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Birth Date

September 22, 1921

Education

A. B., Magna cum Laude with High Honors in Chemistry, Brown University, 1942.
Ph.D., Physical Chemistry, University of Minnesota, 1947.
D.h.c. University of Leuven, 1986; Jagiellonian University, 1996.

Academic Positions

Assistant Professor of Chemistry, University of Minnesota, 1947-48; Assistant Professor to Professor of Chemistry, Carnegie Institute of Technology, 1948-1962; Visiting Professor of Chemistry and Member of Center of Advanced Study, University of Illinois, 1962; Professor of Chemistry, The Johns Hopkins University, 1962-1974; Chairman, Department of Chemistry, 1969-1972; William R. Kenan, Jr. Professor of Theoretical Chemistry, University of North Carolina, 1974-1990; Wassily Hoeffding Professor of Chemical Physics, 1990-present.

Fellowships, Honors and Awards

Fellow, University of Chicago, 1949, Research Associate, 1957; Visiting Professor, State University of New York at Buffalo and Pennsylvania University, 1967; Japan Society for the Promotion of Science, 1968 and 1979; Technion, University of Berlin, 1977; Duke University 1996-1997; Firth Professor, University of Sheffield, 1976; Coochbehar Professor, Indian Association for the Cultivation of Science, 1990; Sandoval Vallarta Professor, UAM-Iztapalapa, 1992; Mulliken Lecturer, University of Georgia, 1988; Bircher Lecturer, Vanderbilt University, 1990; Crawford Lecturer, University of Minnesota, 1994; Centennial Lecturer of the American Physical Society, 1999; Member, Institute for Theoretical Physics, University of California at Santa Barbara, 1983, 1994.

Guggenheim Fellow and Fulbright Scholar, University of Cambridge, 1953-54; Sloan Fellow, 1956-60. National Science Foundation Senior Postdoctoral Fellow, University of Oxford and CSIRO (Melbourne), 1967-68; Chairman of the General Faculty, Carnegie Institute of Technology, 1960-1961; Chairman of the Faculty Priorities Committee, University of North Carolina, 1986-87; Chancellor's Advisory Committee, 1987-89.

Outstanding Achievement Award of the University of Minnesota, 1968. North Carolina Institute of Chemists Distinguished Chemist Award, 1982. North Carolina Distinguished Speaker Award, North Carolina Section of the American Chemical Society, 1984. Honorary citizen, Taichung City, Taiwan, 1993. Special issues of International Journal of Quantum Chemistry: Volume 37, no. 4, in honor of R. Pariser, R. G. Parr, and J. A. Pople. Volume 49, nos. 3, 4, 5, dedicated to R. G. Parr. Symposium in honor of R. G. Parr, Southeast American Chemical Society Meeting, 1998. Selected by Brown Alumni Magazine as one of the 100 Brown University alumni who most influenced the 20th century, 2000. Book published by World Scientific Publishers in 2002: *Reviews in Modern Quantum Chemistry: Celebration of the Contributions of Robert G. Parr*. Symposium in honor of R. G. Parr, American Chemical Society, March 2006.

Fellowships, Honors and Awards (contd.)

Irving Langmuir Award in Chemical Physics, American Chemical Society, 1994.
North Carolina Award in Science, 1999.
National Academy of Sciences Award in Chemical Sciences, 2004.
Member of International Academy of Quantum Molecular Science. President, 1991-97.
Member of National Academy of Sciences (U.S.)
Member of American Academy of Arts and Sciences
Member of Indian National Science Academy.

Professional Activities

Editorial Boards: Journal of Chemical Physics, 1956-1958; Chemical Reviews, 1961-63; Journal of Physical Chemistry, 1963-67, and 1977-79; American Chemical Society Monographs, 1966-71; Theoretica Chimica Acta, 1966-69, and 1992-96; Chemical Physics Letters, 1967-1979; International Journal of Quantum Chemistry, 1967-present; Chinese Chemical Letters, 1998-present. Associate Editor, Journal of the American Chemical Society, 1969-77.

Organizational Affiliations

Member of Phi Beta Kappa, Sigma Xi, Phi Lambda Upsilon, Pi Mu Epsilon, Sigma Nu, Cosmos Club, Golden Kiwanis. Member of American Chemical Society. Chairman, Division of Physical Chemistry, 1977-78. Fellow of American Physical Society. Chairman of Division of Chemical Physics, 1963-64; Member of Panel on Public Affairs, 1976-77. Fellow of AAAS. Honorary Board Member, International Society for Theoretical Chemical Physics.

Secretary, Shelter Island Conference on Valence Theory, 1951. Chairman, Boulder Quantum Chemistry Conference, 1959. Chairman of Executive Committee, Second International Congress of Quantum Chemistry, New Orleans, 1976. Member-at-Large, Gordon Research Conferences Council, 1974-76. Chairman, Review Committee for the Journal of Chemical Physics, American Institute of Physics, 1979. Honorary Chairman, Cracow Symposium on Thirty Years of Density Functional Theory, 1994.

Chairman, NAS-NRC Committee on Postdoctoral Fellowships in Chemistry, 1961-1963. Chairman, Panel on Theoretical Chemistry of the Westheimer Committee for the Survey of Chemistry, NAS 1964. Member of Commission on Human Resources, National Research Council, 1979-82; Chairman Advisory Committee on Associateships, Office of Scientific and Engineering Personnel, National Research Council, 1983-84; Member of Advisory Committee, Office of Scientific and Engineering Personnel, National Research Council, 1984-87. Member of Council, Institute for Molecular Science, Okazaki, Japan, 1986-88; Board of Trustees, Institute for Fundamental Chemistry, Kyoto, Japan, 1988-2000.

PUBLICATION LIST

1. Simple expressions for the heat capacities of gases. B.L. Crawford, Jr. and R.G. Parr, J. Chem. Phys. 16, 233-236 (1948).

2. Molecular orbital calculations of vibrational force constants. I. Ethylene. R.G. Parr and B.L. Crawford, Jr. J. Chem. Phys. 16, 526-532 (1948).

3. On certain integrals useful in molecular orbital calculations. R.G. Parr and B.L. Crawford, Jr. J. Chem. Phys. 16, 1049-1056 (1948).

4. Molecular orbital calculations of vibrational force constants. II. The ring-twisting constants of benzene. B.L. Crawford, Jr. and R.G. Parr, J. Chem. Phys. 17, 726-733 (1949).

5. On the detection and determination of redundant vibrational coordinates. C.E. Sun, R.G. Parr and B.L. Crawford, Jr., J. Chem. Phys. 17, 840 (1949).

6. Calculations of the lower excited levels of benzene. C.C.J. Roothaan and R.G. Parr, J. Chem. Phys. 17, 1001 (1949).

7. A physical theory of burning of double-base rocket propellants. I. R.G. Parr and B.L. Crawford, Jr. J. Phys. and Colloid Chem. 54, 929-954 (1950).

8. LCAO self-consistent field calculation of the pi-electron energy levels of cis-and trans-1, 3-butadiene. R.G. Parr and R.S. Mulliken, J. Chem. Phys. 18, 1338-1346 (1950).

9. Molecular orbital calculations of the lower excited electronic levels of benzene, configuration interaction included. R.G. Parr, D.P. Craig and I.G. Ross, J. Chem. Phys. 18, 1561-1563 (1950).

10. LCAO self-consistent field calculation of the twisting frequency and pi-electron energy levels of allene. R.G. Parr and G.R. Taylor, J. Chem. Phys. 19, 497-501 (1951).

11. On LCAO molecular orbital schemes and theoretical resonance energies. R.G. Parr, J. Chem. Phys. 19, 799-800 (1951).

12. A mobile electron model for aromatic molecules. K. Ruedenberg and R.G. Parr, J. Chem. Phys. 19, 1268-1270 (1951).

13. LCAO molecular orbital computation of resonance energies of benzene and butadiene with general analysis of theoretical versus thermochemical resonance energies. R.S. Mulliken and R.G. Parr, J. Chem. Phys. 19, 1271-1278 (1951).

14. Superposition of configurations: The helium atom. G.R. Taylor and R.G. Parr, Proc. Natl.Acad. Sci. USA 38, 154-160 (1952).

15. National Academy of Sciences conference on quantum-mechanical methods in valence theory. R.G. Parr and B.L. Crawford, Jr., Proc. Natl. Acad. Sci. USA 38, 547-553 (1952).

16. A method for estimating electronic repulsion integrals over LCAO MOs in complex unsaturated molecules. R.G. Parr, J. Chem. Phys. 20, 1499 (1952).

17. Semi-empirical theory of the electronic spectra and electronic structure of complex unsaturated molecules. I. R. Pariser and R.G. Parr, J. Chem. Phys. 21, 466-471 (1953).

18. A semi-empirical theory of electronic spectra and electronic structure of complex unsaturated molecules. II. R. Pariser and R.G. Parr, J. Chem. Phys. 21, 767-776 (1953).

19. Electronic states of diatomic molecules: the oxygen molecule. F.G. Fumi and R.G. Parr. Chem. Phys. 21, 1864-1868 (1953).

20. On the electronic structure and electronic spectra of ethylene-like molecules. R.G. Parr and R. Pariser, J. Chem. Phys. 23, 711-725 (1955).

21. The quantum theory of valence. R.G. Parr and F.O. Ellison, Annu. Rev. Phys. Chem. 6, 171-192 (1955).

22. Generalized antisymmetrized product wave functions for atoms and molecules. R.G. Parr, F.O. Ellison and P.G. Lykos, J. Chem. Phys. 24, 1106 (1956).

23. On the pi-electron approximation and its possible refinement. P.G. Lykos and R.G. Parr, Chem. Phys. 24, 1166-1173 (1956); 25, 1301 (1956).

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25. 1s orbitals as basis functions for molecular calculations. R.G. Parr, J. Chem. Phys. 26, 428 (1957).

26. Book review: Mécanique Ondulatoire Appliquée a l'Étude des Atomes et des Molecules, by Raymond Daudel. R.G. Parr, J. Am. Chem. Soc. 79, 5586 (1957).

27. Theory of separated electron pairs. J.M. Parks and R.G. Parr, J. Chem. Phys. 28, 335-345 (1958).

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29. A one-center wave function for the hydrogen molecule. H.W. Joy and R.G. Parr, J. Chem. Phys. 28, 448-453 (1958).

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37. Three remarks on molecular orbital theory of complex molecules. R.G. Parr, J. Chem. Phys. 33, 1184-1199 (1960).

38. Problems in perturbation theory calculation of diamagnetic susceptibility and nuclear magnetic shielding in molecules: illustration with the hydrogen atom. L.C. Snyder and R.G. Parr, J. Chem. Phys. 34, 837-842 (1961).

39. Extraordinary basis functions in valence theory. L.C. Snyder and R.G. Parr, J. Chem. Phys. 34, 1661-1665 (1961).

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41. Perturbation theory calculations. R.G. Parr and L.C. Snyder, J. Chem. Phys. 35, 1898-1899 (1961).

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47. An approach to the internal rotation problem. M. Karplus and R.G. Parr, J. Chem. Phys. 38, 1547-1552 (1963).

48. Magnetic properties of molecules from one-center wave functions. Theory and application to the hydrogen molecule. J.R. Hoyland and R. G. Parr, J. Chem. Phys. 38, 2991-2998 (1963).

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56. Off-center hydrogen atom calculations. A.G. Turner, B.H. Honig, R.G. Parr and J.R. Hoyland, J. Chem. Phys. 40, 3216-3220 (1964).

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61. Integral Hellmann-Feynman theorem. H. Kim and R.G. Parr, J. Chem. Phys. 41, 2892-2897 (1964).

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63. Range of electron correlation in the helium atom. B.M. Gimarc, W.A. Cooney and R.G. Parr. J. Chem. Phys. 42, 21-25 (1965).

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66. Time-dependent Hellmann-Feynman theorems. E.F. Hayes and R.G. Parr, J. Chem. Phys. 43, 1831-1832 (1965).

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68. Book review: Molecular Orbital Theory, by C.J. Ballhausen and H.B. Gray. R.G. Parr, J. Franklin Inst. 280, 287 (1965).

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70. Integral Hellmann-Feynman theorem, barriers to internal rotation, and iso-electronic processes. R.G. Parr, in Modern Quantum Chemistry, Part I (Academic Press, Inc., New York, 1965), pp. 101-105.

71. General survey of pi-electron methods and problems. R.G. Parr, in Modern Quantum Chemistry, Part I (Academic Press, Inc., New York, 1965), pp. 107-112.

72. Book review: Electrons and Chemical Bonding, by H.B. Gray, and Chemical Bonding, by A.L. Companion. R.G. Parr, Science 150, 738 (1965).

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74. Chemical bond theory. R.G. Parr, McGraw-Hill Encyclopedia of Science and Technology (McGraw-Hill Co., Inc., New York, 1965), Vol. 3, pp. 26A-26B.

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77. Theoretical chemistry: a current review. R.G. Parr, R.B. Bernstein, H.S. Gutowsky, S.A.Rice, H.E. Simmons and O. Sinanoglu, National Academy of Sciences-National Research Council Publication 1292-D, 1966.

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80. Energy differences from the integral Hellmann-Feynman formula: Application to HeH^+. E.F. Hayes and R.G. Parr, J. Chem. Phys. 44, 4650-4651 (1966).

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82. Hulthén orbital and Hulthén correlation factor for the ground state of helium-like systems. R.G. Parr and J.H. Weare, Prog. Theor. Phys. (Kyoto) 36, 854-855 (1966).

83. Book review: Methods of Quantum Chemistry, by Veselov et al., R.G. Parr, J. Chem. Ed. 44, A162 (1967).

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85. Chemical binding and potential energy functions for molecules. R.G. Parr and R.F. Borkman. Chem. Phys. 46, 3683-3685 (1967).

86. Single-center expansions of molecular electronic wave functions. E.F. Hayes and R.G. Parr, Prog. Theor. Phys. (Kyoto), Supplement 40, 78-105 (1967).

87. Some integral Hellmann-Feynman calculations on hydrogen peroxide and ammonia. M.P. Melrose and R.G. Parr, Theoret. Chim. Acta 8, 150-156 (1967).

88. Integrated and integral Hellmann-Feynman formulas. S.T. Epstein, A.C. Hurley, R.E. Wyatt and R.G. Parr, J. Chem. Phys. 47, 1275-1286 (1967).

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90. One-center perturbation approach to molecular electronic energies. III. One-electron systems. P. Hauk, H. Kim, R.G. Parr and H.F. Hameka, J. Chem. Phys. 47, 2677-2684 (1967).

91. A stationary principle for discontinuous trial functions and a framework for zero-differential overlap theories of electronic structure. J.H. Weare and R.G. Parr, Chem. Phys. Lett. 1, 349-350 (1967).

92. Remark on the analytical form of 1s orbitals in atoms and molecules. J.H. Weare and R.G. Parr, Intern. J. Quantum Chem. Symposium 1, 163-165 (1967).

93. Book review: Valence Theory, by J.N. Murrell, S.F.A. Kettle, and J.M. Tedder. R.G. Parr, American Scientist 55, 489A-490A (1967).

94. Determination of accurate single-center expansions with Slater-type orbitals: the H_3 system. E.F. Hayes and R.G. Parr, J. Chem. Phys. 47, 3961-3967 (1967).

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96. Integral virial theorem and generalized differential Hellmann-Feynman formula. R.G. Parr, F. Borkman and M.T. Marron, J. Chem. Phys. 48, 1425-1426 (1968).

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100. Toward understanding vibrations of polyatomic molecules. R.G. Parr and J.E. Brown, J. Chem. Phys, 49, 4849-4852 (1968).

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110. Single-center variational calculations with basis functions depending on $r_<$ and $r_>$. A.B. Anderson and R.G. Parr, J. Chem. Phys. 53, 4098-4100 (1970).

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114. Vibrational potential functions for CO_2, OCS, HCN, and N_2O. J.E. Brown and R.G. Parr, J. Chem. Phys. 54, 3429-3438 (1971).

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