
J. Gerratt, 1938–1997

This volume is a celebration of the scientific achievements of the late Joseph Gerratt. These were indeed considerable for Gerratt was a pioneering researcher. In his graduate work, with I. M. Mills, he introduced the direct evaluation of force constants and energy derivatives [1, 2]. The determination of analytic energy derivatives with respect to nuclear coordinates has facilitated detailed studies of potential energy hypersurfaces by quantum chemical methods. This work was published in 1968 but did not become widely appreciated until almost a decade later. In the late 1970s and early 1980s the practical calculation of analytical energy derivatives became a reality. Today, it is part of “everyday” quantum chemistry. His paper, with I. M. Mills, entitled “Force constants and dipole-moment derivatives of molecules from perturbed Hartree–Fock calculations.” [1] was included in the list of “landmark” papers in *ab initio* molecular electronic structure methods selected by H. F. Schaefer III in *Quantum Chemistry: The Development of ab initio Methods in Molecular Electronic Structure Theory* [3]. Schaefer writes:

It goes almost without saying that certain scientific papers while recognized as important upon publication, become much more important as time passes. This is certainly true of the paper by Gerratt and Mills, who set out to determine the derivatives of each occupied SCF molecular orbital with respect to each nuclear coordinate. As methods have developed since 1978 for the determination of analytic SCF energy second derivatives . . . and analytic CI energy first derivatives, the solution of these ‘coupled-perturbed Hartree–Fock equations’ has become absolutely essential. . . . Accordingly, the Gerratt and Mills paper has become a genuine classic in the history of molecular electronic structure theory [3], p. 56.

Gerratt and Mills recognized the difficulties which arise in the numerical evaluation of derivatives. Indeed, they quoted from Hartree’s treatise on *Numerical Analysis* [4] in their work:

The differentiation of a function specified only by a table of values . . . is a notoriously unsatisfactory process, particularly if higher derivatives than the first are required [1].

In a review published in 1987 by another pioneer of analytical derivative methods in molecular electronic structure calculations, Pulay [5] was able to write [6]:

Since their introduction in the late 1960s, gradient methods, or more properly analytical derivative methods, have become one of the most vigorously developing topics on modern quantum chemistry [6], p. 241.

Most often analytical derivative methods are employed in structure optimizations via energy minimization. Gerratt’s interest lay in the application of theoretical techniques in molecular spectroscopy, and he recognized the importance of molecular wave functions which provided a useful description of molecular dissociative processes.

Gerratt’s main interest was in the calculation of potential energy curves and surfaces, in the description of intermolecular forces, and in the nature of chemical bonding. He recognized at an early stage the inadequacies of the Hartree–Fock molecular orbital theory and advocated the use of valence bond theory, which, in another landmark paper [7] published in 1971, he cast into its “modern” form. With an encyclopedic knowledge of the work of prewar pioneers, such as Heitler [8] and van Vleck [9], he laid the foundations of a practical

ab initio valence bond theory. His theory of spin-coupled wave functions employed the spin permutation group and the symmetric group to construct spin eigenvalues. He built on the work of Racah [10], Wigner [11], Kotani [12], Serber [13], Jahn [14], Löwdin [15], Kaplan [16], and others in developing his general theory, which, in more recent years, has seen a wide range of applications.

The importance of the work, which Gerratt was beginning when he arrived in Bristol in 1968, on what is now called "modern" valence bond theory has only been recognized in recent years. Over the past 10 years, a range of applications have demonstrated the advantages of the method [17–20]. Many have become aware of the "simple elegance" afforded by this approach to the molecular electronic structure problem and its power in describing the dissociative chemical process. The essential ingredients of the method were given in his paper with Lipscomb [21] which is reproduced in this volume [22]. Single-handedly, Gerratt developed the basic equations for his "General theory of spin-coupled wave functions for atoms and molecules" published in *Advances in Atomic and Molecular Physics* [7]. In his article, he begins:

The object of any useful theory of natural phenomena are threefold: to give quantitative answers that are in reasonable agreement with experiment, to provide a logically self-consistent physical model, and to predict correctly the results of further experiments. The Hartree–Fock molecular orbital theory of the electronic structure of atoms and molecules may claim to be a substantial success on all these three counts.

The theory still possesses a number of shortcomings, however. As is well-known, it gives an adequate account of chemical binding both qualitatively and quantitatively [7], p. 141.

The spin-coupled wave function for an N -electron system is written

$$\Psi_{SM}^0 = \sum_{k=1}^{f_S^N} C_{Sk} \sqrt{N!} \mathcal{A}(\phi_1 \phi_2 \dots \phi_N \Theta_{S,M;k}^N),$$

where the spatial orbitals are $\phi_\mu(\mathbf{r})$, $\mu = 1, 2, \dots, N$ and the N -electron spin function, $\Theta_{S,M;k}^N$ is an eigenfunction of S^2 and S_z formed by coupling the one-electron spins according to a scheme k ; \mathcal{A} is the antisymmetrizing projection operator, and the coefficients C_{Sk} are determined by solution of a secular equation. The orbitals $\phi_\mu(\mathbf{r})$ are not sub-

jected to any restrictions other than normalization. In practice this leads to functions which often reflect the chemist's intuitive picture of the bonding mechanism. Gerratt's article set up a general scheme for carrying out a calculation with such a wave function. It was arranged as follows:

- I. Introduction
 - II. Properties of the Exact Electronic Eigenfunction
 - III. Construction of the Spin Functions
 - IV. The Spin-Coupled Wave Functions
 - V. Calculation of Matrix Elements of the Hamiltonian
 - VI. The Orbital Equations
 - VII. Symmetry Properties of the Spin-Coupled Wave Functions
 - VIII. The Hund's Rule Coupling
 - IX. The General Recoupling Problem and Bonding in Molecules
 - X. Conclusions
- Note Added in Proof

In the late 1960s and early 1970s, Gerratt was not alone in his efforts to develop a "modern" valence bond theory. In particular, Goddard, in California, was independently following a similar approach. In his 1971 article, Gerratt writes:

The object of this article is to develop a theory that is as general as possible and to examine its consequences thoroughly. In particular, an extensive analysis of the spatial symmetry properties of the orbitals is given. This is of some importance since much of the physical content of the theory reveals itself through this.... Some progress in this direction has been made in a recent series of papers by Goddard and his work is referred to at various points. His results, however, have been disappointing, with total energies differing very little from the corresponding HFMO results. This is due to the particular formalism used, which obscures the physical significance of the different possible coupling schemes for the orbitals [7], p. 143.

Goddard [23–26] formulated the problem in terms of the Young diagrams and Young tableaux of the symmetric group. Gerratt used the more physical spin-coupling techniques taken from angular momentum theory. In Bristol, the use of orbital orthogonality restrictions was explored as a means of

rendering calculations computationally tractable [27, 28]. [For example, the adoption of a $(\mu - 1, \mu)$ orthogonality condition facilitated calculations of the diborane molecule and a unique representation of the three-center bond [29].] A very similar approach was followed by Goddard and his co-workers, and his generalized valence bond (GVB) approach [30] was widely adopted in the mid-1970s. One of the many consequences of Gerratt's detailed and thorough examination of the theoretical apparatus of spin-coupled wave functions was the recognition that

the form of the orbital equations... shows that an electron assigned to an orbital ϕ_μ may be interpreted as moving in an average field... due to all the other electrons in the molecule. We observe that the operator is different for each orbital, so that each electron experiences a different average field [7], p. 167.

This means that for each occupied orbital there is a distinct set of virtual orbitals [31]. These orbitals are used to construct a nonorthogonal configuration interaction (CI) wave function in the spin-coupled valence bond (SCVB) method. This method has proved extremely powerful in the accurate description of excited states, sometimes supporting a range of more than 40 eV.

An essential ingredient of spin-coupled valence bond theory is a knowledge of the theory of the symmetric group and spin algebras. Gerratt translated [34] Kaplan's *Symmetry of Many-Electron Systems* from the original Russian [35]. The total electronic wave function of an atom or molecule, Ψ_{SM} , with spin quantum numbers S and M must satisfy

$$P\Psi_{SM} = \varepsilon_p\Psi_{SM},$$

where P is the operator which simultaneously permutes space and spin coordinates and $\varepsilon_p = \pm 1$, depending on whether the permutation is odd or even. We can write

$$P = P^r P^\sigma,$$

where $P^r(P^\sigma)$ permutes only space (spin) coordinates and, since the Hamiltonian, \mathcal{H} , is completely symmetric under all permutations of the spatial coordinates:

$$[\mathcal{H}, P^r] = 0, \quad \forall P \in \mathcal{S}_N.$$

The N -electron spatial wave function, Φ_{Sl}^N , must satisfy

$$P^r\Phi_{Sk}^N = \sum_{l=1}^{f_S^N} U_{lk}^{S,N}(P)\Phi_{Sl}^N,$$

and the N -electron spin function, $\Theta_{S,N;l}^N$ must satisfy

$$P^\sigma\Theta_{S,N;k}^N = \varepsilon_p \sum_{l=1}^{f_S^N} U_{lk}^{S,N}(P)\Theta_{S,M;l}^N,$$

where the matrices $U^{SN}(P)$ form an irreducible representation of the symmetric group, S_N . The most general form that the wave function Ψ_{SM} can have is then [11]

$$\Psi_{SM} = \frac{1}{f_S^N} \sum_{k=1}^{f_S^N} \Phi_{Sk}^N(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \times \Theta_{S,M;k}^N(\sigma_1, \sigma_2, \dots, \sigma_N).$$

These equations are fundamental to the spin-coupled wave function method, and Gerratt's translation of Kaplan's book did much to increase understanding of these fundamentals.

Inevitably, the practical realization of an ab initio valence bond theory faced significant computational challenges. Often these required a completely new approach as, for example, in the development of the quasi-second-order methods which he introduced, together with Pyper [32, 33], for the optimization of the molecular wave functions constructed from nonorthogonal orbitals. Increased computing power, coupled with improved algorithms, has heralded a resurgence of interest in calculations based on valence bond theory not only because it supports a simple intuitive picture of chemical bonding, but also because it correctly describes molecular dissociative processes. Both of these features had originally inspired Gerratt's seminal work.

Although programs for performing calculations based on Gerratt's general theory were operational in the mid-1970s [32, 33], it is only in more recent years that he, in collaboration with Raimondi and then Cooper, Karadakov, and others, demonstrated the power of the approach [17–20]. There are at least two reasons for this delay in realizing the full potential of the method: (i) only relatively recently have computers of sufficient power to handle the demands of modern valence bond calculations become available, and (ii) increasingly

Hartree–Fock calculations have become “routine” and only in more recent times has it been recognized that in order to improve our description of molecular electronic structure, particularly in situation involving bond breaking, one needed more than mere computing time; one needs new theories which encapsulate the essential physics and chemistry of the target system.

In 1986, the theory of spin-coupled wave functions was brought to the attention of a wider audience by a paper published [36] (see also [37]) in *Nature* concerning the electronic structure of the benzene molecule, the quintessential aromatic molecule. The spin-coupled approach successfully challenged the established quantum chemical explanation of aromaticity based on molecular orbital theory. In subsequent work [38, 39], a particularly simple and highly visual interpretation of the effect of substituents on the energy and electron distribution of the arenium intermediates in aromatic electrophilic substitutions was afforded by the spin-coupled wave function theory. Antiaromaticity arises in cyclobutadiene from the formation of a triplet spin state from a pair of electrons in two distinct orbitals of the C_4 ring. Gerratt and his co-workers [40] demonstrated that, in addition to the characteristic orbitals, it is the particular spin-coupling scheme in which two triplet pairs are coupled to an overall singlet that provides the key to understanding the antiaromaticity of this system. A generalization of this picture came from studies of systems in which two H atoms of cyclobutadiene are substituted by methylene groups or further cyclobutadiene units. Further generalization of these ideas led to the antiferromagnetic spin-coupling model exemplified in a study on cyclobutadiene chains [41].

Gerratt had a long-standing interest in the mechanisms of cycloaddition reactions and their theoretical description. The first spin-coupled wave function studies were of the reaction of CH_2 with molecular hydrogen to form methane [42] and with ethene to form cyclopropane [43]. Along the reaction path there was found to be a region in which orbitals, originally centered on ethene, are substantially deformed toward the more electrophilic CH_2 . In the orbital picture furnished by the spin-coupled wave function, there is a point in the reaction where one can detect “the action of a hook or claw” and the term “chelotropic reaction” appears appropriate. A study of the ethene + ethene addition reaction [44] provides a further example of the use of spin-coupled wave function

theory in the description of both the qualitative changes of the orbitals and of the spin-recoupling processes which usually accompany such reactions.

Calculations based on the theory of spin-coupled wave functions afford unique and compelling evidence suggesting that the familiar octet rule for main group elements should be replaced by a “democracy principle,” according to which any valence electron can participate in chemical bonding, depending only on the availability of sufficient energetic incentives [45].

For the N_2S_2 molecule, a spin-coupled wave function study revealed that this molecule has the character of a singlet radical [46]. The two N atoms at the two opposite vertices of the square each have a negative charge while the two S atoms have a complementary positive charges. The electronic structure of the six-electron p system is described in this model by two orbitals on each N paired to form singlets and by two orbitals highly localized on each S, but possessing a nodal surface, roughly half way between the two S atoms; the spins associated with these two orbitals are again coupled to form a singlet.

As a graduate student in the early 1960s, Gerratt recognized the importance of “high-performance” computing to his work. He had coded the Barnett–Coulson algorithm [47] for integrals over exponential-type basis functions in ALGOL at Reading University. He was one of the first users of the Ferranti Atlas computer, the United Kingdom’s first supercomputer, installed in the Atlas Computer Laboratory, sited less than 30 miles from Reading, next door to the Atomic Energy Research Establishment, Harwell, in 1964. He was a frequent visitor and enthusiastic supporter of C.E.C.A.M., the Centre Européen Calcul Atomique et Moléculaire (European Centre for Atomic and Molecular Computations), an institute founded in Paris in 1969, but now operating in Lyons with the aim of promoting “advanced study and application of computational science in atomic, molecular and condensed-matter physics and chemistry.” Gerratt was a founding member of what was to become the first UK Collaborative Computational Project. This project, entitled, “Electron correlation in molecules,” was inaugurated in the mid-1970s. Under the auspices of “four wise men” [48] (C. A. Coulson, R. McWeeny, P. G. Burke, and B. H. Bransdon), it was originally known as the Meeting House project. In a review of the development of computational chemistry in the United Kingdom,

Smith and Sutcliffe [48] describe how the then director of the Atlas Computing Laboratory, Dr. J. Howlett,

proposed... for the first meeting house to be one which would study "molecular correlation errors in theories which surpass the Hartree–Fock theory in accuracy" ... The first Project 1 working group consisted of... [Roy] McWeeny and [John] Murrell ... and J. (Joe) Gerratt (Bristol), N.C. (Nicholas) Handy (Cambridge), M.A. (Mike) Robb (Queen Elizabeth, London) and B.T. (Brian) Sutcliffe (York). ...

The first meeting of the Working Group took place ... on 28 March 1974. ... The agenda for that meeting began as follows:

1. THE SCIENTIFIC SCOPE OF THE PROJECT ...

- i. Valence Bond Theory and Its Variants
- ii. Multiconfigurational Self-Consistent Field Theory
- iii. Geminal and Group Function Methods
- iv. Large Scale Configuration Interaction
- v. Transcorrelated Wave Functions
- vi. Many Body Perturbation Theory and Green's Function Methods
- vii. Time-Dependent Hartree–Fock Theory, Response Functions, and Related Methods

However, although valence bond theory headed the list of possible projects, it was not until a meeting on 4 December, 1975, that [48] "Joe Gerratt was invited to inaugurate a pilot study on the viability of the VB method."

At that time, his "modern" valence bond theory was not accepted as "mainstream" by the UK quantum chemistry community. Nevertheless Gerratt's work was followed with interest and, in more recent times, has been more widely accepted and appreciated.

Over the years, Gerratt and his colleagues developed a number of techniques for the practical determination of spin-coupled wave functions beginning with the quasi-second-order methods which he introduced, together with Pyper [32, 33]. At present, there are three main strategies for the optimization of spin-coupled wave functions:

1. The symmetric group strategy, which has been extended to handle the optimization of

a set of doubly occupied, "inactive" orbitals [49].

2. Expansion in Slater determinants constructed from nonorthogonal orbitals [50], a strategy which can handle up to 14 "active" electrons [51], together with "inactive" electrons [52].
3. "CASVB" [53, 54], which may be used either to generate compact representations of complete active space self-consistent field (CAS-SCF) wave functions or to perform fully variational optimization of various types of modern valence bond wave function, such as spin-coupled and multiconfiguration spin-coupled wave functions.

Gerratt's other scientific interests were as wide and varied as they were original and insightful. The study of intermolecular forces and van der Waals interactions, the use of the L^2 R -matrix theory, and charge transfer were among the areas to which he made significant contributions. A complete list of the scientific publications of J. Gerratt follows this article.

Born in 1938, J. Gerratt grew up in Northampton, the county town of Northamptonshire in the English East Midlands. He was educated at Oxford University. Gaining a place at Hertford College, he read chemistry and graduated from the university in 1961. He left Oxfordshire and moved, some 30 miles or so, south to the neighboring county of Berkshire where, at the University of Reading, he carried out research for his doctorate under the supervision of Professor I. M. Mills, a molecular spectroscopist, in the Chemistry Department. He was awarded his doctorate in 1966. His thesis examiner was Professor R. McWeeny. Then, he crossed the Atlantic to undertake postdoctoral research with Professor W. N. Lipscomb in the Chemistry Department of Harvard University. His study in the Proceedings of the National Academy of Science (U.S.A.) [21] entitled "Spin-coupled wave functions for atoms and molecules," is reproduced in this volume [22]. Returning to England in 1967, he took up a post as lecturer in the University of East Anglia in Norwich. After a year, he moved to the west of England, to the University of Bristol where he joined the newly formed Department of Theoretical Chemistry under the leadership of Professor A. D. Buckingham. He remained in Bristol for the rest of his life being promoted in due course to Reader in Theoretical Chemistry.

J. Gerratt died on 16th October, 1997, aged 59. He is survived by his wife Zaga, three daughters, and a son.

References

- Gerratt, J.; Mills, I. M. *J Chem Phys* 1968, 49, 1719.
- Gerratt, J.; Mills, I. M. *J Chem Phys* 1968, 49, 1730.
- Schaefer III, H. F. *Quantum Chemistry. The Development of ab initio Methods in Molecular Electronic Structure Theory*; Clarendon: Oxford, 1984.
- Hartree, D. R. *Numerical Analysis*; Oxford University Press: Oxford, 1958.
- Pulay, P. *Molec Phys* 1969, 17, 197.
- Pulay, P. *Adv Chem Phys* 1987, 69, 241.
- Gerratt, J. *Adv At Mol Phys* 1971, 7, 141.
- Heitler, W. *Marx Handb Radiologie* 1934, II, 485.
- van Vleck, J. H.; Sherman, A. *Rev Mod Phys* 1935, 7, 167.
- Racah, G. *Phys Rev* 1942, 61, 186; 1942, 62, 438; 1943, 63, 367; 1949, 76, 1352.
- Wigner, E. P. *Group Theory and its Application to the Quantum Mechanics of Atomic Spectra*; Academic: New York, 1959.
- (a) Kotani, M.; Siga, M. *Proc Phys Math Soc Jpn* 1937, 19, 471. (b) Kotani, M.; Amemiya, A.; Ishiguro, E.; Kimura, T. *Table of Molecular Integrals*, 2nd ed.; Maruzen: Tokyo, 1963.
- Serber, R. *Phys Rev* 1934, 45, 461; *J Chem Phys* 1935, 2, 697.
- Jahn, H. A. *Proc Roy Soc* 1950, A201, 516; *Proc Roy Soc* 1951, A205, 192; *Phys Rev* 1954, 96, 989.
- Löwdin, P.-O. *Phys Rev* 1955, 97, 1509.
- Kaplan, I. G. *Liet Fiz Rinkiny* 1963, III, 227; *Teor Eksp Khim* 1965, 1, 608, 619; 1965, 2, 441; 1967, 3, 150, 287; *Zh Eksp Teor Fiz* 1966, 51, 169.
- Cooper, D. L.; Gerratt, J.; Raimondi, M. *Adv Chem Phys* 1987, 69, 319.
- Gerratt, J.; Cooper, D. L.; Raimondi, M. In *Valence Bond Theory and Chemical Structure*, Klein, D. J.; Trinajstić, N., Eds.; Elsevier: Amsterdam, 1990, p. 287.
- Cooper, D. L.; Gerratt, J.; Raimondi, M. *Chem Rev* 1991, 91, 929.
- Gerratt, J.; Cooper, D. L.; Karadakov, P. B.; Raimondi, M. *Chem Soc Rev* 1997, 26, 87.
- Gerratt, J.; Lipscomb, W. N. *Proc Natl Acad Sci (USA)* 1968, 59, 332.
- Gerratt, J.; Lipscomb, W. N. *Int J Quant Chem* 1999, 74, 83.
- Goddard III, W. A. *Phys Rev* 1967, 157, 73.
- Goddard III, W. A. *Phys Rev* 1967, 157, 81.
- Goddard III, W. A. *J Chem Phys* 1968, 48, 450.
- Goddard III, W. A. *J Chem Phys* 1968, 48, 5337.
- Wilson, S.; Gerratt, J. *Proc SRC Atlas Symposium: Quantum Chemistry: The State of the Art*, Saunders, V. R.; Brown, J., Ed.; Atlas Computer Laboratory, Science Research Council, Chilton, Oxfordshire, 1974, p. 109.
- Wilson, S. Ph.D. Thesis, University of Bristol, 1975.
- Wilson, S.; Gerratt, J. *Molec Phys* 30, 765.
- Bobrowicz, F.; Goddard III, W. A. In *Methods of Electronic Structure Theory*, Schaefer III, H. F., Ed.; Plenum: New York, 1977, p. 79.
- Gerratt, J.; Raimondi, M. *Proc Roy Soc* 1980, A371, 525.
- Pyper, N. C.; Gerratt, J. *Proc SRC Atlas Symposium: Quantum Chemistry: The State of the Art*, Saunders, V. R.; Brown, J., Eds.; Atlas Computer Laboratory, Science Research Council, Chilton, Oxfordshire, 1974, p. 93.
- Pyper, N. C.; Gerratt, J. *Proc Roy Soc* 1977, A355, 407.
- Kaplan, I. G. *Symmetry of Many-Electron Systems*, Academic: London, 1975.
- Kaplan, I. G. *Simmetrii mnogoélektronnykh sistem*, Izdatel'stvo "Nauka": Moscow, 1969.
- Cooper, D. L.; Gerratt, J.; Raimondi, M. *Nature* 1986, 323, 699.
- Gerratt, J. *Chem Britain* 1987, 23, 327.
- Raos, G.; Gerratt, J.; Karadakov, P. B.; Cooper, D. L.; Raimondi, M. *J Chem Soc Faraday Trans* 1995, 91, 4011.
- Raos, G.; Astorri, L.; Raimondi, M.; Cooper, D. L.; Gerratt, J.; Karadakov, P. B. *J Phys Chem A* 1997, 101, 2886.
- Wright, S. C.; Cooper, D. L.; Gerratt, J.; Raimondi, M. *J Phys Chem* 1992, 96, 7943.
- Raos, G.; McNicholas, S. J.; Gerratt, J.; Cooper, D. L.; Karadakov, P. B. *J Phys Chem B* 1997, 101, 6688.
- Sironi, M.; Cooper, D. L.; Gerratt, J.; Raimondi, M. *J Am Chem Soc* 1990, 112, 5054.
- Sironi, M.; Raimondi, M.; Cooper, D. L.; Gerratt, J. *J Chem Soc Faraday Trans 2* 1987, 83, 1651.
- Karadakov, P. B.; Gerratt, J.; Cooper, D. L.; Raimondi, M. *J Chem Soc Faraday Trans* 1994, 90, 1643.
- Cooper, D. L.; Cunningham, T. P.; Gerratt, J.; Karadakov, P. B.; Raimondi, M. *J Am Chem Soc* 1994, 116, 4114.
- Gerratt, J.; McNicholas, S. J.; Karadakov, P. B.; Sironi, M.; Raimondi, M.; Cooper, D. L. *J Am Chem Soc* 1996, 118, 6472.
- Barnett, M. P.; Coulson, C. A. *Phil Trans Roy Soc Lond* 1951, A243, 221.
- Smith, S. J.; Sutcliffe, B. T. *Rev Comput Chem* 1997, 10, 271.
- Karadakov, P. B.; Gerratt, J.; Cooper, D. L.; Raimondi, M. *J Chem Phys* 1992, 97, 7635.
- Cooper, D. L.; Gerratt, J.; Raimondi, M.; Sironi, M.; Thorsteinsson, T. *Theor Chim Acta* 1993, 85, 261.
- Sironi, M.; Raimondi, M.; Cooper, D. L.; Gerratt, J. *J Mol Struct (THEOCHEM)* 1995, 338, 257.
- McNicholas, S. J. Ph.D. Thesis, University of Bristol, 1997.
- Thorsteinsson, T.; Cooper, D. L. *Theor Chim Acta* 1996, 94, 233.
- Cooper, D. L.; Thorsteinsson, T.; Gerratt, J. *Adv Quant Chem* 1998, 32, 51.

S. Wilson
M. Raimondi
D. L. Cooper