Invited Lecture)

44. *Chemistry by Computer: A Theoretical Approach to Structure and Mechanism*
Organic Reactivity: Physical and Biological Aspects
Newcastle upon Tyne, England, July 1993
(Plenary Lecture)

45. *Theoretical Studies of Strained-Ring Systems*
World Association of Theoretical Organic Chemists
Third World Congress
Toyohashi, Japan, July 1993
(Invited Lecture)

46. *Chemistry by Computer: A Theoretical Approach to Structure and Mechanism*
Symposium on Computational Chemistry: Methods and Applications
Fifth Asian Chemical Congress
Kuala Lumpur, Malaysia, November 1993
(Plenary Lecture)

47. *The Mechanism of Radical Addition to Alkenes*
Symposium on Computational Organic Chemistry
American Chemical Society, 207th National Meeting
San Diego, California, U.S.A., March 1994
(Invited Lecture)

48. *Towards Planar Carbon*
The 2nd Heron Island Conference on Unusual Molecules and Reactive Intermediates
Heron Island, July 1994
(Invited Lecture)

49. *A Computational Approach to Gas-Phase Ion Chemistry*
45th Conference of the American Society for Mass Spectrometry
Atlanta, Georgia, U.S.A., May 1995
(Keynote Lecture)

50. *A Computational Approach to Gas-Phase Ion Chemistry*
78th Canadian Society for Chemistry Conference
Guelph, Ontario, Canada, June 1995
(Invited Lecture)

51. *Towards Planar Carbon*
Forty Years of Ab Initio Polyatomic Quantum Chemistry
Cambridge, England, September 1995
(Plenary Lecture)

52. *Radical Addition to Alkenes: A Theoretical Approach*
Symposium on Organic Radical Chemistry
1995 International Chemical Congress of Pacific Basin Societies
Honolulu, Hawaii, U.S.A., December 1995

(Plenary Lecture)

53. *Radical-Addition and Radical-Transfer Reactions: A Theoretical Perspective*
VII International Symposium on Organic Free Radicals
Lake Garda, Italy, June 1996
(Plenary Lecture)

54. *Theoretical Studies of Reactions Involving Ion-Molecule Complexes*
International Workshop on Weakly-Bonded Species in Gas-Phase Ionic Reactions
Ecole Polytechnique, Palaiseau Cedex, France, June 1996
(Invited Lecture)

55. *Distonic Radical Cations and Their Conventional Isomers: A Theoretical Perspective*
14th International Conference on Radical Ions
Uppsala, Sweden, July 1996
(Invited Lecture)

56. *Planar Tetracoordinate Carbon*
World Association of Theoretical Organic Chemists
Fourth World Congress
Jerusalem, Israel, July 1996
(Invited Lecture)

57. *Theoretical Aspects of Free Radical Reactions*
Symposium on Advances in Free Radical Polymerization
American Chemical Society, 213th National Meeting
San Francisco, California, U.S.A., April 1997
(Invited Lecture)

58. *Theoretical Studies Related to B_{12}-Mediated Reactions*
TMR Symposium on the Action of Coenzyme B_{12}
Berne, Switzerland, November 1997
(Invited Lecture)

59. *Theoretical Adventures in Gas-Phase Ion Chemistry*
Workshop on Computational Chemistry
Miraflores, Spain, June 1998
(Invited Lecture)

60. *Catalysis of Molecular Rearrangements: A Theoretical Study*
Synergism of Experimental and Theoretical Chemistry
Mexico City, August, 1998
(Invited Lecture)

61. *The Planar Carbon Story*
14th IUPAC Conference on Physical Organic Chemistry
Florianopolis, Brazil, August 1998
(Plenary Lecture)

62. *Metal-Free Catalysis*
PPP Conference in Honor of John A. Pople
Amelia Island, Florida, U.S.A., March 1999
(Invited Lecture)

63. *Theoretical Studies of Radical Stabilities and Reactions*
Gordon Research Conference on Free Radical Reactions

Plymouth, New Hampshire, U.S.A., July 1999
(Invited Lecture)

64. *B_{12}-Mediated Reactions: A Theoretical Examination*
Modern Electronic Structure Theory: Celebrating the 1998 Nobel Prize in Chemistry
218th National Meeting of the American Chemical Society
New Orleans, Louisiana, U.S.A., August 1999
(Invited Lecture)

65. *Reactions Mediated by Coenzyme B_{12}: A Theoretical Examination*
Workshop on Computational Chemistry
Hong Kong, February, 2000
(Invited Lecture)

66. *DFT Studies of Radical Stability and Reactivity*
Satellite Symposium on Density Functional Theory
Menton, France, June 2000
(Invited Lecture)

67. *Theoretical Studies of B_{12}-Mediated Reactions*
5th European Symposium on Vitamin B_{12} and B_{12}-Proteins
Marburg, Germany, September 2000
(Invited Lecture)

68. *Planar Tetracoordinate Carbon and Related Systems*
Symposium on Reactive Intermediates and Unusual Molecules
2000 International Chemical Congress of Pacific Basin Societies
Honolulu, Hawaii, U.S.A., December 2000
(Invited Lecture)

69. *The Mechanism of Action of Coenzyme B_{12}*
Molecular Quantum Mechanics
Seattle, Washington, USA, July 2001
(Invited Lecture)

70. *B_{12}-Mediated Reactions: Radical Chemistry in Action*
Organic Free Radicals – EUCHEM 2002
York, England, July 2002
(Plenary Lecture)

71. *Adventures with Metal Oxides and Hydroxides*
Exploring Modern Computational Chemistry
Nottingham, England, July/August, 2002
(Invited Lecture)

72. *The Mechanism of Action of Coenzyme B_{12}*
Sixth World Congress of the World Association of Theoretically Oriented Chemists
Lugarno, Switzerland, August 2002
(Plenary Lecture)

73. *The Mechanism of Action of Coenzyme B_{12}*
9th European Symposium on Organic Reactivity (ESOR 9)
Oslo, Norway, July 2003
(Plenary Lecture)

74. *Free Radical Chemistry: Stability and Reactions*

Singapore International Chemical Conference 3
Singapore, December 2003
(Keynote Lecture)

75. *Stabilities and Reactivities of Free Radicals*
Theory and Applications of Computational Chemistry
Gyeongju, Korea, February 2004
(Invited Lecture)

76. *The Mechanism of Action of Coenzyme B_{12}*
Asian Pacific Symposium on Theoretical and Computational Chemistry
Okazaki, Japan, May 2004
(Plenary Lecture)

77. *The Mechanism of B_{12}-Mediated Reactions*
MM2004
Sydney, Australia, July 2004
(Invited Lecture)

78. *Thermochemistry of Calcium-Containing Molecules: An Examination of the Performance of High-Level Theoretical Procedures*
Symposium in Honor of Professor H.F. Schaefer III
228th National Meeting of the American Chemical Society
Philadelphia, USA, August 2004
(Invited Lecture)

79. *Adventures in B_{12} Chemistry: A Theoretical Mechanistic Study*
One-Day Symposium Honoring Professor Lew Mander
Canberra, Australia, September 2004
(Invited Lecture)

80. *Suicide Inactivation in B_{12}-Mediated Reactions*
Seventh World Congress of the World Association of Theoretically Oriented Chemists
Cape Town, South Africa, January 2005
(Invited Lecture)

81. *Transition-Metal-Free Hydrogenation*
Second Asian Pacific Conference on Theoretical and Computational Chemistry
Bangkok, Thailand, May 2005
(Invited Lecture)

82. *Reflections on 35 Years in Computational Quantum Chemistry*
Symposium on Computational Quantum Chemistry: Methodology and Application
2005 International Chemical Congress of Pacific Basin Societies
Honolulu, Hawaii, U.S.A., December 2005
(Invited Lecture)

83. *Theoretical Adventures in Peptide Radical Chemistry*
Symposium on Large Molecular Systems, Satellite Symposium to the XIIth International Congress of Quantum Chemistry
Okazaki, Japan, May 2006
(Invited Lecture)

84. *An Overview of Free Radical Chemistry at the University of Sydney: A Computational Approach*

Free Radical Winter Carnival
Canberra, Australia, June 2006

85. *Adventures in Peptide Radical Chemistry: A Theoretical Approach*
Theory of Molecular and Macromolecular Kinetics:
A Symposium in Honour of Professor Bob Gilbert's 60th Birthday
Sydney, Australia, October 2006
(Invited Lecture)

86. *Adventures in Peptide Radical Chemistry: A Theoretical Approach*
Practicing Chemistry with Theoretical Tools:
A Symposium in Honour of Professor Mark Gordon's 65th Birthday
Maui, USA January 2007
(Invited Lecture)

87. *Transition-Metal-Free Hydrogenation*
Molecular Quantum Mechanics: Analytical Gradients and Beyond. A Conference in Honour of Peter Pulay
Budapest, Hungary, May-June, 2007
(Invited Lecture)

88. *Hydrogenation Without Transition Metals*
Third Asian Pacific Conference on Theoretical and Computational Chemistry
Beijing, China, September 2007
(Plenary Lecture)

89. *Chemistry Without Test Tubes: Using Quantum Mechanics and Computers*
Twelfth Annual Symposium on Computational Science and Engineering
Ubonratchathani, Thailand, March 2008
(Plenary Lecture)

90. *Transition-Metal-Free Hydrogenation and Hydrogenolysis*
Nineteenth IUPAC International Conference on Physical Organic Chemistry (ICPOC-19)
Santiago de Compostela, Spain, July 2008
(Plenary Lecture)

91. *The Role of Radicals in Coenzyme-B_{12}-Mediated Reactions: A Computational Approach*
10th International Symposium on Organic Free Radicals (ISOFR 10) and 3rd Pacific Symposium on Radical Chemistry (PSRC 3)
Heron Island, Queensland, August 2008
(Invited Lecture)

92. *The Role of Radicals in Coenzyme-B_{12}-Mediated Reactions: A Computational Approach*
International Conference on Simulations and Dynamics for Nanoscale and Biological Systems
Tokyo, Japan, March 2009
(Invited Lecture)

93. *The Role of Radicals in Coenzyme-B_{12}-Mediated Reactions: A Computational Approach*
7th Canadian Computational Chemistry Conference
Halifax, Canada, July 2009

(Invited Lecture)

94. *The Mechanism Of Action Of Coenzyme B_{12}: A Computational Approach*
Third Adriatic Meeting on Computational Solutions in the Life Sciences
Primosten, Croatia, September 2009
(Invited Lecture)

95. *Transition-Metal-Free Hydrogenation and Hydrogenolysis: A Computational Approach*
Modelling 09: A Symposium in Honor of Professor Tim Clark's 60th Birthday
Erlangen, Germany, September 2009
(Plenary Lecture)

96. *Structure and Mechanism in Free Radical Chemistry: A Computational Approach*
Perspectives of a Radical Chemist: A Symposium in Honour of Professor Athel Beckwith's 80th Birthday
Canberra, Australia, February 2010
(Invited Lecture)

97. *Fritz Down Under*
Molecular Quantum Mechanics 2010: An International Conference in Honor of Professor Henry F. Schaefer
Berkeley, USA, May 2010
(Invited Lecture)

98. *Adventures in Free Radical Chemistry: A Computational Approach*
EUCHEM 2010 Conference on Organic Free Radicals
Bologna, Italy, June 2010
(Plenary Lecture)

99. *Adventures in Free Radical Chemistry: A Computational Approach*
Molecular Modelling – 2010: Advances in Biomolecular and Materials Modelling
Melbourne, Australia, November–December 2010
(Plenary Lecture)

100. *Analysis of the Effect of Multiple Substitution on the Stability of Carbon-Centered Radicals*
Symposium on Computational Quantum Chemistry: Theory and Interactions with Experiment
2010 International Chemical Congress of Pacific Basin Societies
Honolulu, Hawaii, U.S.A., December 2010
(Invited Lecture)

101. *Hydrogen Abstraction by Chlorine Atom from Amino Acids: The Remarkable Influence of Polar Effects on Regioselectivity*
Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2011)
Santiago de Compostela, Spain, July 2011
(Invited Lecture)

102. *A Computational Approach to the Study of Free Radical Chemistry*
Seventh Congress of the International Society for Theoretical Chemical Physics (ISTCP-VII)
Tokyo, Japan, September 2011

(Plenary Lecture)

103. *Some Shared Adventures on Potential Energy Surfaces*
Symposium on Theoretical and Computational Chemical Physics in Honour of Professor Michael Collins
Canberra, Australia, November 2011
(Invited Lecture)

104. *Adventures In Free Radical Chemistry: A Computational Approach*
BioPhysChem 2011
Wollongong, Australia, December 2011
(Physical Chemistry Division Medal Lecture)

105. *The Contrathermodynamic Abstraction of Hydrogen By Chlorine Atom From Amino Acids*
Fifth Asia Pacific Conference on Theoretical and Computational Chemistry (APCTCC-5)
Rotorua, New Zealand, December 2011
(Invited Lecture)

106. *DFT Calculations on Radicals*
Challenges in Density Matrix and Density Functional Theory
Ghent, Belgium, April 2012
(Plenary Lecture)

107. *Influence of Connector Groups on the Stabilities of Radicals*
Beckwith Memorial Symposium on Free Radical Chemistry
244th National Meeting of the American Chemical Society
Philadelphia, USA, August 2012
(Invited Lecture)

108. *Water-Catalyzed Proton-Transfer Reactions: Identification of Shortcomings in G2(MP2)-Type Procedures*
Symposium in Honor of Professor H.B. Schlegel
244th National Meeting of the American Chemical Society
Philadelphia, USA, August 2012
(Invited Lecture)

109. *A Computational Exploration of the Stabilities of Free Radicals*
Sixth Asia Pacific Conference on Theoretical and Computational Chemistry (APCTCC-6)
Gyeongju, South Korea, July 2013
(Keynote Lecture)

CONFERENCE ORGANIZATION

Secretary, "Organic Synthesis: A Symposium in Honour of Professor A.J. Birch", Canberra, February 198l

Convenor, "Minisymposium in Theoretical Organic Chemistry/Computational Quantum Chemistry", Canberra, February 1982

Secretary, "Royal Australian Chemical Institute, Organic Division, 7th National Conference", Canberra, August 1982

Committee Member, "Summer School in Theoretical Chemistry", Canberra, February 1983

Committee Member , "Third Australian Conference on Atomic and Molecular Physics and Quantum Chemistry", Canberra, February 1984

Convenor, "The Interface Between Theory and Experiment: A Symposium in Honour of Professor D.P. Craig", Canberra, February 1985

International Advisory Committee Member, "World Congress of Theoretical Organic Chemists", Budapest, Hungary, August 1987

International Advisory Committe Member, "10th IUPAC Conference on Physical Organic Chemistry

International Advisory Committee Member, "Second World Congress of Theoretical Organic Chemists", Toronto, Canada, July 1990

Convenor, "RSC-25: Reflections on the Past and Visions for the Future", Canberra, September 1992

Co-Chair, "Computational Quantum Chemistry: A Viable Partner to Experiment in Chemical Research", Honolulu, USA, December 1995

International Advisory Committee Member, "Fourth World Congress of Theoretical Organic Chemists", Jerusalem, Israel, July 1996

International Advisory Committee Member, "Fifth World Congress of Theoretical Organic Chemists", London, England, August 1999

Co-Chair, "Computational Quantum Chemistry: Theoretical and Experimental Perspectives", Honolulu, USA, December 2000

International Advisory Committee Member, "16th IUPAC Conference on Physical Organic Chemistry", San Diego, USA, August 2002

Co-organiser, "Computational Chemistry in the 21st Century", Melbourne, Australia, June 2003

International Advisory Board, "Singapore International Chemistry Conference 3", Singapore, December 2003

International Advisory Board, "1st Asia-Pacific Conference on Theoretical & Computational Chemistry", Okazaki, Japan, May 2004,

International Advisory Board Member, "17th IUPAC Conference on Physical Organic Chemistry", Shanghai, China, August 2004

Co-organiser, "Symposium in Honor of Professor H.F. Schaefer III", 228th National Meeting of the American Chemical Society, Philadelphia, USA, August 2004

Co-organiser, "Symposium in Memory of Professor John Pople", 229th National Meeting of the American Chemical Society, San Diego, USA, March 2005

International Advisory Board, "2nd Asian Pacific Conference on Theoretical & Computational Chemistry", Bangkok, Thailand, May 2005.

International Advisory Board Member, "18th IUPAC Conference on Physical Organic Chemistry", Warsaw, Poland, August 2006

International Advisory Board Member, "19th IUPAC Conference on Physical Organic Chemistry", Santiago de Compostela, Spain, July 2008

Chair, Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists, Sydney, September 2008

International Advisory Board Member, "20th IUPAC Conference on Physical Organic Chemistry", Busan, Korea, August 2010

Co-Chair, "Computational Quantum Chemistry: Theory and Interactions with Experiment", Honolulu, USA, December 2010

International Advisory Board Member, "21st IUPAC Conference on Physical Organic Chemistry", Durham, England, September 2012

International Advisory Board Member, "22nd IUPAC Conference on Physical Organic Chemistry", Ottawa, Canada, August 2014

Co-Chair, "Computational Quantum Chemistry: Theoretical and Experimental Perspectives", Honolulu, USA, December 2015

International Advisory Board Member, "23rd IUPAC Conference on Physical Organic Chemistry", Sydney, Australia, July 2016