Supporting Information:
A Fully Referenced Version of the Tribute Article:

Richard F. W. Bader: A True Pioneer

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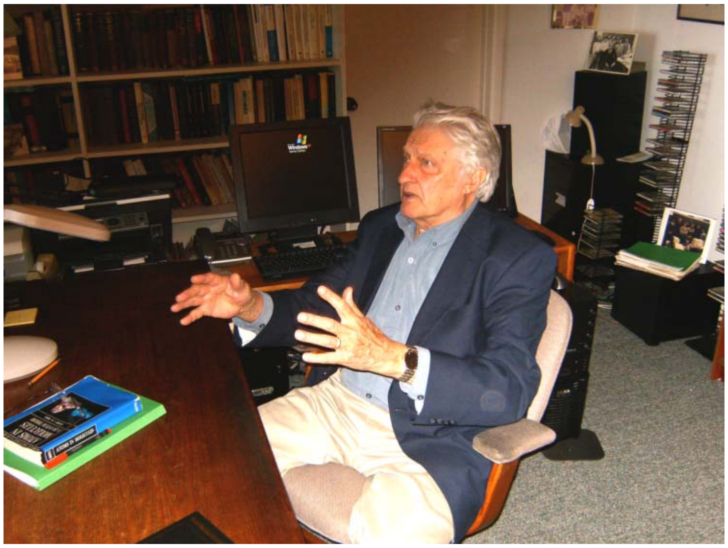

Professor Richard F. W. Bader in his home-study (Burlington, June 2009).

It is an honour to be able pay tribute here to the remarkable career of Professor Richard F. W. Bader. Two of us (C.F.M. and T.A.K.) had the privilege to be among Richard's many former graduate students and one of us (L.M.) has been a close friend to Richard and an admirer of his work since he first met him in 1974 during a crystallography symposium in Melbourne, Australia.

It is neither common nor easy to do something that is fundamentally new in science. This can be due both to inherent difficulties of the subject as well to biases that most of us have in favour of the familiar and against the unfamiliar. Richard Bader has been doing fundamentally new things for much of his career (See **Table 1**). At times this has been met with considerable resistance. Fortunately, Richard has never wavered in his pursuit of new and useful ideas and, equally important, their publication. His hard work and persistence have led to explanations and quantification tools for many of the central concepts of chemistry and to the opening of an entire field of research – the topological analysis of electron density distributions - that has crossed the boundaries of theoretical chemistry[1-8] to the laboratory bench of X-ray crystallography.[9-14]

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Table 1 Milestones in Richard F. W. Bader's Scientific Career.[a]

Contribution	Years[b]	Principal References
• Experimental and theoretic studies of solvent isotope effects. Librational model of water solvent isotope effects.	1954-1961	15-21
• Discovery of the first symmetry rules for predicting signs of vibrational interaction force constants and courses of chemical reactions.	1962	22
• Detailed analyses of molecular charge density distributions.	1963-1969	23-32
• Detailed analyses of Feynman forces on nuclei and studies of Berlin binding and anti-binding regions.	1968	29
• Detailed analyses of kinetic energy densities.	1969,1978	32,33
• First theoretical discovery of a Teller conical intersection.	1971	34
• Discovery of relationship between regional transferability of charge densities and kinetic energy densities.	1972	35
• Discovery of natural partitioning of molecules into mono-nuclear regions bounded by surfaces having zero flux of the gradient of the electron density.	1971-1975	35-38
• The postulation of the existence of an atomic virial theorem. That is, the realization that fragments bounded by zero-flux surfaces have unique kinetic energy and for which a virial relationships $-2T(\Omega) = V(\Omega)$ and $E(\Omega) = -T(\Omega)$ appear to apply.	1971-1974	35-37
• Variational derivation of the significance of the zero-flux boundary condition and atomic hypervirial theorem.	1975,1978	38,39
• Proof of the atomic virial theorem and Ehrenfest theorem.	1975,1978	38,39
• Generalization of Schwinger's principle of stationary action to open systems (atoms in molecules).	1978, 1994	39,40
• Discovery of the bond path.	1977, 1998	41-43
• Topological analyses of molecular charge distributions, topological theory of molecular structure and its change.	1977-1982	7,41,44-48
• Localization and delocalization of electrons in molecules through analyses of pair density distributions and Fermi Hole distributions.	1975, 1989, 1996, 1999	49-56
• Development of AIMPAC, a freely distributed computer program package for QTAIM analyses.	1981–	63
• Laplacian of the electron density. Atomic shell structure, regions of charge concentration and depletion, and appearance in a local virial relationship. Characterization of bonding. Prediction of reactive sites.	1984-1989	57-62
• Recovery of group additivity schemes via atomic and group contributions to molecular energies, volumes, dipole moments, vibrational absorption intensities, polarizabilities, magnetizabilities, *etc.*	1993-2002	5,57,64-90
• Discovery of importance of atomic polarization, in addition to atomic charges or charge transfer, in interpreting molecular dipole moments and dipole moment changes.	1992	68,81,83, 173,174
• Development of the IGAIM and CSGT methods. Analysis of magnetically induced current densities and atomic contributions to molecular magnetic response properties.	1992-1996	69,70,91-93

Contribution	Years(b)	Principal References
• Discovery of structural homeomorphism between the electron density and the virial field.	1996	94
• Discovery of non-nuclear attractors.	1987	95-97
• Discovery of the source function.	1998	98-105
• Development of the localization and delocalization indices.	1999	53
• Elucidation of the atomic origins of rotational and inversion barriers.	1990	84,106,107
• First analysis of topology of crystalline charge density distributions.	1994, 1995	108-111
• Discovery of the stabilizing nature of closed-shell hydrogen-hydrogen (H–H) bonding interactions in molecules and crystals.	2003	84

(a) The ordering of this list is not strictly chronological, but rather mainly logical and topical.
(b) The listed years or range of years are only indicative of the period where the groundwork related to the listed contribution has been published. In several instances, the work has been further developed at later dates and in some cases is still being actively developed at the time of writing.

Founded on solid bases of quantum mechanics and observation, his seminal work, the *Quantum Theory of Atoms in Molecules* (QTAIM), is applied today by thousands of chemists, physicists, material scientists, molecular biologists, crystallographers and others all over the world and has found applications from the physics of crystals (see for example Refs. 11,109,110,112) to chemical biology and in the formulation of new strategies to design drugs (See for example Refs. 87-89,113-125, and the literature cited therein). QTAIM has inspired the topological analysis of functions other than the electron density, a widely used example being the electron localization function (ELF).[126-131]

Richard Bader is a true pioneer, being among the first to seriously ask and answer a number of fundamental questions about the physical basis for such powerful chemical concepts as atoms in molecules, functional groups, bonding, electron pairs and electron localization and delocalization, concepts that chemists and other scientists use every day. In 1963, a year before the historical discovery of the foundations of modern density functional theory (DFT),[132-134] R. F. W. Bader and G. A. Jones wrote:[24]

> *"The manner in which the electron density is disposed in a molecule has not received the attention its importance would seem to merit. Unlike the energy of a molecular system which requires a knowledge of the second-order density matrix for its evaluation[a] many of the observable properties of a molecule are determined in whole or in part by the simple three-dimensional electron-density distribution. In fact, these properties provide a direct measure of a wide spectrum of different moments averaged directly over the density distribution. Thus the diamagnetic susceptibility, the dipole moment, the diamagnetic contribution to the nuclear screening constant, the electric field, and the electric field gradient (as obtained from nuclear quadrupole coupling constants) provide a measure of (aside from any angular dependencies)* $\langle r_i^2 \rangle$, $\langle r_i \rangle$, $\langle r_i^{-1} \rangle$, $\langle r_i^{-2} \rangle$, *and* $\langle r_i^{-3} \rangle$, *respectively. The electric field at a nucleus due to the electron density distribution is of particular interest due to the theorem derived by Hellmann[b] and Feynman.[c] They have demonstrated that the force acting on a nucleus in a molecule is determined by the electric field at that nucleus due to the other nuclei and to the electron-density distribution."*
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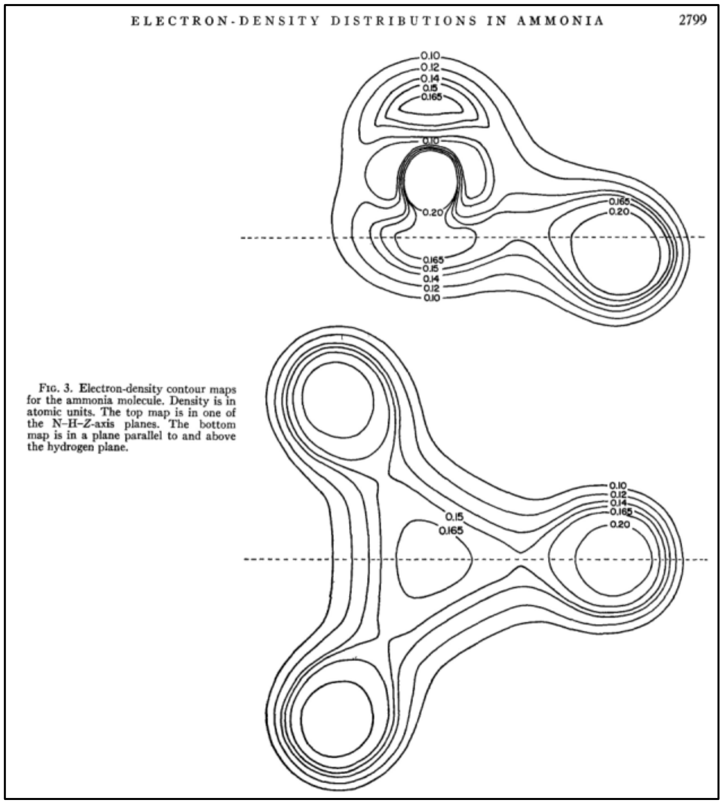
> [a] P.-O.Löwdin, *Adv. Chem. Phys.* **2**, 207 (1959); [b] J. Hellman, *Einführung in die Quantenchemie* (Detiche and Company,

Leipzig, Germany, 1937); [c] R. P. Feynman, *Phys. Rev.* **56**, 340 (1939).

This statement comes at a time when few were interested in the total electron density and its topography and topology as a vehicle for understanding and predicting chemistry. The first contour plots of electron densities in molecules, now common place, were published by the Bader group already in the early sixties (**Fig. 1**) along with deep discussions on their significance as carriers of key physical information about structure, bonding, and reactivity.[23-32]



ELECTRON-DENSITY DISTRIBUTIONS IN AMMONIA 2799

FIG. 3. Electron-density contour maps for the ammonia molecule. Density is in atomic units. The top map is in one of the N–H–Z-axis planes. The bottom map is in a plane parallel to and above the hydrogen plane.

Fig. 1 An example of Bader's early total electron density distribution maps (of the NH3 molecule) published in the *Journal of Chemical Physics'* issue of 15 June 1963. Nowadays, 48 years later, plots of the density and of its associated gradient vector field and Laplacian fill journals of computational and theoretical chemistry and crystallography alike. (Reproduced with permission from Ref. [24]. Copyright 1963, *American Institute of Physics)*.

Early studies of the electron density as well as kinetic energy densities by Bader and co-workers in the 60s and early 70s were enabled through a collaboration with Clemens C. J. Roothaan and his then former PhD advisor and Nobel Laureate Robert S. Mulliken, both at the University of Chicago. Careful examination of the density maps ultimately led Richard and his coworkers to the realization that a regional similarity (transferability) of the electron densities between different molecules is associated with a corresponding transferability of kinetic energy densities.

Bader and Bedall discovered in 1972 that the real space of a molecule is naturally partitioned into mononuclear atomic regions, each bounded by surfaces having the property of zero-flux in the gradient of the electron density. This partitioning appeared to result in a maximal and paralleling transferability of the electron and kinetic energy densities for each atom in a molecule. Since their can be multiple definitions of kinetic energy density, it is equally important that this unique partitioning yields the same atomic kinetic energy regardless of the kinetic energy density definition. On the basis of these observations, together with the implied transferability of atomic energies associated with experimental additivity schemes for heats of formation, Bader and Bedall postulated that the molecular virial relationship $2T + V = 0$ (for stationary point molecular geometries) between electronic kinetic energy T and potential energy V may also apply to individual atoms in a molecule, $2T(\Omega) + V(\Omega) = 0$, and thus the energy $E(\Omega)$ of an atom Ω in a molecule could be defined as $E(\Omega) = -T(\Omega)$ in analogy with the molecular result $E = -T$ that follows from the molecular virial theorem and $E = T + V$.[35]

Bader and coworkers later proved the postulated atomic virial relationship between the atomic kinetic energy and the atomic virial of the Ehrenfest force density acting on an atom and its surface, the total atomic potential energy.[1,36,38,39] The *virial theorem for an atom in a molecule* provided the basis for defining what had previously been thought unattainable, that is, a local, unique, straightforward and relatively easily calculable energy of an atom in a molecule. Atomic energies so defined are transferable in a manner paralleling the atomic electron density distribution and, for stationary point geometries (and provided the molecular virial theorem is satisfied) are additive to give the total molecular energy when the sum runs over all the atoms or the energy of a group of atoms within the molecules if that sum runs over the atoms forming that group. This partitioning has allowed researchers a new perspective on understanding the energies of molecules, and the changes of these energies in different conformers or at different local minima or saddle points on the accessible potential energy surface. Such discussions of energy at an atomic resolution were previously thought to be impossible - but Richard sought the solution outside the traditional box taking the starting point the *observable* electron density.

The virial theorem has been generalized in a second way by Bader *et al.* into a *local* version.[1,46] The *local virial theorem* relates a potential energy density and the gradient form of the kinetic energy density,[33,135,136] to the Laplacian of the electron density.[1,46] The Laplacian of the electron density plays a central role in QTAIM and its topology faithfully recovers the atomic shell structure of isolated atoms as well as the Lewis and VSEPR models of bonded and nonbonded electron pairs of atoms in molecules and is useful for characterizing bonded interactions in molecules and for predicting reactive sites in molecules.[58,61] Maps of the Laplacian of the electron density obtained from X-ray diffraction experiments followed by multipolar refinement fill the crystallographic literature since these maps and their topography are now recognized to provide deep insight into the nature of chemical bonding.[9,12-14,137] A noted example for such insight is the development of a complete real-space theory of the solid state by the group at *Universidad de Oviedo* (Spain) on the bases provided by QTAIM and its analysis of the electron density.[96,138-144]

The atomic virial theorem was shown to be but one of many atomic theorems that follow from the atomic hypervirial theorem that was derived variationally by Bader and coworkers from Schrodinger's energy functional generalized to subspaces bounded by surfaces having zero-flux of the gradient of the electron density. The variational derivation of the atomic hypervirial theorem, followed shortly thereafter by the generalization of Schwinger's principle of stationary action to an atom in a molecule, marked the birth of QTAIM.[1,39,40]

Simultaneously with solidification of the quantum mechanical underpinnings of QTAIM, the topological properties of the electron density were thoroughly explored by Richard and coworkers[41,44,45,47] and this work quickly blossomed into an entire coherent and consistent theory of molecular structure and structural stability used by theorists and experimentalists alike. The most important organizing principle in chemistry, that a molecule is a collection of atoms in real space with characteristic properties and linked together by bonds, and that a chemical reaction involves a rearrangement of atoms and making and breaking of bonds, was given full, quantifiable backing by QTAIM. Long before electron density functional theory became popular, or even generally known, among quantum chemists, Richard and his group had embarked on a program of thoroughly investigating electron density distributions in molecules. By the time density functional theory became mainstream, Richard and his group had developed an extensive and useable theory of the fundamental concepts of chemistry in terms of the electron density.

Another important development came from detailed analyses of electron pair density distributions by Bader and co-workers:[49] the realization that the localization of an electron in a region within a molecule is determined by the corresponding localization of its associated Fermi hole.[49,50,52,53] As a corollary, the delocalization of the Fermi hole reflects the delocalization of the electron in the molecule.[51,145] This finding, combined with QTAIM, ultimately led to a precise determinations of the extent to which the electron population of an atom in a molecule is localized in the atom, the localization index, and the extent to which the electron population of an atom is shared with other atoms in a molecule, the delocalization indices.[53] Interestingly and significantly, Bader and Heard discovered that the Laplacian of the electron density faithfully reproduces the spatial characteristics of electron localization and delocalization as revealed by the topology of the Laplacian of the conditional pair density.[54]

It seems that whatever field Richard was involved in, however briefly, new ideas emerged. Another example is magnetic response properties. In their endeavour to understand molecular magnetic response properties of closed-shell molecules in terms of atomic contributions, Richard and a graduate student were led to calculate and analyze magnetically induced current density distributions. Using conventional single-gauge methods available to them at the time proved inadequate due to the practical problem of gauge-origin dependence, but the use of QTAIM saved the day because it encouraged the calculation of the current density distribution an atom at a time, with the nucleus of each atom serving as the gauge origin for the current density distribution within the atom. This Individual Gauges for Atoms In Molecules (IGAIM) approach proved to be quite reliable in eliminating the gauge problem and predicting relatively accurate molecular magnetic response properties. The IGAIM method was soon generalized to the Continuous Set of Gauge Transformations (CSGT) method, a novel and practical method whereby a different gauge origin is used for each point in space to calculate molecular current density distributions and the molecular magnetic response properties they determine.[91] The IGAIM and CSGT methods enabled the thorough and correct topological analyses of magnetically induced current densities for the first time and the investigation of molecular magnetic response properties in terms of atomic and bonding contributions.

Besides pure and applied theoretical chemistry, perhaps no field has been impacted more by the work of Richard and co-workers than X–ray crystallography. The foundations of QTAIM emanate from the electron density which is the very object of experimental X–ray analysis. In the early days of electron density measurements by crystallographers, interpretation of results was hampered by an over-dependence on “difference density” methods, which however useful heuristically, suffered from ambiguous reference atomic densities and had little connection with quantum mechanical theorems. It is a fortunate circumstance that major advances in the ability to measure high resolution crystalline electron densities in the past few decades have coincided with the parallel development of the theoretical tools necessary to analyze and interpret them, *viz.*, QTAIM. It is fitting that Richard and one of his graduate students at the time, P. F. Zou, were among the first to discuss and perform full QTAIM analyses of crystalline electron densities.[108,111,146]

It is no exaggeration to point out that QTAIM analysis has revolutionized the understanding of accurate coherent X–ray electron density measurements, by bringing them into strong correspondence with the quantum mechanical theorems that underlie and make understandable molecular structure. The experimentally measured electron density zero-flux surfaces partition a crystal into atoms and functional groups with transferability properties that track experimental behaviour and has led to the development of several transferable multipolar databases (see for example Refs. 147-165).

The electron density critical points allow quantitative analysis of bonding properties in crystals. It is of utmost significance to crystallographers to find that ridges of maximal electron density between nuclei, bond paths, unfailingly characterize attractive interactions, of every kind, weak and strong. To be emphasized is that all these topological properties of the electron density are available from analysis of the measurements obtained from X-ray diffraction experiments. Indeed the fact that the analysis is exactly the same for densities whether experimental or theoretical is of importance. It is just such direct comparison of experimental and theoretical objects which makes understanding most complete and prediction possible.[108,111]

In the earlier years of his career, Richard was an experimental physical organic chemist, before he switched to theory in the sixties. Even though Richard has spent most of his career as a theorist, his skill at the wet laboratory bench and outside the realm of quantum chemistry was equally exceptional. Together with his PhD advisor C.G. Swain, he published a series of important papers on solvent isotope effects.[16-21]

Perhaps one of the most significant early contributions of Richard was the use of molecular vibration theory, perturbation theory and molecular orbital theory to formulate the first symmetry rules to predict the signs of vibrational interaction force constants as well as possible pathways of chemical reactions.[22] In this work, Richard cleverly showed that the lowest-lying excited state of a molecule or transition state that gives a non-zero transition density determines, by symmetry, the normal vibrational mode(s) that can lead to decomposition of a molecule or a transition state, thus allowing predictions of the course of some chemical reactions. A reading of these papers illustrates Richard's detailed knowledge and appreciation of molecular orbital theory in classifying electronic states of molecules. The significance of Richard's work did not escape the notice of Kenichi Fukui, who stated in his 1981 Nobel Lecture:[166]

> "*In this way, it turned out in the course of time that the electron delocalization between HOMO and LUMO generally became the principal factor determining he easiness of a chemical reaction and the stereoselective path, irrespective of intra- and intermolecular processes, as illustrated in Fig. 3. Besides our own school, a number of other chemists made contributions. I want to refer to several names which are worthy of special mention.*
>
> *First of all, the general perturbation theory of the HOMO-LUMO interaction between two molecules was built up by Salem.[23-25] One of Salem's papers[25] was in line with the important theory of Bader,[26] which specified the mode of decomposition of a molecule or a transition complex by means of the symmetry of the normal vibration. Furthermore Pearson[27] investigated the relation between the symmetry of reaction coordinates in general and that of HOMO and LUMO.*" (References in this passage as in Fukui's Nobel Lecture, where Fukui's Ref. 26 is the present's article Ref. 22).

It is particularly fitting to see a festschrift in this *Journal* where Richard has published 60 out of his 220 papers. Richard's papers are often listed among the "Most Read" on the *Journal*'s web page. At the time of this writing, for example, his paper "*Definition of Molecular Structure: By Choice or by Appeal to Observation?*"[167] is listed among the *Journal*'s "Most Read" in the past 12 months, while his paper in the present festchrift in his honor "*Worlds Apart in Chemistry: A Personal Tribute to J. C. Slater*"[168] is the most read paper in the past month (June-August 2011). His papers are also often very highly cited (**Table 2**). For example, his paper "*Bond Paths Are Not Chemical Bonds*"[43] is listed among the *Journal*'s "Most Cited Papers" in the last three years. And two of his classic papers are listed among the "All Time Top 20 Most Cited Articles published by the *Journal*", his paper entitled "*A Bond Path: A Universal Indicator of Bonded Interactions*"[42] (482 citations) and the one he co-authored with his co-workers, now Professors Xavier Fradera and Maggie A. Austen, entitled "*The Lewis Model and Beyond*"[53] (348 citations). A third paper, also in the "*All Time Top 20 Most Cited*" is one on the "*Characterization of a Dihydrogen Bond on the Basis of the Electron Density*"[169] by Professor Paul L. A. Popelier (428 citations)[1] is also based on QTAIM.

In closing, it is an impossible task to do justice to a scientist of the standing of Richard F. W. Bader in a short tribute such as this. We wish him and his family, affectionately, a happy 80th birthday and thank him for his friendship and invaluable and lasting contributions to chemistry and physics.

Table 2 Bibliographic data of Professor Richard F. W. Bader as of 24 August 2011 according to ISI Web of Knowledge.(a)

Item	Count
Results found (number of papers published)	215
Sum of the times cited (without the book[1])	18,942
Sum of times cited without self-citations (and without the book[1])	16,973
Sum of times cited of the book[1](a)	5,906
Total citations (articles and the book[1])(b)	22,879
Citing articles	8,882
Average citations per item	88.10
h-index(c)	70

(a) The standard automated citation count of the ISI does not include books or book chapters, only citations to papers are counted and summed.

(b) This count was obtained by summing all citation variants of Ref. 1. Citation variants are the different manners of citing the same reference. Variants are summed separately by the ISI automated counting engine.

(c) This index is the number of papers that are cited at least *that* number of times. So in this case, 70 papers are cited 70 times or more. Richard's five most cited papers are cited 1160,[6] 1116,[63] 632,[170] 622,[171] and 501[92] times respectively to date.

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[1] Another paper using QTAIM to characterize hydrogen bonds (by Koch and Popelier) in this *Journal* entitled "*Characterization of C-H-O Hydrogen-Bonds on the Basis of the Charge-Density*",[172] has received 776 citations, according to the ISI at the time of writing.

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