Total Bond Energies of Exact Classical Solutions of Molecules Generated by Millsian 1.0 Compared to Those Computed Using Modern 3-21G and 6-31G* Basis Sets

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ABSTRACT

Mills [1-12] solved the structure of the bound electron using classical laws and subsequently developed a unification theory based on those laws called the Grand Unified Theory of Classical Physics (GUTCP) with results that match observations for the basic phenomena of physics and chemistry from the scale of the quarks to cosmos. Millsian 1.0 is a program comprising molecular modeling applications of GUTCP, solving atomic and molecular structures based on applying the classical laws of physics, (Newton's and Maxwell's Laws) to the atomic scale. The functional groups of all major classes of chemical bonding including those involved in most organic molecules have been solved exactly in closed-form solutions. By using these functional groups as building blocks, or independent units, a potentially infinite number of molecules can be solved. As a result, Millsian software can visualize the exact three-dimensional structure and calculate physical characteristics of almost any molecule of any length and complexity. Even complex proteins and DNA (the molecules that encode genetic information) can be solved in real-time interactively on a personal computer. By contrast, previous software based on traditional quantum methods must resort to approximations and run on powerful computers for even the simplest systems. The energies of exact classical solutions of molecules generated by Millsian 1.0 and those from a modern quantum mechanics-based program, Spartan's pre-computed database using 3-21G and 6-31G* basis sets at the Hartree-Fock level of theory, were compared to experimental values. The Millsian results were consistently within an average relative deviation of about 0.1% of the experimentally values. In contrast, the 3-21G and 6-31G* results deviated over a wide range of relative error, typically being >30-150% with a large percentage of catastrophic failures, depending on functional group type and basis set.

I. INTRODUCTION

In this paper, the old view that the electron is a zero or one-dimensional point in an all-space probability wave function $\Psi(x)$ is not taken for granted. Rather, atomic and molecular physics theory, derived from first principles, must successfully and consistently apply physical laws on all scales [1-12]. Stability to radiation was ignored by all past atomic models, but in this case, it is the basis of the solutions wherein the structure of the electron is first solved and the result determines the nature of the atomic and molecular electrons involved in chemical bonds.

Historically, the point at which quantum mechanics broke with classical laws can be traced to the issue of nonradiation of the one electron atom. Bohr just postulated orbits stable to radiation with the further postulate that the bound electron of the hydrogen atom does not obey Maxwell's equations—rather it obeys different physics [1-12]. Later physics was replaced by "pure mathematics" based on the notion of the inexplicable wave-particle duality nature of electrons which lead to the Schrödinger equation wherein the consequences of radiation predicted by Maxwell's equations were ignored. Ironically, Bohr, Schrödinger, and Dirac used the Coulomb potential, and Dirac used the vector potential of Maxwell's equations. But, all ignored electrodynamics and the corresponding radiative consequences. Dirac originally attempted to solve the bound electron physically with stability with respect to radiation according to Maxwell's equations with the further constraints that it was relativistically invariant and gave rise to electron spin [13]. He and many founders of QM such as Sommerfeld, Bohm, and Weinstein wrongly pursued a planetary model, were unsuccessful, and resorted to the current mathematical-probability-wave model that has many problems [1-17]. Consequently, Feynman for example, attempted to use first principles including Maxwell's equations to discover new physics to replace quantum mechanics [18].

Starting with the same essential physics as Bohr, Schrödinger, and Dirac of e^- moving in the Coulombic field of the proton and an electromagnetic wave equation and matching electron source current rather than an energy diffusion equation originally sought by Schrödinger, advancements in the understanding of the stability of the bound electron to radiation are applied to solve for the exact nature of the electron. Rather than using the postulated Schrödinger boundary condition: "$\Psi \to 0$ as $r \to \infty$", which leads to a purely mathematical model of the electron, the constraint is based on experimental observation. *Using Maxwell's equations, the structure of the electron is derived as a boundary-value problem wherein the electron comprises the source current of time-varying electromagnetic fields during transitions with the constraint that the bound $n = 1$ state electron cannot radiate energy.* Although it is well known that an accelerated *point* particle radiates, an *extended distribution* modeled as a superposition of accelerating charges does not have to radiate. The physical boundary condition of nonradiation

of that was imposed on the bound electron follows from a derivation by Haus [19]. The function that describes the motion of the electron must not possess spacetime Fourier components that are synchronous with waves traveling at the speed of light. Similarly, nonradiation is demonstrated based on the electron's electromagnetic fields and the Poynting power vector. A simple invariant physical model arises naturally wherein the results are extremely straightforward, internally consistent, and predictive of conjugate parameters for the first time, requiring minimal math as in the case of the most famous exact equations (no uncertainty) of Newton and Maxwell on which the model is based. No new physics is needed; only the known physical laws based on direct observation are used.

The structure of the bound atomic electron was solved by first considering one-electron atoms [1-12]. Since the hydrogen atom is stable and nonradiative, the electron has constant energy. Furthermore, it is time dynamic with a corresponding current that serves as a source of electromagnetic radiation during transitions. The wave equation solutions of the radiation fields permit the source currents to be determined as a boundary-value problem. These source currents match the field solutions of the wave equation for two dimensions plus time and the nonradiative $n = 1$ state when the nonradiation condition is applied. Then, the mechanics of the electron can be solved from the two-dimensional wave equation plus time in the form of an energy equation wherein it provides for conservation of energy and angular momentum as given in the Electron Mechanics and the Corresponding Classical Wave Equation for the Derivation of the Rotational Parameters of the Electron section of Ref. [1]. Once the nature of the electron is solved, all problems involving electrons can be solved in principle. Thus, in the case of one-electron atoms, the electron radius, binding energy, and other parameters are solved after solving for the nature of the bound electron.

For time-varying spherical electromagnetic fields, Jackson [20] gives a generalized expansion in vector spherical waves that are convenient for electromagnetic boundary-value problems possessing spherical symmetry properties and for analyzing multipole radiation from a localized source distribution. The Green function $G(\mathbf{x'}, \mathbf{x})$ which is appropriate to the equation

$$\left(\nabla^2 + k^2 \right) G\left(\mathbf{x'}, \mathbf{x}\right) = -\delta\left(\mathbf{x'} - \mathbf{x}\right) \tag{1}$$

in the infinite domain with the spherical wave expansion for the outgoing wave Green function is

$$G\left(\mathbf{x'}, \mathbf{x}\right) = \frac{e^{-ik|\mathbf{x}-\mathbf{x'}|}}{4\pi |\mathbf{x}-\mathbf{x'}|} = ik \sum_{\ell=0}^{\infty} j_\ell\left(kr_<\right) h_\ell^{(1)}\left(kr_>\right) \sum_{m=-\ell}^{\ell} Y_{\ell,m}^*\left(\theta', \phi'\right) Y_{\ell,m}\left(\theta, \phi\right) \tag{2}$$

Jackson [20] further gives the general multipole field solution to Maxwell's equations in a source-free region of empty space with the assumption of a time dependence $e^{i\omega_n t}$:

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$$\mathbf{B} = \sum_{\ell,m} \left[a_E(\ell,m) f_\ell(kr) \mathbf{X}_{\ell.m} - \frac{i}{k} a_M(\ell,m) \nabla \times g_\ell(kr) \mathbf{X}_{\ell.m} \right]$$

$$\mathbf{E} = \sum_{\ell,m} \left[\frac{i}{k} a_E(\ell,m) \nabla \times f_\ell(kr) \mathbf{X}_{\ell.m} + a_M(\ell,m) g_\ell(kr) \mathbf{X}_{\ell.m} \right]$$

(3)

where the cgs units used by Jackson are retained in this section. The radial functions $f_\ell(kr)$ and $g_\ell(kr)$ are of the form:

$$g_\ell(kr) = A_\ell^{(1)} h_\ell^{(1)} + A_\ell^{(2)} h_\ell^{(2)}$$

(4)

$\mathbf{X}_{\ell.m}$ is the vector spherical harmonic defined by

$$\mathbf{X}_{\ell,m}(\theta,\phi) = \frac{1}{\sqrt{\ell(\ell+1)}} \mathbf{L} Y_{\ell,m}(\theta,\phi)$$

(5)

where

$$\mathbf{L} = \frac{1}{i}(\mathbf{r} \times \nabla)$$

(6)

The coefficients $a_E(\ell,m)$ and $a_M(\ell,m)$ of Eq. (3) specify the amounts of electric (ℓ,m) multipole and magnetic (ℓ,m) multipole fields, and are determined by sources and boundary conditions as are the relative proportions in Eq. (4). Jackson gives the result of the electric and magnetic coefficients from the sources as

$$a_E(\ell,m) = \frac{4\pi k^2}{i\sqrt{\ell(\ell+1)}} \int Y_\ell^{m*} \left\{ \rho \frac{\partial}{\partial r} [r j_\ell(kr)] + \frac{ik}{c}(\mathbf{r} \cdot \mathbf{J}) j_\ell(kr) - ik\nabla \cdot (r \times \boldsymbol{M}) j_\ell(kr) \right\} d^3x$$

(7)

and

$$a_M(\ell,m) = \frac{-4\pi k^2}{\sqrt{\ell(\ell+1)}} \int j_\ell(kr) Y_\ell^{m*} \mathbf{L} \cdot \left(\frac{\mathbf{J}}{c} + \nabla \times \boldsymbol{M} \right) d^3x$$

(8)

respectively, where the distribution of charge $\rho(\mathbf{x},t)$, current $\mathbf{J}(\mathbf{x},t)$, and intrinsic magnetization $\boldsymbol{M}(\mathbf{x},t)$ are harmonically varying sources: $\rho(\mathbf{x})e^{-i\omega t}$, $\mathbf{J}(\mathbf{x})e^{-i\omega t}$, and $\boldsymbol{M}(\mathbf{x})e^{-i\omega t}$.

The electron current-density function can be solved as a boundary value problem regarding the time varying corresponding source current $\mathbf{J}(\mathbf{x})e^{-i\omega t}$ that gives rise to the time-varying spherical electromagnetic fields during transitions between states with the further constraint that the electron is nonradiative in a state defined as the $n=1$ state. The potential energy, $V(\mathbf{r})$, is an inverse-radius-squared relationship given by given by Gauss' law which for a point charge or a two-dimensional spherical shell at a distance r from the nucleus the potential is

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$$

(9)

Thus, consideration of conservation of energy would require that the electron radius must be fixed. Addition constraints requiring a two-dimensional source current of fixed radius are matching the delta function of Eq. (1) with no singularity, no time dependence and consequently no radiation, absence of self-interaction (See Appendix IV of Ref. [1]), and exact electroneutrality of the hydrogen atom wherein the electric field is given by

$$\mathbf{n} \bullet \left(\mathbf{E}_1 - \mathbf{E}_2 \right) = \frac{\sigma_s}{\varepsilon_0} \tag{10}$$

where $\mathbf{n}$ is the normal unit vector, $\mathbf{E}_1$ and $\mathbf{E}_2$ are the electric field vectors that are discontinuous at the opposite surfaces, σ_s is the discontinuous two-dimensional surface charge density, and $\mathbf{E}_2 = 0$. Then, the solution for the radial electron function, which satisfies the boundary conditions is a delta function in spherical coordinates—a spherical shell [21]

$$f(r) = \frac{1}{r^2} \delta(r - r_n) \tag{11}$$

where r_n is an allowed radius. This function defines the charge density on a spherical shell of a fixed radius (See Figure 1), not yet determined, with the charge motion confined to the two-dimensional spherical surface. The integer subscript n is *determined during photon absorption* as given in the Excited States of the One-Electron Atom (Quantization) section of Ref. [1]. It is shown in this section that the force balance between the electric fields of the electron and proton plus any resonantly absorbed photons gives the result that $r_n = nr_1$ wherein n is an integer in an excited state.

Given time harmonic motion and a radial delta function, the relationship between an allowed radius and the electron wavelength is given by

$$2\pi r_n = \lambda_n \tag{12}$$

Based on conservation of the electron's angular momentum of $\hbar$, the magnitude of the velocity and the angular frequency for *every* point on the surface of the bound electron are

$$v_n = \frac{h}{m_e \lambda_n} = \frac{h}{m_e 2\pi r_n} = \frac{\hbar}{m_e r_n} \tag{13}$$

$$\omega_n = \frac{\hbar}{m_e r_n^2} \tag{14}$$

To further match the required multipole electromagnetic fields between transitions of states, the trial nonradiative source current functions are time and spherical harmonics, each having an exact radius and an exact energy. Then, each allowed electron charge-density (mass-density) function is the product of a radial delta function $(f(r) = \frac{1}{r^2} \delta(r - r_n))$, two angular functions (spherical harmonic functions $Y_\ell^m(\theta, \phi) = P_\ell^m(\cos\theta)e^{im\phi}$), and a time-harmonic function $e^{im\omega_n t}$. The spherical harmonic $Y_0^0(\theta, \phi) = 1$ is also an allowed solution that is in fact required in order

for the electron charge and mass densities to be positive definite and to give rise to the phenomena of electron spin. The real parts of the spherical harmonics vary between -1 and 1. But the mass of the electron cannot be negative; and the charge cannot be positive. Thus, to insure that the function is positive definite, the form of the angular solution must be a superposition:

$$Y_0^0(\theta,\phi) + Y_\ell^m(\theta,\phi) \tag{15}$$

The current is constant at every point on the surface for the s orbital corresponding to $Y_0^0(\theta,\phi)$. The quantum numbers of the spherical harmonic currents can be related to the observed electron orbital angular momentum states. The currents corresponding to s, p, d, f, etc. orbitals are

$\ell = 0$

$$\rho(r,\theta,\phi,t) = \frac{e}{8\pi r^2}[\delta(r-r_n)]\left[Y_0^0(\theta,\phi) + Y_\ell^m(\theta,\phi) \right] \tag{16}$$

$\ell \neq 0$

$$\rho(r,\theta,\phi,t) = \frac{e}{4\pi r^2}[\delta(r-r_n)]\left[Y_0^0(\theta,\phi) + \mathrm{Re}\left\{Y_\ell^m(\theta,\phi) e^{im\omega_n t}\right\} \right] \tag{17}$$

where $Y_\ell^m(\theta,\phi)$ are the spherical harmonic functions that spin about the z-axis with angular frequency ω_n with $Y_0^0(\theta,\phi)$ the constant function and $\mathrm{Re}\left\{Y_\ell^m(\theta,\phi) e^{im\omega_n t}\right\} = P_\ell^m(\cos\theta)\cos(m\phi + m\omega_n t)$.

The Fourier transform of the electron charge-density function is a solution of the four-dimensional wave equation in frequency space ($\mathbf{k}$, ω-space). Then the corresponding Fourier transform of the current-density function $K(s,\Theta,\Phi,\omega)$ is given by multiplying by the constant angular frequency corresponding to a potentially emitted photon.

$$K(s,\Theta,\Phi,\omega) = 4\pi\omega_n \frac{\sin(2s_n r_n)}{2s_n r_n} \otimes 2\pi \sum_{\upsilon=1}^{\infty} \frac{(-1)^{\upsilon-1}\left(\pi\sin\Theta\right)^{2(\upsilon-1)}}{(\upsilon-1)!(\upsilon-1)!} \frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\upsilon+\frac{1}{2}\right)}{\left(\pi\cos\Theta\right)^{2\upsilon+1}2^{\upsilon+1}} \frac{2\upsilon!}{(\upsilon-1)!} s^{-2\upsilon}$$

$$\otimes 2\pi \sum_{\upsilon=1}^{\infty} \frac{(-1)^{\upsilon-1}\left(\pi\sin\Phi\right)^{2(\upsilon-1)}}{(\upsilon-1)!(\upsilon-1)!} \frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\upsilon+\frac{1}{2}\right)}{\left(\pi\cos\Phi\right)^{2\upsilon+1}2^{\upsilon+1}} \frac{2\upsilon!}{(\upsilon-1)!} s^{-2\upsilon} \frac{1}{4\pi}[\delta(\omega-\omega_n)+\delta(\omega+\omega_n)] \tag{18}$$

The motion on the orbitsphere is angular; however, a radial correction exists due to special relativistic effects. When the velocity is c corresponding to a potentially emitted photon

$$\mathbf{s}_n \bullet \mathbf{v}_n = \mathbf{s}_n \bullet \mathbf{c} = \omega_n \tag{19}$$

the relativistically corrected wavelength is (Eq. (1.247) of Ref. [1])

$$r_n = \lambda_n \tag{20}$$

Substitution of Eq. (20) into the sinc function results in the vanishing of the entire Fourier

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transform of the current-density function. Thus, spacetime harmonics of $\dfrac{\omega_n}{c} = k$ or $\dfrac{\omega_n}{c}\sqrt{\dfrac{\varepsilon}{\varepsilon_o}} = k$

for which the Fourier transform of the current-density function is nonzero do not exist. Radiation due to charge motion does not occur in any medium when this boundary condition is met. There is acceleration without radiation. (Also see Abbott and Griffiths and Goedecke [22-23]). Nonradiation is also shown directly using Maxwell's equations directly in Appendix I of Ref. [1]. However, in the case that such a state arises as an excited state by photon absorption, it is radiative due to a radial dipole term in its current-density function since it possesses spacetime Fourier transform components synchronous with waves traveling at the speed of light as shown in the Instability of Excited States section of Ref. [1]. The *radiation emitted or absorbed during electron transitions is the multipole radiation given by Eq. (2)* as given in the Excited States of the One-Electron Atom (Quantization) section and the Equation of the Photon section of Ref. [1] wherein Eqs. (4.18-4.23) give a macro-spherical wave in the far-field.

In Chapter 1 of Ref. [1], the uniform current density function $Y_0^0(\theta,\phi)$ (Eqs. (16-17)) that gives rise to the spin of the electron is generated from two current-vector fields (CVFs). Each CVF comprises a continuum of correlated *orthogonal great circle current-density elements (one dimensional "current loops")*. The current pattern comprising each CVF is generated over a half-sphere surface by a set of rotations of two orthogonal great circle current loops that serve as basis elements about each of the $\left(-\mathbf{i_x},\mathbf{i_y},0\mathbf{i_z}\right)$ and $\left(-\dfrac{1}{\sqrt{2}}\mathbf{i_x},\dfrac{1}{\sqrt{2}}\mathbf{i_y},\mathbf{i_z}\right)$-axis; the span being π radians. Then, the two CVFs are convoluted, and the result is normalized to exactly generate the *continuous* uniform electron current density function $Y_0^0(\theta,\phi)$ covering a spherical shell and having the three angular momentum components of $\mathbf{L}_{xy} = +/-\dfrac{\hbar}{4}$ ($+/-$ designates both the positive and negative vector directions along an axis in the xy-plane) and $\mathbf{L}_z = \dfrac{\hbar}{2}$. The z-axis view of a representation of the total current pattern of the $Y_0^0(\theta,\phi)$ orbitsphere comprising the superposition of 144 current elements is shown in Figure 2A. As the number of great circles goes to infinity the current distribution becomes continuous and is exactly uniform following normalization. A representation of the $\left(-\dfrac{1}{\sqrt{2}}\mathbf{i_x},\dfrac{1}{\sqrt{2}}\mathbf{i_y},\mathbf{i_z}\right)$-axis view of the total uniform current-density pattern of the $Y_0^0(\phi,\theta)$ orbitsphere with 144 vectors overlaid on the continuous bound-electron current density giving the direction of the current of each great circle element is shown in Figure 2B. This superconducting current pattern is confined to two spatial dimensions.

Thus, a bound electron is a constant two-dimensional spherical surface of charge (zero thickness and total charge $= -e$), called an electron orbitsphere that can exist in a bound state at only specified distances from the nucleus determined by an energy minimum for the $n = 1$ state and integer multiples of this radius due to the action of resonant photons as shown in the

Determination of Orbitsphere Radii section and Excited States of the One-Electron Atom (Quantization) section of Ref. [1], respectively. The bound electron is not a point, but it is point-like (behaves like a point at the origin). The free electron is continuous with the bound electron as it is ionized and is also point-like as shown in the Electron in Free Space section of Ref. [1]. The total function that describes the spinning motion of each electron orbitsphere is composed of two functions. One function, the spin function (see Figure 1 for the charge function and Figure 2 for the current function), is spatially uniform over the orbitsphere, where each point moves on the surface with the same quantized angular and linear velocity, and gives rise to spin angular momentum. It corresponds to the nonradiative $n = 1$, $\ell = 0$ state of atomic hydrogen which is well known as an s state or orbital. The other function, the modulation function, can be spatially uniform—in which case there is no orbital angular momentum and the magnetic moment of the electron orbitsphere is one Bohr magneton—or not spatially uniform—in which case there is orbital angular momentum. The modulation function rotates with a quantized angular velocity about a specific (by convention) z-axis. The constant spin function that is modulated by a time and spherical harmonic function as given by Eq. (17) is shown in Figure 3 for several ℓ values. The modulation or traveling charge-density wave that corresponds to an orbital angular momentum in addition to a spin angular momentum are typically referred to as p, d, f, etc. orbitals and correspond to an ℓ quantum number not equal to zero.

It was shown previously [1-12] that classical physics gives closed form solutions for the atom including the stability of the $n = 1$ state and the instability of the excited states, the equation of the photon and electron in excited states, the equation of the free electron, and photon which predict the wave particle duality behavior of particles and light. The current and charge density functions of the electron may be directly physically interpreted. For example, spin angular momentum results from the motion of negatively charged mass moving systematically, and the equation for angular momentum, $\mathbf{r} \times \mathbf{p}$, can be applied directly to the wavefunction (a current density function) that describes the electron. The magnetic moment of a Bohr magneton, Stern Gerlach experiment, g factor, Lamb shift, resonant line width and shape, selection rules, correspondence principle, wave-particle duality, excited states, reduced mass, rotational energies, and momenta, orbital and spin splitting, spin-orbital coupling, Knight shift, and spin-nuclear coupling, and elastic electron scattering from helium atoms, are derived in closed form equations based on Maxwell's equations. The agreement between observations and predictions based on closed-form equations with fundamental constants only matches to the limit permitted by the error in the measured fundamental constants.

In contrast to the failure of the Bohr theory and the nonphysical, unpredictive, adjustable-parameter approach of quantum mechanics, multielectron atoms [1, 4] and the nature of the chemical bond [1, 5] are given by exact closed-form solutions containing fundamental constants

only. Using the nonradiative electron current-density functions, the radii are determined from the force balance of the electric, magnetic, and centrifugal forces that correspond to the minimum of energy of the atomic or ionic system. The ionization energies are then given by the electric and magnetic energies at these radii. The spreadsheets to calculate the energies from exact solutions of one through twenty-electron atoms are available from the internet [24]. For 400 atoms and ions the agreement between the predicted and experimental results are remarkable [4]. In this paper, we extend these results to the nature of the chemical bond. In this regard, quantum mechanics has historically sought the lowest energy of the molecular system, but this is trivially the case of the electrons inside the nuclei. Obviously, the electrons must obey additional physical laws since matter does not exist in a state with the electrons collapsed into the nuclei. Specifically, molecular bonding is due to the physics of Newton's and Maxwell's laws together with achieving an energy minimum.

The structure of the bound molecular electron was solved by first considering the one-electron molecule H_2^+ and then the simplest molecule H_2 [1, 5]. The nature of the chemical bond was solved in the same fashion as that of the bound atomic electron. First principles including stability to radiation requires that the electron charge of the molecular orbital is a prolate spheroid, a solution of the Laplacian as an equipotential minimum energy surface in the natural ellipsoidal coordinates compared to spheroidal in the atomic case, and the current is time harmonic and obeys Newton's laws of mechanics in the central field of the nuclei at the foci of the spheroid. There is no a priori reason why the electron position must be a solution of the three-dimensional wave equation plus time and cannot comprise source currents of electromagnetic waves that are solutions of the three-dimensional wave equation plus time. Then, the special case of nonradiation determines that the current functions are confined to two-spatial dimensions plus time and match the electromagnetic wave-equation solutions for these dimensions. In addition to the important result of stability to radiation, several more very important physical results are subsequently realized: (i) The charge is distributed on a two-dimension surface; thus, there are no infinities in the corresponding fields (Eq. (10)). Infinite fields are simply renormalized in the case of the point-particles of quantum mechanics, but it is physically gratifying that none arise in this case since infinite fields have never been measured or realized in the laboratory. (ii) The hydrogen molecular ion or molecule has finite dimensions rather than extending over all space. From measurements of the resistivity of hydrogen as a function of pressure, the finite dimensions of the hydrogen molecule are evident in the plateau of the resistivity versus pressure curve of metallic hydrogen [25]. This is in contradiction to the predictions of quantum probability functions such as an exponential radial distribution in space. Furthermore, despite the predictions of quantum mechanics that preclude the imaging of a

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molecule orbital, the full three-dimensional structure of the outer molecular orbital of N_2 has been recently tomographically reconstructed [26]. The charge-density surface observed is similar to that shown in Figure 4 for H_2 which is direct evidence that MO's electrons are not point-particle probability waves that have no form until they are "collapsed to a point" by measurement. Rather they are physical, two-dimensional equipotential charge density functions as derived herein. (iii) Consistent with experiments, neutral scattering is predicted without violation of special relativity and causality wherein a point must be everywhere at once as required in the QM case. (iv) There is no electron self-interaction. The continuous charge-density function is a two-dimensional equipotential energy surface with an electric field that is strictly normal for the elliptic parameter $\xi > 0$ according to Gauss' law and Faraday's law. The relationship between the electric field equation and the electron source charge-density function is given by Maxwell's equation in two dimensions [27,28] (Eq. (10)). This relation shows that only a two-dimensional geometry meets the criterion for a fundamental particle. This is the nonsingularity geometry that is no longer divisible. It is the dimension from which it is not possible to lower dimensionality. In this case, there is no electrostatic self-interaction since the corresponding potential is continuous across the surface according to Faraday's law in the electrostatic limit, and the field is discontinuous, normal to the charge according to Gauss' law [27-29]. (v) The instability of electron-electron repulsion of molecular hydrogen is eliminated since the central field of the hydrogen molecular ion relative to a second electron at $\xi > 0$ which binds to form the hydrogen molecule is that of a single charge at the foci. (vi) The ellipsoidal MOs allow exact spin pairing over all time that is consistent with experimental observation. This aspect is not possible in the QM model.

Current algorithms to solve molecules are based on nonphysical models based on the concept that the electron is a zero or one-dimensional point in an all-space probability wave function $\Psi(x)$ that permits the electron to be over all space simultaneously and give output based on trial and error or direct empirical adjustment of parameters. These models ultimately cannot be the actual description of a physical electron in that they inherently violate physical laws. They suffer from the same shortcomings that plague atomic quantum theory, infinities, instability with respect to radiation according to Maxwell's equations, violation of conservation of linear and angular momentum, lack of physical relativistic invariance, and the electron is unbounded such that the edge of molecues does not exist. There is no uniqueness, as exemplified by the average of 150 internally inconsistent programs per molecule for each of the 788 molecules posted on the NIST website [30]. Furthermore, from a physical perspective, the implication for the basis of the chemical bond according to quantum mechanics being the exchange integral and the requirement of zero-point vibration, "strictly quantum mechanical

phenomena," is that the theory cannot be a correct description of reality as described for even the simple bond of molecular hydrogen as reported previous [1, 5]. Even the premise that "electron overlap" is responsible for bonding is opposite to the physical reality that negative charges repel each other with an inverse-distance-squared force dependence that becomes infinite. A proposed solution based on physical laws and fully compliant with Maxwell's equations solves the parameters of molecules even to infinite length and complexity in closed form equations with fundamental constants only.

For the first time in history, the key building blocks of organic chemistry have been solved from two basic equations. Now, the true physical structure and parameters of an infinite number of organic molecules up to infinite length and complexity can be obtained to permit the engineering of new pharmaceuticals and materials at the molecular level. The solutions of the basic functional groups of organic chemistry were obtained by using generalized forms of a geometrical and an energy equation for the nature of the $H-H$ bond. The geometrical parameters and total bond energies of about 800 exemplary organic molecules were calculated using the functional group composition. The results obtained essentially instantaneously match the experimental values typically to the limit of measurement [1]. The solved function groups are given in Table 1.

The two basic equations that solves organic molecules, one for geometrical parameters and the other for energy parameters, were applied to bulk forms of matter containing trillions of trillions of electrons. For example, using the same alkane- and alkene-bond solutions as elements in an infinite network, the nature of the solid molecular bond for all known allotropes of carbon (graphite, diamond, C_{60}, and their combinations) were solved. By further extension of this modular approach, the solid molecular bond of silicon and the nature of semiconductor bond were solved. The nature of other fundamental forms of matter such as the nature of the ionic bond, the metallic bond, and additional major fields of chemistry such as that of silicon, organometallics, and boron were solved exactly such that the position and energy of each and every electron is precisely specified. The implication of these results is that it is possible using physical laws to solve the structure of all types of matter. Some of the solved forms of matter of infinite extent as well as additional major fields of chemistry are given in Table 2. In all cases, the agreement with experiment is remarkable [1].

II. METHODOLOGICAL OUTLINE
A. The Nature of the Chemical Bond of Hydrogen

The nature of the chemical bond of functional groups is solved by first solving the simplest molecule, molecular hydrogen as given in the Nature of the Chemical Bond of Hydrogen-Type Molecules section of Ref. [1]. The hydrogen molecule charge and current

density functions, bond distance, and energies are solved from the Laplacian in ellipsoidal coordinates with the constraint of nonradiation [1, 5].

$$(\eta - \zeta)R_\xi \frac{\partial}{\partial\xi}(R_\xi \frac{\partial\phi}{\partial\xi}) + (\zeta - \xi)R_\eta \frac{\partial}{\partial\eta}(R_\eta \frac{\partial\phi}{\partial\eta}) + (\xi - \eta)R_\zeta \frac{\partial}{\partial\zeta}(R_\zeta \frac{\partial\phi}{\partial\zeta}) = 0 \qquad (21)$$

a. The Geometrical Parameters of the Hydrogen Molecule

As shown in Figure 4, the nuclei are at the foci of the electrons comprising a two-dimensional, equipotential-energy, charge- and current-density surface that obeys Maxwell's equations including stability to radiation and Newton's laws of motion. The force balance equation for the hydrogen molecule is

$$\frac{\hbar^2}{m_e a^2 b^2}D = \frac{e^2}{8\pi\varepsilon_o ab^2}D + \frac{\hbar^2}{2m_e a^2 b^2}D \qquad (22)$$

where

$$D = \mathbf{r}(t) \cdot \mathbf{i}_\zeta \qquad (23)$$

is the time dependent distance from the origin to the tangent plane at a point on the ellipsoidal MO. Eq. (22) has the parametric solution

$$r(t) = \mathbf{i}a\cos\omega t + \mathbf{j}b\sin\omega t \qquad (24)$$

when the semimajor axis, a, is

$$a = a_o \qquad (25)$$

The internuclear distance, $2c'$, which is the distance between the foci is

$$2c' = \sqrt{2}a_o \qquad (26)$$

The experimental internuclear distance is $\sqrt{2}a_o$. The semiminor axis is

$$b = \frac{1}{\sqrt{2}}a_o \qquad (27)$$

The eccentricity, e, is

$$e = \frac{1}{\sqrt{2}} \qquad (28)$$

b. The Energies of the Hydrogen Molecule

The potential energy of the two electrons in the central field of the protons at the foci is

$$V_e = \frac{-2e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} = -67.836\ eV \qquad (29)$$

The potential energy of the two protons is

$$V_p = \frac{e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}} = 19.242\ eV \qquad (30)$$

The kinetic energy of the electrons is

$$T = \frac{\hbar^2}{2m_e a \sqrt{a^2 - b^2}} \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} = 33.918 \ eV \tag{31}$$

The energy, V_m, of the magnetic force between the electrons is

$$V_m = \frac{-\hbar^2}{4m_e a \sqrt{a^2 - b^2}} \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} = -16.959 \ eV \tag{32}$$

During bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the protons. The corresponding energy $\bar{E}_{osc}$ is the difference between the Doppler and average vibrational kinetic energies:

$$\bar{E}_{osc} = \bar{E}_D + \bar{E}_{Kvib} = \left(V_e + T + V_m + V_p \right) \sqrt{\frac{2\bar{E}_K}{Mc^2}} + \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}} \tag{33}$$

The total energy is

$$E_T = V_e + T + V_m + V_p + \bar{E}_{osc} \tag{34}$$

$$E_T = -\frac{e^2}{8\pi\varepsilon_o a_0} \left[\left(2\sqrt{2} - \sqrt{2} + \frac{\sqrt{2}}{2} \right) \ln \frac{\sqrt{2} + 1}{\sqrt{2} - 1} - \sqrt{2} \right] \left[1 + \sqrt{\frac{2\hbar \sqrt{\frac{e^2}{4\pi\varepsilon_o a_0^3}}}{m_e c^2}} \right] - \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}} = -31.689 \ eV$$

$$\tag{35}$$

The energy of two hydrogen atoms is

$$E(2H[a_H]) = -27.21 \ eV \tag{36}$$

The bond dissociation energy, E_D, is the difference between the total energy of the corresponding hydrogen atoms (Eq. (36)) and E_T (Eq. (35)).

$$E_D = E(2H[a_H]) - E_T = 4.478 \ eV \tag{37}$$

The experimental energy is $E_D = 4.478 \ eV$. The calculated and experimental parameters of H_2, D_2, H_2^+, and D_2^+ from Ref. [5] and Chp. 11 of Ref. [1] are given in Table 3.

B. Derivation of the General Geometrical and Energy Equations of Organic Chemistry

Organic molecules comprising an arbitrary number of atoms can be solved using similar principles and procedures as those used to solve alkanes of arbitrary length. Alkanes can be considered to be comprised of the functional groups of CH_3, CH_2, and $C-C$. These groups with the corresponding geometrical parameters and energies can be added as a linear sum to give the solution of any straight chain alkane as shown in the Continuous-Chain Alkanes section of Ref. [1]. Similarly, the geometrical parameters and energies of all functional groups such as those given in Table 1 can be solved. The functional-group solutions can be made into a linear superposition and sum, respectively, to give the solution of any organic molecule. The solutions of the functional groups can be conveniently obtained by using generalized forms of the geometrical and energy equations. The derivation of the dimensional parameters and energies of the function groups are given in the Nature of the Chemical Bond of Hydrogen-Type Molecules, Polyatomic Molecular Ions and Molecules, More Polyatomic Molecules and Hydrocarbons, and Organic Molecular Functional Groups and Molecules sections of Ref. [1]. *(Reference to equations of the form Eq. (15.number), Eq. (11.number), Eq. (13.number), and Eq. (14.number) will refer to the corresponding equations of Ref. [1].)* Additional derivations for other non-organic function groups given in Table 2 are derived in the following sections of Ref. [1]: Applications: Pharmaceuticals, Specialty Molecular Functional Groups and Molecules, Dipole Moments, and Interactions, Nature of the Solid Molecular Bond of the Three Allotropes of Carbon, Silicon Molecular Functional Groups and Molecules, Nature of the Solid Semiconductor Bond of Silicon, Boron Molecues, and Organometallic Molecular Functional Groups and Molecules sections.

Consider the case wherein at least two atomic orbital hybridize as a linear combination of electrons at the same energy in order to achieve a bond at an energy minimum, and the sharing of electrons between two or more such orbitals to form a MO permits the participating hybridized orbitals to decrease in energy through a decrease in the radius of one or more of the participating orbitals. The force-generalized constant k' of a H_2-type ellipsoidal MO due to the equivalent of two point charges of at the foci is given by:

$$k' = \frac{C_1 C_2 2e^2}{4\pi\varepsilon_0} \tag{38}$$

where C_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the molecule or molecular ion which is 0.75 (Eq. (13.59)) in the case of H bonding to a central atom and 0.5 (Eq. (14.152)) otherwise, and C_2 is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of the chemical bond. From Eqs. (13.58-13.63), the distance from the origin of the MO to each focus c' is given by:

$$c' = a\sqrt{\frac{\hbar^2 4\pi\varepsilon_0}{m_e e^2 2C_1 C_2 a}} = \sqrt{\frac{a a_0}{2C_1 C_2}} \tag{39}$$

The internuclear distance is

$$2c' = 2\sqrt{\frac{a a_0}{2C_1 C_2}} \tag{40}$$

The length of the semiminor axis of the prolate spheroidal MO $b = c$ is given by

$$b = \sqrt{a^2 - c'^2} \tag{41}$$

And, the eccentricity, e, is

$$e = \frac{c'}{a} \tag{42}$$

From Eqs. (11.207-11.212), the potential energy of the two electrons in the central field of the nuclei at the foci is

$$V_e = n_1 c_1 c_2 \frac{-2e^2}{8\pi\varepsilon_o \sqrt{a^2 - b^2}} \ln\frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} \tag{43}$$

The potential energy of the two nuclei is

$$V_p = n_1 \frac{e^2}{8\pi\varepsilon_o \sqrt{a^2 - b^2}} \tag{44}$$

The kinetic energy of the electrons is

$$T = n_1 c_1 c_2 \frac{\hbar^2}{2m_e a\sqrt{a^2 - b^2}} \ln\frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} \tag{45}$$

And, the energy, V_m, of the magnetic force between the electrons is

$$V_m = n_1 c_1 c_2 \frac{-\hbar^2}{4m_e a\sqrt{a^2 - b^2}} \ln\frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} \tag{46}$$

The total energy of the H_2-type prolate spheroidal MO, $E_T(H_2MO)$, is given by the sum of the energy terms:

$$E_T(H_2MO) = V_e + T + V_m + V_p \tag{47}$$

$$E_T(H_2MO) = -\frac{n_1 e^2}{8\pi\varepsilon_o \sqrt{a^2 - b^2}}\left[c_1 c_2\left(2 - \frac{a_0}{a}\right)\ln\frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} - 1\right]$$

$$= -\frac{n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1 c_2\left(2 - \frac{a_0}{a}\right)\ln\frac{a + c'}{a - c'} - 1\right] \tag{48}$$

where n_1 is the number of equivalent bonds of the MO. c_1 is the fraction of the H_2-type ellipsoidal MO basis function of an MO which is 0.75 (Eqs. (13.67-13.73)) in the case of H bonding to an unhybridized central atom and 1 otherwise, and c_2 is the factor that results in an equipotential energy match of the participating the MO and the at least two atomic orbitals of the

chemical bond. Specifically, to meet the equipotential condition and energy matching conditions for the union of the H_2-type-ellipsoidal-MO and the HOs or AOs of the bonding atoms, the factor c_2 of a H_2-type ellipsoidal MO may given by (i) one, (ii) the ratio of the Coulombic or valence energy of the AO or HO of at least one atom of the bond and $13.605804\ eV$, the Coulombic energy between the electron and proton of H, (iii) the ratio of the valence energy of the AO or HO of one atom and the Coulombic energy of another, (iv) the ratio of the valence energies of the AOs or HOs of two atoms, (v) the ratio of two c_2 factors corresponding to any of cases (ii)-(iv), and (vi) the product of two different c_2 factors corresponding to any of the cases (i)-(v). Specific examples of the factor c_2 of a H_2-type ellipsoidal MO given in previously [1] are

0.936127, the ratio of the ionization energy of N $14.53414\ eV$ and $13.605804\ eV$, the Coulombic energy between the electron and proton of H;

0.91771, the ratio of $14.82575\ eV$, $-E_{Coulomb}\left(C, 2sp^3\right)$, and $13.605804\ eV$;

0.87495, the ratio of $15.55033\ eV$, $-E_{Coulomb}\left(C_{ethane}, 2sp^3\right)$, and $13.605804\ eV$;

0.85252, the ratio of $15.95955\ eV$, $-E_{Coulomb}\left(C_{ethylene}, 2sp^3\right)$, and $13.605804\ eV$;

0.85252, the ratio of $15.95955\ eV$, $-E_{Coulomb}\left(C_{benzene}, 2sp^3\right)$, and $13.605804\ eV$, and

0.86359, the ratio of $15.55033\ eV$, $-E_{Coulomb}\left(C_{alkane}, 2sp^3\right)$, and $13.605804\ eV$.

In the generalization of the hybridization of at least two atomic-orbital shells to form a shell of hybrid orbitals, the hybridized shell comprises a linear combination of the electrons of the atomic-orbital shells. The radius of the hybridized shell is calculated from the total Coulombic energy equation by considering that the central field decreases by an integer for each successive electron of the shell and that the total energy of the shell is equal to the total Coulombic energy of the initial AO electrons. The total energy $E_T\left(atom, msp^3\right)$ (m is the integer of the valence shell) of the AO electrons and the hybridized shell is given by the sum of energies of successive ions of the atom over the n electrons comprising total electrons of the at least one AO shell.

$$E_T\left(atom, msp^3\right) = -\sum_{m=1}^{n} IP_m \qquad (49)$$

where IP_m is the mth ionization energy (positive) of the atom. The radius r_{msp^3} of the hybridized shell is given by:

$$r_{msp^3} = \sum_{q=Z-n}^{Z-1} \frac{-(Z-q)e^2}{8\pi\varepsilon_0 E_T\left(atom, msp^3\right)} \qquad (50)$$

Then, the Coulombic energy $E_{Coulomb}\left(atom, msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by

$$E_{Coulomb}\left(atom,msp^3\right)=\frac{-e^2}{8\pi\varepsilon_0 r_{msp^3}} \tag{51}$$

In the case that during hybridization at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy $E(magnetic)$ at the initial radius r of the AO electron:

$$E(magnetic)=\frac{2\pi\mu_0 e^2\hbar^2}{m_e^2 r^3}=\frac{8\pi\mu_o\mu_B^2}{r^3} \tag{52}$$

Then, the energy $E\left(atom,msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by the sum of $E_{Coulomb}\left(atom,msp^3\right)$ and $E(magnetic)$:

$$E\left(atom,msp^3\right)=\frac{-e^2}{8\pi\varepsilon_0 r_{msp^3}}+\frac{2\pi\mu_0 e^2\hbar^2}{m_e^2 r^3} \tag{53}$$

Consider next that the at least two atomic orbitals hybridize as a linear combination of electrons at the same energy in order to achieve a bond at an energy minimum with another atomic orbital or hybridized orbital. As a further generalization of the basis of the stability of the MO, the sharing of electrons between two or more such hybridized orbitals to form a MO permits the participating hybridized orbitals to decrease in energy through a decrease in the radius of one or more of the participating orbitals. In this case, the total energy of the hybridized orbitals is given by the sum of $E\left(atom,msp^3\right)$ and the next energies of successive ions of the atom over the n electrons comprising the total electrons of the at least two initial AO shells. Here, $E\left(atom,msp^3\right)$ is the sum of the first ionization energy of the atom and the hybridization energy. An example of $E\left(atom,msp^3\right)$ for $E\left(C,2sp^3\right)$ is given in Eq. (14.503) where the sum of the negative of the first ionization energy of C, $-11.27671\ eV$, plus the hybridization energy to form the $C2sp^3$ shell given by Eq. (14.146) is $E\left(C,2sp^3\right)=-14.63489\ eV$.

Thus, the sharing of electrons between two *atom* msp^3 HOs to form an atom-atom-bond MO permits each participating hybridized orbital to decrease in radius and energy. In order to further satisfy the potential, kinetic, and orbital energy relationships, each *atom* msp^3 HO donates an excess of 25% per bond of its electron density to the atom-atom-bond MO to form an energy minimum wherein the atom-atom bond comprises one of a single, double, or triple bond. In each case, the radius of the hybridized shell is calculated from the Coulombic energy equation by considering that the central field decreases by an integer for each successive electron of the shell and the total energy of the shell is equal to the total Coulombic energy of the initial AO electrons plus the hybridization energy. The total energy $E_T\left(mol.atom,msp^3\right)$ (m is the integer of the valence shell) of the HO electrons is given by the sum of energies of successive ions of the atom over the n electrons comprising total electrons of the at least one initial AO shell and the

hybridization energy:

$$E_T\left(mol.atom, msp^3\right) = E\left(atom, msp^3\right) - \sum_{m=2}^{n} IP_m \tag{54}$$

where IP_m is the mth ionization energy (positive) of the atom and the sum of $-IP_1$ plus the hybridization energy is $E\left(atom, msp^3\right)$. Thus, the radius r_{msp^3} of the hybridized shell due to its donation of a total charge $-Qe$ to the corresponding MO is given by is given by:

$$
\begin{aligned}
r_{msp^3} &= \left(\sum_{q=Z-n}^{Z-1} (Z-q) - Q\right) \frac{-e^2}{8\pi\varepsilon_0 E_T\left(mol.atom, msp^3\right)} \\
&= \left(\sum_{q=Z-n}^{Z-1} (Z-q) - s(0.25)\right) \frac{-e^2}{8\pi\varepsilon_0 E_T\left(mol.atom, msp^3\right)}
\end{aligned}
\tag{55}
$$

where $-e$ is the fundamental electron charge and $s = 1, 2, 3$ for a single, double, and triple bond, respectively. The Coulombic energy $E_{Coulomb}\left(mol.atom, msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by

$$E_{Coulomb}\left(mol.atom, msp^3\right) = \frac{-e^2}{8\pi\varepsilon_0 r_{msp^3}} \tag{56}$$

In the case that during hybridization at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy $E(magnetic)$ at the initial radius r of the AO electron given by Eq. (52). Then, the energy $E\left(mol.atom, msp^3\right)$ of the outer electron of the *atom* msp^3 shell is given by the sum of $E_{Coulomb}\left(mol.atom, msp^3\right)$ and $E(magnetic)$:

$$E\left(mol.atom, msp^3\right) = \frac{-e^2}{8\pi\varepsilon_0 r_{msp^3}} + \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 r^3} \tag{57}$$

$E_T\left(atom - atom, msp^3\right)$, the energy change of each *atom* msp^3 shell with the formation of the atom-atom-bond MO is given by the difference between $E\left(mol.atom, msp^3\right)$ and $E\left(atom, msp^3\right)$:

$$E_T\left(atom - atom, msp^3\right) = E\left(mol.atom, msp^3\right) - E\left(atom, msp^3\right) \tag{58}$$

In the case of the $C2sp^3$ HO, the initial parameters (Eqs. (14.142-14.146)) are

$$r_{2sp^3} = \sum_{n=2}^{5} \frac{(Z-n)e^2}{8\pi\varepsilon_0 (e148.25751\ eV)} = \frac{10e^2}{8\pi\varepsilon_0 (e148.25751\ eV)} = 0.91771a_0 \tag{59}$$

$$E_{Coulomb}\left(C, 2sp^3\right) = \frac{-e^2}{8\pi\varepsilon_0 r_{2sp^3}} = \frac{-e^2}{8\pi\varepsilon_0 0.91771a_0} = -14.82575\ eV \tag{60}$$

$$E(magnetic) = \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 \left(r_3\right)^3} = \frac{8\pi\mu_o \mu_B^2}{\left(0.84317a_0\right)^3} = 0.19086\ eV \tag{61}$$

$$E\left(C, 2sp^3\right) = \frac{-e^2}{8\pi\varepsilon_0 r_{2sp^3}} + \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 \left(r_3\right)^3}$$

$$= -14.82575 \ eV + 0.19086 \ eV \tag{62}$$

$$= -14.63489 \ eV$$

In Eq. (55),

$$\sum_{q=Z-n}^{Z-1} (Z-q) = 10 \tag{63}$$

Eqs. (14.147) and (54) give

$$E_T\left(mol.atom, msp^3\right) = E_T\left(C_{ethane}, 2sp^3\right) = -151.61569 \ eV \tag{64}$$

Using Eqs. (55-65), the final values of r_{C2sp^3}, $E_{Coulomb}\left(C2sp^3\right)$, and $E\left(C2sp^3\right)$, and the resulting $E_T\left(\overset{BO}{C-C}, C2sp^3\right)$ of the MO due to charge donation from the HO to the MO where $\overset{BO}{C-C}$

refers to the bond order of the carbon-carbon bond for different values of the parameter s are given in Table 4.

In another generalized case of the basis of forming a minimum-energy bond with the constraint that it must meet the energy matching condition for all MOs at all HOs or AOs, the energy $E\left(mol.atom, msp^3\right)$ of the outer electron of the *atom msp*^{3} shell of each bonding atom must be the average of $E\left(mol.atom, msp^3\right)$ for two different values of s:

$$E\left(mol.atom, msp^3\right) = \frac{E\left(mol.atom(s_1), msp^3\right) + E\left(mol.atom(s_2), msp^3\right)}{2} \tag{65}$$

In this case, $E_T\left(atom-atom, msp^3\right)$, the energy change of each *atom msp*^{3} shell with the formation of each atom-atom-bond MO, is average for two different values of s:

$$E_T\left(atom-atom, msp^3\right) = \frac{E_T\left(atom-atom(s_1), msp^3\right) + E_T\left(atom-atom(s_2), msp^3\right)}{2} \tag{66}$$

Consider an aromatic molecule such as benzene given in the Benzene Molecule section of Ref. [1]. Each $C=C$ double bond comprises a linear combination of a factor of 0.75 of four paired electrons (three electrons) from two sets of two $C2sp^3$ HOs of the participating carbon atoms. Each $C-H$ bond of CH having two spin-paired electrons, one from an initially unpaired electron of the carbon atom and the other from the hydrogen atom, comprises the linear combination of 75% H_2-type ellipsoidal MO and 25% $C2sp^3$ HO as given by Eq. (13.439). However, $E_T\left(atom-atom, msp^3\right)$ of the $C-H$-bond MO is given by $0.5E_T\left(C=C, 2sp^3\right)$ (Eq. (14.247)) corresponding to one half of a double bond that matches the condition for a single-bond order for $C-H$ that is lowered in energy due to the aromatic character of the bond.

A further general possibility is that a minimum-energy bond is achieved with satisfaction of the potential, kinetic, and orbital energy relationships by the formation of an MO comprising an allowed multiple of a linear combination of H_2-type ellipsoidal MOs and corresponding HOs or AOs that contribute a corresponding allowed multiple (e.g. 0.5, 0.75, 1) of the bond order given in Table 4. For example, the alkane MO given in the Continuous-Chain Alkanes section of Ref. [1] comprises a linear combination of factors of 0.5 of a single bond and 0.5 of a double bond.

Consider a first MO and its HOs comprising a linear combination of bond orders and a second MO that shares a HO with the first. In addition to the mutual HO, the second MO comprises another AO or HO having a single bond order or a mixed bond order. Then, in order for the two MOs to be energy matched, the bond order of the second MO and its HOs or its HO and AO is a linear combination of the terms corresponding to the bond order of the mutual HO and the bond order of the independent HO or AO. Then, in general, $E_T\left(atom-atom, msp^3\right)$, the energy change of each $atom\ msp^3$ shell with the formation of each atom-atom-bond MO, is a weighted linear sum for different values of s that matches the energy of the bonded MOs, HOs, and AOs:

$$E_T\left(atom-atom, msp^3\right) = \sum_{n=1}^{N} c_{s_n} E_T\left(atom-atom\left(s_n\right), msp^3\right) \tag{67}$$

where c_{s_n} is the multiple of the BO of s_n. The radius r_{msp^3} of the $atom\ msp^3$ shell of each bonding atom is given by the Coulombic energy using the initial energy $E_{Coulomb}\left(atom, msp^3\right)$ and $E_T\left(atom-atom, msp^3\right)$, the energy change of each $atom\ msp^3$ shell with the formation of each atom-atom-bond MO:

$$r_{msp^3} = \frac{-e^2}{8\pi\varepsilon_0 a_0 \left(E_{Coulomb}\left(atom, msp^3\right) + E_T\left(atom-atom, msp^3\right)\right)} \tag{68}$$

where $E_{Coulomb}\left(C2sp^3\right) = -14.825751\ eV$. The Coulombic energy $E_{Coulomb}\left(mol.atom, msp^3\right)$ of the outer electron of the $atom\ msp^3$ shell is given by Eq. (56). In the case that during hybridization, at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy $E(magnetic)$ (Eq. (52)) at the initial radius r of the AO electron. Then, the energy $E\left(mol.atom, msp^3\right)$ of the outer electron of the $atom\ msp^3$ shell is given by the sum of $E_{Coulomb}\left(mol.atom, msp^3\right)$ and $E(magnetic)$ (Eq. (57)). $E_T\left(atom-atom, msp^3\right)$, the energy change of each $atom\ msp^3$ shell with the formation of the atom-atom-bond MO is given by the difference between $E\left(mol.atom, msp^3\right)$ and $E\left(atom, msp^3\right)$ given by Eq. (58). Using Eq. (60)

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for $E_{Coulomb}\left(C, 2sp^3\right)$ in Eq. (68), the single bond order energies given by Eqs. (55-64) and shown in Table 4, and the linear combination energies (Eqs. (65-67)), the parameters of linear combinations of bond orders and linear combinations of mixed bond orders are given in Table 5.

Consider next the radius of the AO or HO due to the contribution of charge to more than one bond. The energy contribution due to the charge donation at each atom such as carbon superimposes linearly. In general, the radius r_{mol2sp^3} of the $C2sp^3$ HO of a carbon atom of a given molecule is calculated using Eq. (14.514) by considering $\sum E_{T_{mol}}\left(MO, 2sp^3\right)$, the total energy donation to all bonds with which it participates in bonding. The general equation for the radius is given by

$$r_{mol2sp^3} = \frac{-e^2}{8\pi\varepsilon_0\left(E_{Coulomb}\left(C, 2sp^3\right) + \sum E_{T_{mol}}\left(MO, 2sp^3\right)\right)}$$

$$= \frac{e^2}{8\pi\varepsilon_0\left(e14.825751\ eV + \sum\left|E_{T_{mol}}\left(MO, 2sp^3\right)\right|\right)} \tag{69}$$

The Coulombic energy $E_{Coulomb}\left(mol.atom, msp^3\right)$ of the outer electron of the *atom msp³* shell is given by Eq. (56). In the case that during hybridization, at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy $E(magnetic)$ (Eq. (52)) at the initial radius r of the AO electron. Then, the energy $E\left(mol.atom, msp^3\right)$ of the outer electron of the *atom msp³* shell is given by the sum of $E_{Coulomb}\left(mol.atom, msp^3\right)$ and $E(magnetic)$ (Eq. (57)).

For example, the $C2sp^3$ HO of each methyl group of an alkane contributes $-0.92918\ eV$ (Eq. (14.513)) to the corresponding single $C-C$ bond; thus, the corresponding $C2sp^3$ HO radius is given by Eq. (14.514). The $C2sp^3$ HO of each methylene group of C_nH_{2n+2} contributes $-0.92918\ eV$ to each of the two corresponding $C-C$ bond MOs. Thus, the radius (Eq. (69)), the Coulombic energy (Eq. (56)), and the energy (Eq. (57)) of each alkane methylene group are

$$r_{alkaneC_{methylene}2sp^3} = \frac{-e^2}{8\pi\varepsilon_0\left(E_{Coulomb}\left(C, 2sp^3\right) + \sum E_{T_{alkane}}\left(methylene\ C-C, 2sp^3\right)\right)}$$

$$= \frac{e^2}{8\pi\varepsilon_0\left(e14.825751\ eV + e0.92918\ eV + e0.92918\ eV\right)} \tag{70}$$

$$= 0.81549 a_0$$

$$E_{Coulomb}\left(C_{methylene}2sp^3\right) = \frac{-e^2}{8\pi\varepsilon_0\left(0.81549a_0\right)} = -16.68412\ eV \tag{71}$$

$$E\left(C_{methylene}2sp^3\right) = \frac{-e^2}{8\pi\varepsilon_0\left(0.81549a_0\right)} + \frac{2\pi\mu_0 e^2\hbar^2}{m_e^2\left(0.84317a_0\right)^3} = -16.49325\ eV \tag{72}$$

In the determination of the parameters of functional groups, heteroatoms bonding to $C2sp^3$ HOs to form MOs are energy matched to the $C2sp^3$ HOs. Thus, the radius and the energy parameters of a bonding heteroatom are given by the same equations as those for $C2sp^3$ HOs. Using Eqs. (52), (56-57), (61), and (69) in a generalized fashion, the final values of the radius of the HO or AO, $r_{Atom.HO.AO}$, $E_{Coulomb}\left(mol.atom, msp^3\right)$, and $E\left(C_{mol}2sp^3\right)$ are calculated using $\sum E_{T_{group}}\left(MO, 2sp^3\right)$, the total energy donation to each bond with which an atom participates in bonding corresponding to the values of $E_T\left(C \overset{BO}{-} C, C2sp^3\right)$ of the MO due to charge donation from the AO or HO to the MO given in Tables 4 and 5.

The energy of the MO is matched to each of the participating outermost atomic or hybridized orbitals of the bonding atoms wherein the energy match includes the energy contribution due to the AO or HO's donation of charge to the MO. The force constant k' (Eq. (38)) is used to determine the ellipsoidal parameter c' (Eq. (39)) of the each H_2-type-ellipsoidal-MO in terms of the central force of the foci. Then, c' is substituted into the energy equation (from Eq. (48))) which is set equal to n_1 times the total energy of H_2 where n_1 is the number of equivalent bonds of the MO and the energy of H_2, $-31.63536831\ eV$, Eq. (11.212) is the minimum energy possible for a prolate spheroidal MO. From the energy equation and the relationship between the axes, the dimensions of the MO are solved. The energy equation has the semimajor axis a as it only parameter. The solution of the semimajor axis a then allows for the solution of the other axes of each prolate spheroid and eccentricity of each MO (Eqs. (40-42)). The parameter solutions then allow for the component and total energies of the MO to be determined.

The total energy, $E_T\left(_{H_2MO}\right)$, is given by the sum of the energy terms (Eqs. (43-48)) plus $E_T\left(AO/HO\right)$:

$$E_T\left(_{H_2MO}\right) = V_e + T + V_m + V_p + E_T\left(AO/HO\right) \tag{73}$$

$$E_T\left(_{H_2MO}\right) = -\frac{n_1 e^2}{8\pi\varepsilon_o\sqrt{a^2-b^2}}\left[c_1 c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}-1\right] + E_T\left(AO/HO\right)$$

$$= -\frac{n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1 c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1\right] + E_T\left(AO/HO\right) \tag{74}$$

where n_1 is the number of equivalent bonds of the MO, c_1 is the fraction of the H_2-type ellipsoidal MO basis function of a chemical bond of the group, c_2 is the factor that results in an equipotential energy match of the participating at least two atomic orbitals of each chemical bond, and $E_T\left(AO/HO\right)$ is the total energy comprising the difference of the energy $E\left(AO/HO\right)$ of at least one atomic or hybrid orbital to which the MO is energy matched and any

energy component $\Delta E_{H_2MO}(AO/HO)$ due to the AO or HO's charge donation to the MO.

$$E_T(AO/HO) = E(AO/HO) - \Delta E_{H_2MO}(AO/HO) \tag{75}$$

To solve the bond parameters and energies, $c' = a\sqrt{\dfrac{\hbar^2 4\pi\varepsilon_0}{m_e e^2 2C_1 C_2 a}} = \sqrt{\dfrac{aa_0}{2C_1 C_2}}$ (Eq. (39)) is

substituted into $E_T(H_2MO)$ to give

$$
\begin{aligned}
E_T(H_2MO) &= -\frac{n_1 e^2}{8\pi\varepsilon_o \sqrt{a^2-b^2}}\left[c_1 c_2 \left(2 - \frac{a_0}{a}\right)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} - 1\right] + E_T(AO/HO) \\
&= -\frac{n_1 e^2}{8\pi\varepsilon_0 c'}\left[c_1 c_2 \left(2 - \frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'} - 1\right] + E_T(AO/HO) \\
&= -\frac{n_1 e^2}{8\pi\varepsilon_0 \sqrt{\dfrac{aa_0}{2C_1 C_2}}}\left[c_1 c_2 \left(2 - \frac{a_0}{a}\right)\ln\frac{a+\sqrt{\dfrac{aa_0}{2C_1 C_2}}}{a-\sqrt{\dfrac{aa_0}{2C_1 C_2}}} - 1\right] + E_T(AO/HO)
\end{aligned}
\tag{76}
$$

The total energy is set equal to $E(basis\ energies)$ which in the most general case is given by the sum of a first integer n_1 times the total energy of H_2 minus a second integer n_2 times the total energy of H, minus a third integer n_3 times the valence energy of $E(AO)$ (e.g. $E(N) = -14.53414\ eV$) where the first integer can be $1, 2, 3...$, and each of the second and third integers can be $0, 1, 2, 3...$.

$$E(basis\ energies) = n_1(-31.63536831\ eV) - n_2(-13.605804\ eV) - n_3 E(AO) \tag{77}$$

In the case that the MO bonds two atoms other than hydrogen, $E(basis\ energies)$ is n_1 times the total energy of H_2 where n_1 is the number of equivalent bonds of the MO and the energy of H_2, $-31.63536831\ eV$, Eq. (11.212) is the minimum energy possible for a prolate spheroidal MO:

$$E(basis\ energies) = n_1(-31.63536831\ eV) \tag{78}$$

$E_T(H_2MO)$, is set equal to $E(basis\ energies)$, and the semimajor axis a is solved. Thus, the semimajor axis a is solved from the equation of the form:

$$-\frac{n_1 e^2}{8\pi\varepsilon_0 \sqrt{\dfrac{aa_0}{2C_1 C_2}}}\left[c_1 c_2 \left(2 - \frac{a_0}{a}\right)\ln\frac{a+\sqrt{\dfrac{aa_0}{2C_1 C_2}}}{a-\sqrt{\dfrac{aa_0}{2C_1 C_2}}} - 1\right] + E_T(AO/HO) = E(basis\ energies) \tag{79}$$

The distance from the origin of the H_2-type-ellipsoidal-MO to each focus c', the internuclear distance $2c'$, and the length of the semiminor axis of the prolate spheroidal H_2-type MO $b = c$ are solved from the semimajor axis a using Eqs. (39-41). Then, the component energies are given by Eqs. (43-46) and (76).

The total energy of the MO of the functional group, $E_T(MO)$, is the sum of the total energy

of the components comprising the energy contribution of the MO formed between the participating atoms and $E_T\left(atom - atom, msp^3.AO\right)$, the change in the energy of the AOs or HOs upon forming the bond. From Eqs. (76-77), $E_T\left(MO\right)$ is

$$E_T\left(MO\right) = E(basis\ energies) + E_T\left(atom - atom, msp^3.AO\right) \tag{80}$$

During bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy $\bar{E}_{osc}$ is the sum of the Doppler, $\bar{E}_D$, and average vibrational kinetic energies, $\bar{E}_{Kvib}$:

$$\bar{E}_{osc} = n_1\left(\bar{E}_D + \bar{E}_{Kvib}\right) = n_1\left(E_{h\nu}\sqrt{\frac{2\bar{E}_K}{m_e c^2}} + \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right) \tag{81}$$

where n_1 is the number of equivalent bonds of the MO , k is the spring constant of the equivalent harmonic oscillator, and μ is the reduced mass. The angular frequency of the reentrant oscillation in the transition state corresponding to $\bar{E}_D$ is determined by the force between the central field and the electrons in the transition state. The force and its derivative are given by

$$f\left(R\right) = -\frac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_0 R^3} \tag{82}$$

and

$$f'\left(a\right) = 2\frac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_0 R^3} \tag{83}$$

such that the angular frequency of the oscillation in the transition state is given by

$$\omega = \sqrt{\frac{\left[\dfrac{-3}{a}f\left(a\right) - f'\left(a\right)\right]}{m_e}} = \sqrt{\frac{k}{m_e}} = \sqrt{\frac{\dfrac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_0 R^3}}{m_e}} \tag{84}$$

where R is the semimajor axis a or the semiminor axis b depending on the eccentricity of the bond that is most representative of the oscillation in the transition state. C_{1o} is the fraction of the H_2-type ellipsoidal MO basis function of the oscillatory transition state of a chemical bond of the group, and C_{2o} is the factor that results in an equipotential energy match of the participating at least two atomic orbitals of the transition state of the chemical bond. Typically, $C_{1o} = C_1$ and $C_{2o} = C_2$. The kinetic energy, E_K, corresponding to $\bar{E}_D$ is given by Planck's equation for functional groups:

$$\bar{E}_K = \hbar\omega = \hbar\sqrt{\frac{\dfrac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_0 R^3}}{m_e}} \tag{85}$$

The Doppler energy of the electrons of the reentrant orbit is

$$\overline{E}_D \cong E_{hv}\sqrt{\frac{2\overline{E}_K}{m_e c^2}} = E_{hv}\sqrt{\frac{2\hbar\sqrt{\dfrac{\dfrac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_0 R^3}}{m_e}}}{m_e c^2}} \tag{86}$$

$\overline{E}_{osc}$ given by the sum of $\overline{E}_D$ and $\overline{E}_{Kvib}$ is

$$\overline{E}_{osc}\,(group) = n_1\left(\overline{E}_D + \overline{E}_{Kvib}\right) = n_1\left(E_{hv}\sqrt{\frac{2\hbar\sqrt{\dfrac{\dfrac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_0 R^3}}{m_e}}}{m_e c^2}} + E_{vib}\right) \tag{87}$$

E_{hv} of a group having n_1 bonds is given by $E_T\,(MO)/n_1$ such that

$$\overline{E}_{osc} = n_1\left(\overline{E}_D + \overline{E}_{Kvib}\right) = n_1\left(E_T\,(MO)/n_1\sqrt{\frac{2\overline{E}_K}{Mc^2}} + \frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right) \tag{88}$$

$E_{T+osc}\,(Group)$ is given by the sum of $E_T\,(MO)$ (Eq. (79)) and $\overline{E}_{osc}$ (Eq. (88)):

$$E_{T+osc}\,(Group) = E_T\,(MO) + \overline{E}_{osc}$$

$$= \left(\begin{pmatrix} -\dfrac{n_1 e^2}{8\pi\varepsilon_0\sqrt{\dfrac{aa_0}{2C_1 C_2}}}\left[c_1 c_2\left(2 - \dfrac{a_0}{a}\right)\ln\dfrac{a + \sqrt{\dfrac{aa_0}{2C_1 C_2}}}{a - \sqrt{\dfrac{aa_0}{2C_1 C_2}}} - 1\right] \\ + E_T\left(AO/HO\right) + E_T\left(atom - atom, msp^3.AO\right) \end{pmatrix} \right.$$
$$\left. \left[1 + \sqrt{\dfrac{2\hbar\sqrt{\dfrac{\dfrac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_o R^3}}{m_e}}}{m_e c^2}}\right] + n_1\frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}\right)$$

$$= \left(E(basis\ energies) + E_T\left(atom - atom, msp^3.AO\right)\right)\left[1 + \sqrt{\frac{2\hbar\sqrt{\dfrac{\dfrac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_o R^3}}{m_e}}}{m_e c^2}}\right] + n_1\frac{1}{2}\hbar\sqrt{\frac{k}{\mu}}$$

$$\tag{89}$$

The total energy of the functional group $E_T\,(group)$ is the sum of the total energy of the components comprising the energy contribution of the MO formed between the participating atoms, $E(basis\ energies)$, the change in the energy of the AOs or HOs upon forming the bond ($E_T\left(atom - atom, msp^3.AO\right)$), the energy of oscillation in the transition state, and the change in

magnetic energy with bond formation, E_{mag}. From Eq. (89), the total energy of the group $E_T\,(Group)$ is

$$E_T\,(Group) = \left(\begin{array}{c} \left(E(basis\ energies) + E_T\left(atom-atom,msp^3.AO\right) \right)\left[1 + \sqrt{\dfrac{2\hbar\sqrt{\dfrac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_oR^3}}}{m_e c^2}} \right] \\ +n_1\overline{E}_{Kvib} + E_{mag} \end{array} \right) \tag{90}$$

The change in magnetic energy E_{mag} which arises due to the formation of unpaired electrons in the corresponding fragments relative to the bonded group is given by

$$E_{mag} = c_3\frac{2\pi\mu_0 e^2\hbar^2}{m_e^2 r^3} = c_3\frac{8\pi\mu_o\mu_B^2}{r^3} \tag{91}$$

where r^3 is the radius of the atom that reacts to form the bond and c_3 is the number of electron pairs.

$$E_T\,(Group) = \left(\begin{array}{c} \left(E(basis\ energies) + E_T\left(atom-atom,msp^3.AO\right) \right)\left[1 + \sqrt{\dfrac{2\hbar\sqrt{\dfrac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_oR^3}}}{m_e c^2}} \right] \\ +n_1\overline{E}_{Kvib} + c_3\dfrac{8\pi\mu_o\mu_B^2}{r^3} \end{array} \right) \tag{92}$$

The total bond energy of the group $E_D\,(Group)$ is the negative difference of the total energy of the group (Eq. (92)) and the total energy of the starting species given by the sum of $c_4 E_{initial}\left(c_4\ AO/HO\right)$ and $c_5 E_{initial}\left(c_5\ AO/HO\right)$:

$$E_D\,(Group) = -\left(\begin{array}{c} \left(E(basis\ energies) + E_T\left(atom-atom,msp^3.AO\right) \right)\left[1 + \sqrt{\dfrac{2\hbar\sqrt{\dfrac{C_{1o}C_{2o}e^2}{4\pi\varepsilon_oR^3}}}{m_e c^2}} \right] \\ +n_1\overline{E}_{Kvib} + c_3\dfrac{8\pi\mu_o\mu_B^2}{r_n^3} - \left(c_4 E_{initial}\left(AO/HO\right) + c_5 E_{initial}\left(c_5\ AO/HO\right)\right) \end{array} \right) \tag{93}$$

In the case of organic molecules, the atoms of the functional groups are energy matched to the $C2sp^3$ HO such that

$$E\left(AO/HO\right) = -14.63489\ eV \tag{94}$$

For example, of E_{mag} of the $C2sp^3$ HO is:

$$E_{mag}\left(C2sp^3\right)=c_3\frac{8\pi\mu_o\mu_B^2}{r^3}=c_3\frac{8\pi\mu_o\mu_B^2}{\left(0.91771a_0\right)^3}=c_3 0.14803\ eV \tag{95}$$

Each molecule, independently of its complexity and size, is comprised of functional groups wherein each present occurs an integer number of times in the molecule. The total bond energy of the molecule is then given by the integer-weighted sum of the energies of the functions groups corresponding to the composition of the molecule. Thus, integer formulas can be constructed easily for molecules for a given class such as straight-chain hydrocarbons considered as an example *infra*. The results demonstrate how simply and instantaneously molecules are solved using the classical exact solutions. In contrast, quantum mechanics requires that wavefunction are nonlinear, and any sum must be squared. The results of Millsian disprove quantum mechanics in this regard, and the linearity and superposition properties of Millsian represent a breakthrough with orders of magnitude reduction in complexity in solving molecues as well as being accurate physical representations rather than pure mathematical curve-fits devoid of a connection to reality.

C. Total Energy of Continuous-Chain Alkanes

$E_D\left(C_nH_{2n+2}\right)$, the total bond dissociation energy of C_nH_{2n+2}, is given as the sum of the energy components due to the two methyl groups, $n-2$ methylene groups, and $n-1$ $C-C$ bonds where each energy component is given by Eqs. (14.590), (14.625), and (14.641), respectively. Thus, the total bond dissociation energy of C_nH_{2n+2} is

$$E_D\left(C_nH_{2n+2}\right)=E_D\left(C-C\right)_{n-1}+2E_{D_{alkane}}\left(^{12}CH_3\right)+\left(n-2\right)E_{D_{alkane}}\left(^{12}CH_2\right)$$
$$=\left(n-1\right)\left(4.32754\ eV\right)+2\left(12.49186\ eV\right)+\left(n-2\right)\left(7.83016\ eV\right) \tag{96}$$

The experimental total bond dissociation energy of C_nH_{2n+2}, $E_{D_{exp}}\left(C_nH_{2n+2}\right)$, is given by the negative difference between the enthalpy of its formation ($\Delta H_f\left(C_nH_{2n+2}\left(gas\right)\right)$) and the sum of the enthalpy of the formation of the reactant gaseous carbons ($\Delta H_f\left(C\left(gas\right)\right)$) and hydrogen ($\Delta H_f\left(H\left(gas\right)\right)$) atoms:

$$E_{D_{exp}}\left(C_nH_{2n+2}\right)=-\left\{\Delta H_f\left(C_nH_{2n+2}\left(gas\right)\right)-\left[n\Delta H_f\left(C\left(gas\right)\right)+\left(2n+2\right)\Delta H_f\left(H\left(gas\right)\right)\right]\right\}$$
$$=-\left\{\Delta H_f\left(C_nH_{2n+2}\left(gas\right)\right)-\left[n7.42774\ eV+\left(2n+2\right)2.259353\ eV\right]\right\} \tag{97}$$

where the heats of formation atomic carbon and hydrogen gas are given by [31-32]

$$\Delta H_f\left(C\left(gas\right)\right)=716.68\ kJ/mole\ \left(7.42774\ eV/molecule\right) \tag{98}$$
$$\Delta H_f\left(H\left(gas\right)\right)=217.998\ kJ/mole\ \left(2.259353\ eV/molecule\right) \tag{99}$$

D. 3-21G and 6-31G* Basis Sets Calculations

The energies of the 3-21G and 6-31G* basis sets were acquired from Spartan's pre-computed database, and the total bond energies E_T were determined using Eqs. (100) and (101). Only those molecules were studied using Spartan for which either the total ionization potentials (IP_{exp}) could be calculated from experimental data [33] or for which quantum mechanical total ionization potentials (IP_{QM}) could be calculated from values obtained from Gaussian. Due to this limitation, many molecules for which experimental data was available were omitted in the comparison between Spartan and these experimental values; although, Millsian solved them including the major classes of organometallics and coordinate compounds to typically within less than 0.1%.

$$E_T = E - Tot \ IP_{exp} \tag{100}$$

$$E_T = E - Tot \ IP_{QM} \tag{101}$$

III. RESULTS AND DISCUSSION

Well over 300 functional groups have been solved classically and comprise the database for Millsian such that the program can provide essentially instant, exact solutions and renderings for practically an infinite number of molecules (for 300 functional groups the approximate number is 300 raised to the $n-1^{th}$ power of molecules each comprising n atoms where $n = 2, 3, 4, ...\infty$). Representative functional groups are given in Tables 1 and 2. For example, using Eq. (96), $E_D\left(C_nH_{2n+2}\right)$ was determined for propane, butane, pentane, hexane, heptane, octane, nonane, decane, undecane, dodecane, and octadecane [1] to compare to the available experimental values. The latter were determined from the corresponding experimental $\Delta H_f\left(C_nH_{2n+2}\left(gas\right)\right)$ [32] and Eqs. (97-99). The results of the determination of the total bond energies are given in Table 6. Similarly, a large array of functional groups and molecules per class for which experimental data was available is given in Tables 6-74. Here, the total bond energies of exemplary organic, silicon, boron, organometallic, and coordinate molecules whose designation is based on the main functional group were calculated using the functional group composition and the corresponding energies derived previously [1] and compared to the experimental values. References for the experimental values are mainly from Ref. [33-36], and they are given for each compound in Ref. [1]. For each molecule, the calculated results is based on first principles and given in closed-form, exact equations containing fundamental constants and integers only. The agreement between the experimental and calculated results is excellent. And, unlike previous curve-fitting approaches, the exact geometric parameters, current densities, and energies are given for every electron. Exact representations based on these solutions are given for some exemplary molecules in Figures 5-14. In the case of a translucent view of the

charge-density, the orbitals of the atoms at their radii, the ellipsoidal surface of each H or H_2-type ellipsoidal MO that transitions to the corresponding outer shell of the atom(s) participating in each bond, and the hydrogen nuclei (red, not to scale) are shown. In the case of a opaque view of the charge-density, the outer orbitals of the atoms at their radii and the ellipsoidal surface of each H or H_2-type ellipsoidal MO that transitions to the corresponding outer shell of the atoms participating in each bond are shown.

The Spartan results were broken down into four sets of tests. The Spartan energy E was obtained for both the 3-21G and 6-31G* basis sets, and the total bond energy E_T was calculated for each basis set using the quantum mechanical ionization potentials (Eq. 101), as is standard practice, and also using experimental ionization potentials (Eq 100) which was a more direct test against experimental data. A relative paucity of Spartan results could actually be tested against experimental data compared to Millsian due to the lack of experimental ionization energy data for higher Z atoms. Table 75 gives the results of Millsian 1.0, the results with 3-21G and 6-31G* basis sets generated from a pre-computed Spartan database, and the experimental values. The Millsian results were consistently within a relative deviation of less than 1%, being typically <0.1%, and the accuracies were very stable across all of the classes of molecules. Where errors of greater than 0.1% occurred, the atypical result was almost always due to the comparison of vacuum theoretical energies to crystalline experimental data since the gas-phase data was not available. In contrast, the Spartan results with 3-21G and 6-31G* deviated by a wide range of relative errors depending on functional group type and basis set and produced large errors even for it best performance. Spartan 3-21G and 6-31G* typically gave >30% relative error compared to experimental values even for simple straight-chain alkanes. Errors for some of the molecule classes were typically greater than 100% and even surpassed 1000% as the functional group complexity increased beyond straight-chain alkanes. Furthermore, the comparison between the two basis sets showed discrepancies with the errors at times of opposite sign indicating even a lack of internal consistency between the basis sets. In fact, as the molecules deviated from the very simple straight-chain alkanes to more complex molecules such as halobenzenes, the results appeared random without any discernible pattern to the failures. The corresponding impact to the fidelity of the data in terms of applications is enormous. Millsian typically gives 3 to 4 significant-figure accuracy compared to 1 to 2 significant figures for Spartan rendering it practically useless.

In the sets where the Spartan results were calculated using quantum mechanical ionization potentials, IP_{QM}, as is standard practice, the relative deviation (>20%) was less than that for the corresponding use of the experimental values, and the trend was highly consistent across classes of molecules. Yet, theoretical calculations that attempt to omit unaccounted for

properties that they might 'cancel out,' producing a better number by the subtraction of two numbers with large errors is of questionable validity. This is evident in the cases of the method using IP_{QM}'s where it was occasionally susceptible to very large discrepancies surpassing 100% and even 1000%.

It is clear from these results that basis-set algorithms such as those using the 3-21G and 6-31G* basis sets can only match experimental results within a limited set of molecules for which they are optimized. Since the results have substantial errors even for the best results, the usefulness to industry application is suspect. This issue is compounded by the fact that the procedures are not based on physical laws; whereas, Millsian is. If electrons do obey physical laws as the results of Millsian confirm, then the basis-set approach is no more useful than curve fitting, and there can be no inherent physical insight or predictiveness to be gained from these computational methods. Without even testing the geometry, it is easy to conclude that quantum mechanical solutions to molecules are not realistic from their inability to correctly render the charge density as well as the predict energy. When comparing the rendering of the simple alkane butane (C_4H_{10}) using the two basis sets (Figures 15A-B) neither shows any resemblance to butane in that they are not even symmetrical, the edge is created artificially and arbitrarily, and the 3-31G basis set rendering has a very different density pattern than that obtained using the 3-21G basis set. This inconsistent and unnatural QM result is contrast with the exact classical solution of butane given in Figure 5 that matches butane for all of its measurable parameters.

IV. CONCLUSION

The current scientific software market is highly fragmented and based on academic-based curve-fitting models; whereas, Millsian 1.0 is the only modeling technology based on fundamental physical laws. In this study we compared the energies of exact classical solutions of molecules generated by Millsian 1.0 to energies from Spartan's pre-computed database using 3-21G and 6-31G* basis sets, and experimental values. The Millsian results were consistently within an average relative deviation of about 0.1% of the experimentally values; whereas, the Spartan 3-21G and 6-31G* results deviated over a wide range of relative error, typically being a factor of three orders of magnitude greater with a large percentage of catastrophic failures, depending on functional group type and basis set. The results indicate that the basis-set computational approach is prone to erroneous numerical results. The failures undermine the premise of using a purely computational model devoid of any physical basis since it cannot render true representations based the underlying physics; consequently, such models lack general predictive utility.

In contrast, Millsian modeling technology based on physical laws predicts exact solutions for molecules for the first time in history. The Millsian competitive advantage includes rendering true molecular structures providing precise bonding characteristics, spatial and temporal charge distributions, and energies of every electron in every bond and bonding atom. These exact solutions can provide precise chemical and engineering properties of molecules and thus materials. Thus, this new technology may create new opportunities for discovery of new chemical processes, new molecules, new synthetic pathways, new materials, and new uses for existing molecules. Exact solutions may facilitate drug design, with the identification of biologically active sites and structures and predict optimal synthetic pathways, products, and yields. This represents a major breakthrough in the chemical and material sciences that may impact nearly all businesses involved in material, chemicals, and drug development. New possibilities are enabled at a time that industries are expanding or changing their focus with a commensurate increased challenge to current modeling capabilities. Pharma, for example, can benefit from the real-time interactive exact rendering of large bio-molecules such as proteins (Figure 13) and DNA (Figure 14) that are enabled by Millsian at a time when the industry is shifting emphasis from small molecules to biotechnology.

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Table 1. Partial List of Organic Functional Groups Solved by Classical Physics.

Continuous-Chain Alkanes	N,N-dialkyl Amides	Aniline
Branched Alkanes	Urea	Aryl Nitro Compounds
Alkenes	Carboxylic Acid Halides	Benzoic Acid Compounds
Branched Alkenes	Carboxylic Acid Anhydrides	Anisole
Alkynes	Nitriles	Pyrrole
Alkyl Fluorides	Thiols	Furan
Alkyl Chlorides	Sulfides	Thiophene
Alkyl Bromides	Disulfides	Imidizole
Alkyl Iodides	Sulfoxides	Pyridine
Alkenyl Halides	Sulfones	Pyrimidine
Aryl Halides	Sulfites	Pyrazine
Alcohols	Sulfates	Quinoline
Ethers	Nitroalkanes	Isoquinoline
Primary Amines	Alkyl Nitrates	Indole
Secondary Amines	Alkyl Nitrites	Adenine
Tertiary Amines	Conjugated Alkenes	Fullerene (C_{60})
Aldehydes	Conjugated Polyenes	Graphite
Ketones	Aromatics	Phosphines
Carboxylic Acids	Naphthalene	Phosphine Oxides
Carboxylic Acid Esters	Toluene	Phosphites
Amides	Chlorobenzene	Phosphates
N-alkyl Amides	Phenol	

Table 2. Partial List of Additional Molecules and Compositions of Matter Solved by Classical Physics.

Solid Molecular Bond of the Three Allotropes of Carbon	Alkyl Borinic Acids
	Tertiary Aminoboranes
Diamond	Quaternary Aminoboranes
Graphite	Borane Amines
Fullerene (C_{60})	Halido Boranes
Dipole-Dipole Bonding	Organometallic Molecular Functional Groups and Molecules
Hydrogen Bonding	
Van der Waals Bonding	Alkyl Aluminum Hydrides
Solid Ionic Bond of Alkali-Hydrides	Bridging Bonds of
Alkali-Hydride Crystal Structures	Organoaluminum Hydrides
Lithium Hydride	Organogermanium and Digermanium
Sodium Hydride	Organolead
Potassium Hydride	Organoarsenic
Rubidium & Cesium Hydride	Organoantimony
Potassium Hydrino Hydride	Organobismuth
Solid Metallic Bond of Alkali Metals	Organic Ions
Alkali Metal Crystal Structures	1° Amino
Lithium Metal	2° Amino
Sodium Metal	Carboxylate
Potassium Metal	Phosphate
Rubidium & Cesium Metals	Nitrate
Alkyl Aluminum Hydrides	Sulfate
Silicon Groups and Molecules	Silicate
Silanes	Proteins
Alkyl Silanes and Disilanes	Amino Acids
Solid Semiconductor Bond of Silicon	Peptide Bonds
Insulator-Type Semiconductor Bond	DNA
Conductor-Type Semiconductor Bond	Bases
Boron Molecules	2-deoxyribose
Boranes	Ribose
Bridging Bonds of Boranes	Phosphate Backbone
Alkoxy Boranes	Water
Alkyl Boranes	Condensed Noble Gases

Table 3. The Maxwellian closed-form calculated and experimental parameters of H_2, D_2, H_2^+ and D_2^+.

Parameter	Calculated	Experimental
H_2 Bond Energy	4.478 eV	4.478 eV
D_2 Bond Energy	4.556 eV	4.556 eV
H_2^+ Bond Energy	2.654 eV	2.651 eV
D_2^+ Bond Energy	2.696 eV	2.691 eV
H_2 Total Energy	31.677 eV	31.675 eV
D_2 Total Energy	31.760 eV	31.760 eV
H_2 Ionization Energy	15.425 eV	15.426 eV
D_2 Ionization Energy	15.463 eV	15.466 eV
H_2^+ Ionization Energy	16.253 eV	16.250 eV
D_2^+ Ionization Energy	16.299 eV	16.294 eV
H_2^+ Magnetic Moment	$9.274 \, X \, 10^{-24} \, JT^{-1} \, \left(\mu_B \right)$	$9.274 \, X \, 10^{-24} \, JT^{-1} \, \left(\mu_B \right)$
Absolute H_2 Gas-Phase NMR Shift	-28.0 ppm	-28.0 ppm
H_2 Internuclear Distance[a]	0.748 Å $\sqrt{2}a_o$	0.741 Å
D_2 Internuclear Distance[a]	0.748 Å $\sqrt{2}a_o$	0.741 Å
H_2^+ Internuclear Distance	1.058 Å $2a_o$	1.06 Å
D_2^+ Internuclear Distance[a]	1.058 Å $2a_o$	1.0559 Å
H_2 Vibrational Energy	0.517 eV	0.516 eV
D_2 Vibrational Energy	0.371 eV	0.371 eV
H_2 $\omega_e x_e$	120.4 cm^{-1}	121.33 cm^{-1}
D_2 $\omega_e x_e$	60.93 cm^{-1}	61.82 cm^{-1}
H_2^+ Vibrational Energy	0.270 eV	0.271 eV
D_2^+ Vibrational Energy	0.193 eV	0.196 eV
H_2 J=1 to J=0 Rotational Energy[a]	0.0148 eV	0.01509 eV
D_2 J=1 to J=0 Rotational Energy[a]	0.00741 eV	0.00755 eV
H_2^+ J=1 to J=0 Rotational Energy	0.00740 eV	0.00739 eV
D_2^+ J=1 to J=0 Rotational Energy[a]	0.00370 eV	0.003723 eV

[a] Not corrected for the slight reduction in internuclear distance due to $\overline{E}_{osc}$.

Table 4. The final values of r_{C2sp^3}, $E_{Coulomb}\left(C2sp^3\right)$, and $E\left(C2sp^3\right)$ and the resulting $E_T\left(C\overset{BO}{-}C, C2sp^3\right)$ of the MO due to charge donation from the HO to the MO where $C\overset{BO}{-}C$ refers to the bond order of the carbon-carbon bond.

MO Bond Order (BO)	s_1	s_2	$r_{C2sp^3}\left(a_0\right)$ Final	$E_{Coulomb}\left(C2sp^3\right)$ (eV) Final	$E\left(C2sp^3\right)$ (eV) Final	$E_T\left(C\overset{BO}{-}C, C2sp^3\right)$ (eV)
I	1	0	0.87495	-15.55033	-15.35946	-0.72457
II	2	0	0.85252	-15.95955	-15.76868	-1.13379
III	3	0	0.83008	-16.39089	-16.20002	-1.56513
IV	4	0	0.80765	-16.84619	-16.65532	-2.02043

Table 5. The final values of r_{C2sp^3}, $E_{Coulomb}(C2sp^3)$, and $E(C2sp^3)$ and the resulting $E_T\left(C\overset{BO}{-}C, C2sp^3\right)$ of the MO comprising a linear combination of H_2-type ellipsoidal MOs and corresponding HOs of single or mixed bond order where c_{s_n} is the multiple of the bond order parameter $E_T\left(atom-atom(s_n), msp^3\right)$ given in Table 4.

MO Bond Order (BO)	s_1	c_{s_1}	s_2	c_{s_2}	s_3	c_{s_3}	$r_{C2sp^3}(a_o)$ Final	$E_{Coulomb}(C2sp^3)$ (eV) Final	$E(C2sp^3)$ (eV) Final	$E_T\left(C\overset{BO}{-}C, C2sp^3\right)$ (eV)
1/2I	1	0.5	0	0	0	0	0.89582	-15.18804	-14.99717	-0.36228
1/2II	2	0.5	0	0	0	0	0.88392	-15.39265	-15.20178	-0.56689
1/2I + 1/4II	1	0.5	2	0.25	0	0	0.87941	-15.47149	-15.28062	-0.64573
1/4II + ¼ (I + II)	2	0.25	1	0.25	2	0.25	0.87363	-15.57379	-15.38293	-0.74804
3/4II	2	0.75	0	0	0	0	0.86793	-15.67610	-15.48523	-0.85034
1/2I + 1/2II	1	0.5	2	0.5	0	0	0.86359	-15.75493	-15.56407	-0.92918
1/2I + 1/2III	1	0.5	3	0.5	0	0	0.85193	-15.97060	-15.77974	-1.14485
1/2I + 1/2IV	1	0.5	4	0.5	0	0	0.83995	-16.19826	-16.00739	-1.37250
1/2II + 1/2III	2	0.5	3	0.5	0	0	0.84115	-16.17521	-15.98435	-1.34946
1/2II + 1/2IV	2	0.5	4	0.5	0	0	0.82948	-16.40286	-16.21200	-1.57711
I+1/2(I + II)	1	1	1	0.5	2	0.5	0.82562	-16.47951	-16.28865	-1.65376
1/2III + 1/2IV	3	0.5	4	0.5	0	0	0.81871	-16.61853	-16.42767	-1.79278
1/2IV + 1/2IV	4	0.5	4	0.5	0	0	0.80765	-16.84619	-16.65532	-2.02043
1/2(I + II)+II	1	0.5	2	0.5	2	1	0.80561	-16.88873	-16.69786	-2.06297

Table 6. Summary results of n-alkanes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_8	propane	41.46896	41.434	-0.00085
C_4H_{10}	butane	53.62666	53.61	-0.00036
C_5H_{12}	pentane	65.78436	65.77	-0.00017
C_6H_{14}	hexane	77.94206	77.93	-0.00019
C_7H_{16}	heptane	90.09976	90.09	-0.00013
C_8H_{18}	octane	102.25746	102.25	-0.00006
C_9H_{20}	nonane	114.41516	114.40	-0.00012
$C_{10}H_{22}$	decane	126.57286	126.57	-0.00003
$C_{11}H_{24}$	undecane	138.73056	138.736	0.00004
$C_{12}H_{26}$	dodecane	150.88826	150.88	-0.00008
$C_{18}H_{38}$	octadecane	223.83446	223.85	0.00008

Table 7. Summary results of branched alkanes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_4H_{10}	isobutane	53.69922	53.695	-0.00007
C_5H_{12}	isopentane	65.85692	65.843	-0.00021
C_5H_{12}	neopentane	65.86336	65.992	0.00195
C_6H_{14}	2-methylpentane	78.01462	78.007	-0.00010
C_6H_{14}	3-methylpentane	78.01462	77.979	-0.00046
C_6H_{14}	2,2-dimethylbutane	78.02106	78.124	0.00132
C_6H_{14}	2,3-dimethylbutane	77.99581	78.043	0.00061
C_7H_{16}	2-methylhexane	90.17232	90.160	-0.00014
C_7H_{16}	3-methylhexane	90.17232	90.127	-0.00051
C_7H_{16}	3-ethylpentane	90.17232	90.108	-0.00072
C_7H_{16}	2,2-dimethylpentane	90.17876	90.276	0.00107
C_7H_{16}	2,2,3-trimethylbutane	90.22301	90.262	0.00044
C_7H_{16}	2,4-dimethylpentane	90.24488	90.233	-0.00013
C_7H_{16}	3,3-dimethylpentane	90.17876	90.227	0.00054
C_8H_{18}	2-methylheptane	102.33002	102.322	-0.00008
C_8H_{18}	3-methylheptane	102.33002	102.293	-0.00036
C_8H_{18}	4-methylheptane	102.33002	102.286	-0.00043
C_8H_{18}	3-ethylhexane	102.33002	102.274	-0.00055
C_8H_{18}	2,2-dimethylhexane	102.33646	102.417	0.00079
C_8H_{18}	2,3-dimethylhexane	102.31121	102.306	-0.00005
C_8H_{18}	2,4-dimethylhexane	102.40258	102.362	-0.00040
C_8H_{18}	2,5-dimethylhexane	102.40258	102.396	-0.00006
C_8H_{18}	3,3-dimethylhexane	102.33646	102.369	0.00032
C_8H_{18}	3,4-dimethylhexane	102.31121	102.296	-0.00015
C_8H_{18}	3-ethyl-2-methylpentane	102.31121	102.277	-0.00033
C_8H_{18}	3-ethyl-3-methylpentane	102.33646	102.317	-0.00019
C_8H_{18}	2,2,3-trimethylpentane	102.38071	102.370	-0.00010
C_8H_{18}	2,2,4-trimethylpentane	102.40902	102.412	0.00003
C_8H_{18}	2,3,3-trimethylpentane	102.38071	102.332	-0.00048
C_8H_{18}	2,3,4-trimethylpentane	102.29240	102.342	0.00049
C_8H_{18}	2,2,3,3-tetramethylbutane	102.41632	102.433	0.00016
C_9H_{20}	2,3,5-trimethylhexane	114.54147	114.551	0.00008
C_9H_{20}	3,3-diethylpentane	114.49416	114.455	-0.00034
C_9H_{20}	2,2,3,3-tetramethylpentane	114.57402	114.494	-0.00070
C_9H_{20}	2,2,3,4-tetramethylpentane	114.51960	114.492	-0.00024
C_9H_{20}	2,2,4,4-tetramethylpentane	114.57316	114.541	-0.00028
C_9H_{20}	2,3,3,4-tetramethylpentane	114.58266	114.484	-0.00086
$C_{10}H_{22}$	2-methylnonane	126.64542	126.680	0.00027
$C_{10}H_{22}$	5-methylnonane	126.64542	126.663	0.00014

Table 8. Summary results of alkenes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_6	propene	35.56033	35.63207	0.00201
C_4H_8	1-butene	47.71803	47.78477	0.00140
C_4H_8	trans-2-butene	47.93116	47.90395	-0.00057
C_4H_8	isobutene	47.90314	47.96096	0.00121
C_5H_{10}	1-pentene	59.87573	59.95094	0.00125
C_5H_{10}	trans-2-pentene	60.08886	60.06287	-0.00043
C_5H_{10}	2-methyl-1-butene	60.06084	60.09707	0.00060
C_5H_{10}	2-methyl-2-butene	60.21433	60.16444	-0.00083
C_5H_{10}	3-methyl-1-butene	59.97662	60.01727	0.00068
C_6H_{12}	1-hexene	72.03343	72.12954	0.00133
C_6H_{12}	trans-2-hexene	72.24656	72.23733	-0.00013
C_6H_{12}	trans-3-hexene	72.24656	72.24251	-0.00006
C_6H_{12}	2-methyl-1-pentene	72.21854	72.29433	0.00105
C_6H_{12}	2-methyl-2-pentene	72.37203	72.37206	0.00000
C_6H_{12}	3-methyl-1-pentene	72.13432	72.19173	0.00080
C_6H_{12}	4-methyl-1-pentene	72.10599	72.21038	0.00145
C_6H_{12}	3-methyl-trans-2-pentene	72.37203	72.33268	-0.00054
C_6H_{12}	4-methyl-trans-2-pentene	72.34745	72.31610	-0.00043
C_6H_{12}	2-ethyl-1-butene	72.21854	72.25909	0.00056
C_6H_{12}	2,3-dimethyl-1-butene	72.31943	72.32543	0.00008
C_6H_{12}	3,3-dimethyl-1-butene	72.31796	72.30366	-0.00020
C_6H_{12}	2,3-dimethyl-2-butene	72.49750	72.38450	-0.00156
C_7H_{14}	1-heptene	84.19113	84.27084	0.00095
C_7H_{14}	5-methyl-1-hexene	84.26369	84.30608	0.00050
C_7H_{14}	trans-3-methyl-3-hexene	84.52973	84.42112	-0.00129
C_7H_{14}	2,4-dimethyl-1-pentene	84.44880	84.49367	0.00053
C_7H_{14}	4,4-dimethyl-1-pentene	84.27012	84.47087	0.00238
C_7H_{14}	2,4-dimethyl-2-pentene	84.63062	84.54445	-0.00102
C_7H_{14}	trans-4,4-dimethyl-2-pentene	84.54076	84.54549	0.00006
C_7H_{14}	2-ethyl-3-methyl-1-butene	84.47713	84.44910	-0.00033
C_7H_{14}	2,3,3-trimethyl-1-butene	84.51274	84.51129	-0.00002
C_8H_{16}	1-octene	96.34883	96.41421	0.00068
C_8H_{16}	trans-2,2-dimethyl-3-hexene	96.69846	96.68782	-0.00011
C_8H_{16}	3-ethyl-2-methyl-1-pentene	96.63483	96.61113	-0.00025
C_8H_{16}	2,4,4-trimethyl-1-pentene	96.61293	96.71684	0.00107
C_8H_{16}	2,4,4-trimethyl-2-pentene	96.67590	96.65880	-0.00018
$C_{10}H_{20}$	1-decene	120.66423	120.74240	0.00065
$C_{12}H_{24}$	1-dodecene	144.97963	145.07163	0.00063
$C_{16}H_{32}$	1-hexadecene	193.61043	193.71766	0.00055

Table 9. Summary results of alkynes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_4	propyne	29.42932	29.40432	-0.00085
C_4H_6	1-butyne	41.58702	41.55495	-0.00077
C_4H_6	2-butyne	41.72765	41.75705	0.00070
C_9H_{16}	1-nonyne	102.37552	102.35367	-0.00021

Table 10. Summary results of alkyl fluorides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CF_4	tetrafluoromethane	21.07992	21.016	-0.00303
CHF_3	trifluoromethane	19.28398	19.362	0.00405
CH_2F_2	difluoromethane	18.22209	18.280	0.00314
C_3H_7F	1-fluoropropane	41.86745	41.885	0.00041
C_3H_7F	2-fluoropropane	41.96834	41.963	-0.00012

Table 11. Summary results of alkyl chlorides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CCl_4	tetrachloromethane	13.43181	13.448	0.00123
$CHCl_3$	trichloromethane	14.49146	14.523	0.00217
CH_2Cl_2	dichloromethane	15.37248	15.450	0.00499
CH_3Cl	chloromethane	16.26302	16.312	0.00299
C_2H_5Cl	chloroethane	28.61064	28.571	-0.00138
C_3H_7Cl	1-chloropropane	40.76834	40.723	-0.00112
C_3H_7Cl	2-chloropropane	40.86923	40.858	-0.00028
C_4H_9Cl	1-chlorobutane	52.92604	52.903	-0.00044
C_4H_9Cl	2-chlorobutane	53.02693	52.972	-0.00104
C_4H_9Cl	1-chloro-2-methylpropane	52.99860	52.953	-0.00085
C_4H_9Cl	2-chloro-2-methylpropane	53.21057	53.191	-0.00037
$C_5H_{11}Cl$	1-chloropentane	65.08374	65.061	-0.00034
$C_5H_{11}Cl$	1-chloro-3-methylbutane	65.15630	65.111	-0.00069
$C_5H_{11}Cl$	2-chloro-2-methylbutane	65.36827	65.344	-0.00037
$C_5H_{11}Cl$	2-chloro-3-methylbutane	65.16582	65.167	0.00002
$C_6H_{13}Cl$	2-chlorohexane	77.34233	77.313	-0.00038
$C_8H_{17}Cl$	1-chlorooctane	101.55684	101.564	0.00007
$C_{12}H_{25}Cl$	1-chlorododecane	150.18764	150.202	0.00009
$C_{18}H_{37}Cl$	1-chlorooctadecane	223.13384	223.175	0.00018

Table 12. Summary results of alkyl bromides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CBr_4	tetrabromomethane	11.25929	11.196	-0.00566
$CHBr_3$	tribromomethane	12.87698	12.919	0.00323
CH_3Br	bromomethane	15.67551	15.732	0.00360
C_2H_5Br	bromoethane	28.03939	27.953	-0.00308
C_3H_7Br	1-bromopropane	40.19709	40.160	-0.00093
C_3H_7Br	2-bromopropane	40.29798	40.288	-0.00024
$C_5H_{10}Br_2$	2,3-dibromo-2-methylbutane	63.53958	63.477	-0.00098
$C_6H_{13}Br$	1-bromohexane	76.67019	76.634	-0.00047
$C_7H_{15}Br$	1-bromoheptane	88.82789	88.783	-0.00051
$C_8H_{17}Br$	1-bromooctane	100.98559	100.952	-0.00033
$C_{12}H_{25}Br$	1-bromododecane	149.61639	149.573	-0.00029
$C_{16}H_{33}Br$	1-bromohexadecane	198.24719	198.192	-0.00028

Table 13. Summary results of alkyl iodides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CHI_3	triiodomethane	10.35888	10.405	0.00444
CH_2I_2	diiodomethane	12.94614	12.921	-0.00195
CH_3I	iodomethane	15.20294	15.163	-0.00263
C_2H_5I	iodoethane	27.36064	27.343	-0.00066
C_3H_7I	1-iodopropane	39.51834	39.516	-0.00006
C_3H_7I	2-iodopropane	39.61923	39.623	0.00009
C_4H_9I	2-iodo-2-methylpropane	51.96057	51.899	-0.00119

Table 14. Summary results of alkene halides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_3Cl	chloroethene	22.46700	22.505	0.00170
C_3H_5Cl	2-chloropropene	35.02984	35.05482	0.00071

Table 15. Summary results of alcohols.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_4O	methanol	21.11038	21.131	0.00097
C_2H_6O	ethanol	33.40563	33.428	0.00066
C_3H_8O	1-propanol	45.56333	45.584	0.00046
C_3H_8O	2-propanol	45.72088	45.766	0.00098
$C_4H_{10}O$	1-butanol	57.72103	57.736	0.00026
$C_4H_{10}O$	2-butanol	57.87858	57.922	0.00074
$C_4H_{10}O$	2-methyl-1-propananol	57.79359	57.828	0.00060
$C_4H_{10}O$	2-methyl-2-propananol	58.15359	58.126	-0.00048
$C_5H_{12}O$	1-pentanol	69.87873	69.887	0.00011
$C_5H_{12}O$	2-pentanol	70.03628	70.057	0.00029
$C_5H_{12}O$	3-pentanol	70.03628	70.097	0.00087
$C_5H_{12}O$	2-methyl-1-butananol	69.95129	69.957	0.00008
$C_5H_{12}O$	3-methyl-1-butananol	69.95129	69.950	-0.00002
$C_5H_{12}O$	2-methyl-2-butananol	70.31129	70.246	-0.00092
$C_5H_{12}O$	3-methyl-2-butananol	69.96081	70.083	0.00174
$C_6H_{14}O$	1-hexanol	82.03643	82.054	0.00021
$C_6H_{14}O$	2-hexanol	82.19398	82.236	0.00052
$C_7H_{16}O$	1-heptanol	94.19413	94.214	0.00021
$C_8H_{18}O$	1-octanol	106.35183	106.358	0.00006
$C_8H_{18}O$	2-ethyl-1-hexananol	106.42439	106.459	0.00032
$C_9H_{20}O$	1-nonanol	118.50953	118.521	0.00010
$C_{10}H_{22}O$	1-decanol	130.66723	130.676	0.00007
$C_{12}H_{26}O$	1-dodecanol	154.98263	154.984	0.00001
$C_{16}H_{34}O$	1-hexadecanol	203.61343	203.603	-0.00005

Table 16. Summary results of ethers.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_6O	dimethyl ether	32.84496	32.902	0.00174
C_3H_8O	ethyl methyl ether	45.19710	45.183	-0.00030
$C_4H_{10}O$	diethyl ether	57.54924	57.500	-0.00086
$C_4H_{10}O$	methyl propyl ether	57.35480	57.355	0.00000
$C_4H_{10}O$	isopropyl methyl ether	57.45569	57.499	0.00075
$C_6H_{14}O$	dipropyl ether	81.86464	81.817	-0.00059
$C_6H_{14}O$	diisopropyl ether	82.06642	82.088	0.00026
$C_6H_{14}O$	t-butyl ethyl ether	82.10276	82.033	-0.00085
$C_7H_{16}O$	t-butyl isopropyl ether	94.36135	94.438	0.00081
$C_8H_{18}O$	dibutyl ether	106.18004	106.122	-0.00055
$C_8H_{18}O$	di-sec-butyl ether	106.38182	106.410	0.00027
$C_8H_{18}O$	di-t-butyl ether	106.36022	106.425	0.00061
$C_8H_{18}O$	t-butyl isobutyl ether	106.65628	106.497	-0.00218

Table 17. Summary results of 1° amines.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_5N	methylamine	23.88297	23.857	-0.00110
C_2H_7N	ethylamine	36.04067	36.062	0.00060
C_3H_9N	propylamine	48.19837	48.243	0.00092
$C_4H_{11}N$	butylamine	60.35607	60.415	0.00098
$C_4H_{11}N$	sec-butylamine	60.45696	60.547	0.00148
$C_4H_{11}N$	t-butylamine	60.78863	60.717	-0.00118
$C_4H_{11}N$	isobutylamine	60.42863	60.486	0.00094

Table 18. Summary results of 2° amines.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_7N	dimethylamine	35.76895	35.765	-0.00012
$C_4H_{11}N$	diethylamine	60.22930	60.211	-0.00030
$C_6H_{15}N$	dipropylamine	84.54470	84.558	0.00016
$C_6H_{15}N$	diisopropylamine	84.74648	84.846	0.00117
$C_8H_{19}N$	dibutylamine	108.86010	108.872	0.00011
$C_8H_{19}N$	diisobutylamine	109.00522	109.106	0.00092

Table 19. Summary results of 3° amines.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_9N	trimethylamine	47.83338	47.761	-0.00152
$C_6H_{15}N$	triethylamine	84.30648	84.316	0.00012
$C_9H_{21}N$	tripropylamine	120.77958	120.864	0.00070

Table 20. Summary results of aldehydes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_2O	formaldehyde	15.64628	15.655	0.00056
C_2H_4O	acetaldehyde	28.18711	28.198	0.00039
C_3H_6O	propanal	40.34481	40.345	0.00000
C_4H_8O	butanal	52.50251	52.491	-0.00022
C_4H_8O	isobutanal	52.60340	52.604	0.00001
$C_5H_{10}O$	pentanal	64.66021	64.682	0.00034
$C_7H_{14}O$	heptanal	88.97561	88.942	-0.00038
$C_8H_{16}O$	octanal	101.13331	101.179	0.00045
$C_8H_{16}O$	2-ethylhexanal	101.23420	101.259	0.00025

Table 21. Summary results of ketones.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_6O	acetone	40.68472	40.672	-0.00031
C_4H_8O	2-butanone	52.84242	52.84	-0.00005
$C_5H_{10}O$	2-pentanone	65.00012	64.997	-0.00005
$C_5H_{10}O$	3-pentanone	65.00012	64.988	-0.00005
$C_5H_{10}O$	3-methyl-2-butanone	65.10101	65.036	-0.00099
$C_6H_{12}O$	2-hexanone	77.15782	77.152	-0.00008
$C_6H_{12}O$	3-hexanone	77.15782	77.138	-0.00025
$C_6H_{12}O$	2-methyl-3-pentanone	77.25871	77.225	-0.00043
$C_6H_{12}O$	3,3-dimethyl-2-butanone	77.29432	77.273	-0.00028
$C_7H_{14}O$	3-heptanone	89.31552	89.287	-0.00032
$C_7H_{14}O$	4-heptanone	89.31552	89.299	-0.00018
$C_7H_{14}O$	2,2-dimethyl-3-pentanone	89.45202	89.458	0.00007
$C_7H_{14}O$	2,4-dimethyl-3-pentanone	89.51730	89.434	-0.00093
$C_8H_{16}O$	2,2,4-trimethyl-3-pentanone	101.71061	101.660	-0.00049
$C_9H_{18}O$	2-nonanone	113.63092	113.632	0.00001
$C_9H_{18}O$	5-nonanone	113.63092	113.675	0.00039
$C_9H_{18}O$	2,6-dimethyl-4-heptanone	113.77604	113.807	0.00027

Table 22. Summary results of carboxylic acids.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_2O_2	formic acid	21.01945	21.036	0.00079
$C_2H_4O_2$	acetic acid	33.55916	33.537	-0.00066
$C_3H_6O_2$	propanoic acid	45.71686	45.727	0.00022
$C_4H_8O_2$	butanoic acid	57.87456	57.883	0.00015
$C_5H_{10}O_2$	pentanoic acid	70.03226	69.995	-0.00053
$C_5H_{10}O_2$	3-methylbutanoic acid	70.10482	70.183	0.00111
$C_5H_{10}O_2$	2,2-dimethylpropanoic acid	70.31679	69.989	-0.00468
$C_6H_{12}O_2$	hexanoic acid	82.18996	82.149	-0.00050
$C_7H_{14}O_2$	heptanoic acid	94.34766	94.347	0.00000
$C_8H_{16}O_2$	octanoic acid	106.50536	106.481	-0.00022
$C_9H_{18}O_2$	nonanoic acid	118.66306	118.666	0.00003
$C_{10}H_{20}O_2$	decanoic acid	130.82076	130.795	-0.00020
$C_{12}H_{24}O_2$	dodecanoic acid	155.13616	155.176	0.00026
$C_{14}H_{28}O_2$	tetradecanoic acid	179.45156	179.605	0.00085
$C_{15}H_{30}O_2$	pentadecanoic acid	191.60926	191.606	-0.00002
$C_{16}H_{32}O_2$	hexadecanoic acid	203.76696	203.948	0.00089
$C_{18}H_{36}O_2$	stearic acid	228.08236	228.298	0.00094
$C_{20}H_{40}O_2$	eicosanoic acid	252.39776	252.514	0.00046

Table 23. Summary results of carboxylic acid esters.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_2H_4O_2$	methyl formate	32.71076	32.762	0.00156
$C_3H_6O_2$	methyl acetate	45.24849	45.288	0.00087
$C_6H_{12}O_2$	methyl pentanoate	81.72159	81.726	0.00005
$C_7H_{14}O_2$	methyl hexanoate	93.87929	93.891	0.00012
$C_8H_{16}O_2$	methyl heptanoate	106.03699	106.079	0.00040
$C_9H_{18}O_2$	methyl octanoate	118.19469	118.217	0.00018
$C_{10}H_{20}O_2$	methyl nonanoate	130.35239	130.373	0.00016
$C_{11}H_{22}O_2$	methyl decanoate	142.51009	142.523	0.00009
$C_{12}H_{24}O_2$	methyl undecanoate	154.66779	154.677	0.00006
$C_{13}H_{26}O_2$	methyl dodecanoate	166.82549	166.842	0.00010
$C_{14}H_{28}O_2$	methyl tridecanoate	178.98319	179.000	0.00009
$C_{15}H_{30}O_2$	methyl tetradecanoate	191.14089	191.170	0.00015
$C_{16}H_{32}O_2$	methyl pentadecanoate	203.29859	203.356	0.00028
$C_4H_8O_2$	propyl formate	57.76366	57.746	-0.00030
$C_4H_8O_2$	ethyl acetate	57.63888	57.548	-0.00157
$C_5H_{10}O_2$	isopropyl acetate	69.89747	69.889	-0.00013
$C_5H_{10}O_2$	ethyl propanoate	69.79658	69.700	-0.00139
$C_6H_{12}O_2$	butyl acetate	81.95428	81.873	-0.00099
$C_6H_{12}O_2$	t-butyl acetate	82.23881	82.197	-0.00051
$C_6H_{12}O_2$	methyl 2,2-dimethylpropanoate	82.00612	81.935	-0.00087
$C_7H_{14}O_2$	ethyl pentanoate	94.11198	94.033	-0.00084
$C_7H_{14}O_2$	ethyl 3-methylbutanoate	94.18454	94.252	0.00072
$C_7H_{14}O_2$	ethyl 2,2-dimethylpropanoate	94.39651	94.345	-0.00054
$C_8H_{16}O_2$	isobutyl isobutanoate	106.44313	106.363	-0.00075
$C_8H_{16}O_2$	propyl pentanoate	106.26968	106.267	-0.00003
$C_8H_{16}O_2$	isopropyl pentanoate	106.37057	106.384	0.00013
$C_9H_{18}O_2$	butyl pentanoate	118.42738	118.489	0.00052
$C_9H_{18}O_2$	sec-butyl pentanoate	118.52827	118.624	0.00081
$C_9H_{18}O_2$	isobutyl pentanoate	118.49994	118.576	0.00064

Table 24. Summary results of amides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_3NO	formamide	23.68712	23.697	0.00041
C_2H_5NO	acetamide	36.15222	36.103	-0.00135
C_3H_7NO	propanamide	48.30992	48.264	-0.00094
C_4H_9NO	butanamide	60.46762	60.449	-0.00030
C_4H_9NO	2-methylpropanamide	60.51509	60.455	-0.00099
$C_5H_{11}NO$	pentanamide	72.62532	72.481	-0.00200
$C_5H_{11}NO$	2,2-dimethylpropanamide	72.67890	72.718	0.00054
$C_6H_{13}NO$	hexanamide	84.78302	84.780	-0.00004
$C_8H_{17}NO$	octanamide	109.09842	109.071	-0.00025

Table 25. Summary results of N-alkyl and N,N-dialkyl amides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_7NO	N,N-dimethylformamide	47.679454	47.574	0.00221
C_4H_9NO	N,N-dimethylacetamide	60.14455	59.890	-0.00426
$C_6H_{13}NO$	N-butylacetamide	84.63649	84.590	-0.00055

Table 26. Summary results of urea.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_4N_2O	urea	31.35919	31.393	0.00108

Table 27. Summary results of acid halide.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_3ClO	acetyl chloride	28.02174	27.990	-0.00115

Table 28. Summary results of acid anhydrides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_4H_6O_3$	acetic anhydride	56.94096	56.948	0.00013
$C_6H_{10}O_3$	propanoic anhydride	81.25636	81.401	0.00177

Table 29. Summary results of nitriles.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_3N	acetonitrile	25.72060	25.77	0.00174
C_3H_5N	Propanenitrile	37.87830	37.94	0.00171
C_4H_7N	butanenitrile	50.03600	50.08	0.00082
C_4H_7N	2-methylpropanenitrile	50.13689	50.18	0.00092
C_5H_9N	pentanenitrile	62.19370	62.26	0.00111
C_5H_9N	2,2-dimethylpropanenitrile	62.47823	62.40	-0.00132
$C_7H_{13}N$	heptanenitrile	86.50910	86.59	0.00089
$C_8H_{15}N$	octanenitrile	98.66680	98.73	0.00069
$C_{10}H_{19}N$	decanenitrile	122.98220	123.05	0.00057
$C_{14}H_{27}N$	tetradecanenitrile	171.61300	171.70	0.00052

Table 30. Summary results of thiols.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
HS	hydrogen sulfide	3.77430	3.653	-0.03320
H_2S	dihydrogen sulfide	7.56058	7.605	0.00582
CH_4S	methanethiol	19.60264	19.575	-0.00141
C_2H_6S	ethanethiol	31.76034	31.762	0.00005
C_3H_8S	1-propanethiol	43.91804	43.933	0.00035
C_3H_8S	2-propanethiol	44.01893	44.020	0.00003
$C_4H_{10}S$	1-butanethiol	56.07574	56.089	0.00024
$C_4H_{10}S$	2-butanethiol	56.17663	56.181	0.00009
$C_4H_{10}S$	2-methyl-1-propanethiol	56.14830	56.186	0.00066
$C_4H_{10}S$	2-methyl-2-propanethiol	56.36027	56.313	-0.00084
$C_5H_{12}S$	2-methyl-1-butanethiol	68.30600	68.314	0.00012
$C_5H_{12}S$	1-pentanethiol	68.23344	68.264	0.00044
$C_5H_{12}S$	2-methyl-2-butanethiol	68.51797	68.441	-0.00113
$C_5H_{12}S$	3-methyl-2-butanethiol	68.31552	68.381	0.00095
$C_5H_{12}S$	2,2-dimethyl-1-propanethiol	68.16441	68.461	0.00433
$C_6H_{14}S$	1-hexanethiol	80.39114	80.416	0.00031
$C_6H_{14}S$	2-methyl-2-pentanethiol	80.67567	80.607	-0.00085
$C_7H_{16}S$	1-heptanethiol	92.54884	92.570	0.00023
$C_{10}H_{22}S$	1-decanethiol	129.02194	129.048	0.00020

Table 31. Summary results of sulfides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_6S	dimethyl sulfide	31.65668	31.672	0.00048
C_3H_8S	ethyl methyl sulfide	43.81438	43.848	0.00078
$C_4H_{10}S$	diethyl sulfide	55.97208	56.043	0.00126
$C_4H_{10}S$	methyl propyl sulfide	55.97208	56.029	0.00102
$C_4H_{10}S$	isopropyl methyl sulfide	56.07297	56.115	0.00075
$C_5H_{12}S$	butyl methyl sulfide	68.12978	68.185	0.00081
$C_5H_{12}S$	t-butyl methyl sulfide	68.28245	68.381	0.00144
$C_5H_{12}S$	ethyl propyl sulfide	68.12978	68.210	0.00117
$C_5H_{12}S$	ethyl isopropyl sulfide	68.23067	68.350	0.00174
$C_6H_{14}S$	diisopropyl sulfide	80.48926	80.542	0.00065
$C_6H_{14}S$	butyl ethyl sulfide	80.28748	80.395	0.00133
$C_6H_{14}S$	methyl pentyl sulfide	80.28748	80.332	0.00056
$C_8H_{18}S$	dibutyl sulfide	104.60288	104.701	0.00094
$C_8H_{18}S$	di-sec-butyl sulfide	104.80466	104.701	-0.00099
$C_8H_{18}S$	di-t-butyl sulfide	104.90822	104.920	0.00011
$C_8H_{18}S$	diisobutyl sulfide	104.74800	104.834	0.00082
$C_{10}H_{22}S$	dipentyl sulfide	128.91828	128.979	0.00047
$C_{10}H_{22}S$	diisopentyl sulfide	129.06340	129.151	0.00068

Table 32. Summary results of disulfides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_2H_6S_2$	dimethyl disulfide	34.48127	34.413	-0.00199
$C_4H_{10}S_2$	diethyl disulfide	58.79667	58.873	0.00129
$C_6H_{14}S_2$	dipropyl disulfide	83.11207	83.169	0.00068
$C_8H_{18}S_2$	di-t-butyl disulfide	107.99653	107.919	-0.00072

Table 33. Summary results of sulfoxides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_6SO	dimethyl sulfoxide	35.52450	35.435	-0.00253
$C_4H_{10}SO$	diethyl sulfoxide	59.83990	59.891	0.00085
$C_6H_{14}SO$	dipropyl sulfoxide	84.15530	84.294	0.00165

Table 34. Summary results of sulfones.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_2H_6SO_2$	dimethyl sulfone	40.27588	40.316	0.00100

Table 35. Summary results of sulfites.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_2H_6SO_3$	dimethyl sulfite	43.95058	44.042	0.00207
$C_4H_{10}SO_3$	diethyl sulfite	68.54939	68.648	0.00143
$C_8H_{18}SO_3$	dibutyl sulfite	117.18019	117.191	0.00009

Table 36. Summary results of sulfates.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_2H_6SO_4$	dimethyl sulfate	48.70196	48.734	0.00067
$C_4H_{10}SO_4$	diethyl sulfate	73.30077	73.346	0.00061
$C_6H_{14}SO_4$	dipropyl sulfate	97.61617	97.609	-0.00008

Table 37. Summary results of nitro alkanes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_3NO_2	nitromethane	25.14934	25.107	-0.00168
$C_2H_5NO_2$	nitroethane	37.30704	37.292	-0.00040
$C_3H_7NO_2$	1-nitropropane	49.46474	49.451	-0.00028
$C_3H_7NO_2$	2-nitropropane	49.56563	49.602	0.00074
$C_4H_9NO_2$	1-nitrobutane	61.62244	61.601	-0.00036
$C_4H_9NO_2$	2-nitroisobutane	61.90697	61.945	0.00061
$C_5H_{11}NO_2$	1-nitropentane	73.78014	73.759	-0.00028

Table 38. Summary results of nitrite.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_3NO_2	methyl nitrite	24.92328	24.955	0.00126

Table 39. Summary results of nitrate.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_3NO_3	methyl nitrate	28.18536	28.117	-0.00244
$C_2H_5NO_3$	ethyl nitrate	40.34306	40.396	0.00131
$C_3H_7NO_3$	propyl nitrate	52.50076	52.550	0.00093
$C_3H_7NO_3$	isopropyl nitrate	52.60165	52.725	0.00233

Table 40. Summary results of conjugated alkenes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_5H_8	cyclopentene	54.83565	54.86117	0.00047
C_4H_6	1,3 butadiene	42.09159	42.12705	0.00084
C_5H_8	1,3 pentadiene	54.40776	54.42484	0.00031
C_5H_8	1,4 pentadiene	54.03745	54.11806	0.00149
C_5H_6	1,3 cyclopentadiene	49.27432	49.30294	0.00058

Table 41. Summary results of aromatics and heterocyclic aromatics.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_6H_6	benzene	57.26008	57.26340	0.00006
C_6H_5Cl	fluorobenzene	57.93510	57.887	-0.00083
C_6H_5Cl	chlorobenzene	56.55263	56.581	0.00051
$C_6H_4Cl_2$	m-dichlorobenzene	55.84518	55.852	0.00012
$C_6H_3Cl_3$	1,2,3-trichlorobenzene	55.13773	55.077	-0.00111
$C_6H_3Cl_3$	1,3,5-trichlorbenzene	55.29542	55.255	-0.00073
C_6Cl_6	hexachlorobenzene	52.57130	52.477	-0.00179
C_6H_5Br	bromobenzene	56.17932	56.391[a]	0.00376
C_6H_5I	iodobenzene	55.25993	55.261	0.00001
$C_6H_5NO_2$	nitrobenzene	65.18754	65.217	0.00046
C_7H_8	toluene	69.48425	69.546	0.00088
$C_7H_6O_2$	benzoic acid	73.76938	73.762	-0.00009
$C_7H_5ClO_2$	2-chlorobenzoic acid	73.06193	73.082	0.00027
$C_7H_5ClO_2$	3-chlorobenzoic acid	73.26820	73.261	-0.00010
C_6H_7N	aniline	64.43373	64.374	-0.00093
C_7H_9N	2-methylaniline	76.62345	76.643	-0.00025
C_7H_9N	3-methylaniline	76.62345	76.661	0.00050
C_7H_9N	4-methylaniline	76.62345	76.654	0.00040
$C_6H_6N_2O_2$	2-nitroaniline	72.47476	72.424	-0.00070
$C_6H_6N_2O_2$	3-nitroaniline	72.47476	72.481	-0.00009
$C_6H_6N_2O_2$	4-nitroaniline	72.47476	72.476	-0.00002
$C_7H_7NO_2$	aniline-2-carboxylic acid	80.90857	80.941	0.00041
$C_7H_7NO_2$	aniline-3-carboxylic acid	80.90857	80.813	-0.00118
$C_7H_7NO_2$	aniline-4-carboxylic acid	80.90857	80.949	0.00050
C_6H_6O	phenol	61.75817	61.704	-0.00087
$C_6H_4N_2O_5$	2,4-dinitrophenol	77.61308	77.642	0.00037
C_6H_8O	anisole	73.39006	73.355	-0.00047
$C_{10}H_8$	naphthalene	90.74658	90.79143	0.00049
C_4H_5N	pyrrole	44.81090	44.785	-0.00057
C_4H_4O	furan	41.67782	41.692	0.00033
C_4H_4S	thiophene	40.42501	40.430	0.00013
$C_3H_4N_2$	imidazole	39.76343	39.74106	-0.00056
C_5H_5N	pyridine	51.91802	51.87927	-0.00075
$C_4H_4N_2$	pyrimidine	46.57597	46.51794	-0.00125
$C_4H_4N_2$	pyrazine	46.57597	46.51380	0.00095
C_9H_7N	quinoline	85.40453	85.48607	0.00178
C_9H_7N	isoquinoline	85.40453	85.44358	0.00046
C_8H_7N	indole	78.52215	78.514	-0.00010

[a] Liquid.

Table 42. Summary results of DNA bases.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_5H_5N_5$	adenine	70.85416	70.79811	-0.00079
$C_5H_6N_2O_2$	thymine	69.08792	69.06438	-0.00034
$C_5H_5N_5O$	guanine	76.88212	77.41849	-0.00055
$C_4H_5N_3O$	cytosine	59.53378	60.58056	0.01728

Table 43. Summary results of alkyl phosphines.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_9P	trimethylphosphine	45.80930	46.87333	0.02270
$C_6H_{15}P$	triethylphosphine	82.28240	82.24869	-0.00041
$C_{18}H_{15}P$	triphenylphosphine	168.40033	167.46591	-0.00558

Table 44. Summary results of alkyl phosphites.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_3H_9O_3P$	trimethyl phosphite	61.06764	60.94329	-0.00204
$C_6H_{15}O_3P$	triethyl phosphite	98.12406	97.97947	-0.00148
$C_9H_{21}O_3P$	tri-isopropyl phosphite	134.89983	135.00698	0.00079

Table 45. Summary results of alkyl phosphine oxides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_9PO	trimethylphosphine oxide	53.00430	52.91192	-0.00175

Table 46. Summary results of alkyl phosphates.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_6H_{15}O_4P$	triethyl phosphate	105.31906	104.40400	-0.00876
$C_9H_{21}O_4P$	tri-n-propyl phosphate	141.79216	140.86778	-0.00656
$C_9H_{21}O_4P$	tri-isopropyl phosphate	142.09483	141.42283	-0.00475
$C_9H_{27}O_4P$	tri-n-butyl phosphate	178.26526	178.07742	-0.00105

Table 47. Summary results of monosaccharides of DNA and RNA.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_5H_{10}O_4$	2-deoxy-D-ribose	77.25842		
$C_5H_{10}O_5$	D-ribose	81.51034	83.498[a]	0.02381
$C_5H_{10}O_4$	alpha-2-deoxy-D-ribose	77.46684		
$C_5H_{10}O_5$	alpha-D-ribose	82.31088		

[a] Crystal

Table 48. Summary results of amino acids.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_4H_7NO_4$	aspartic acid	68.98109	70.843[a]	0.02628
$C_5H_9NO_4$	glutamic acid	81.13879	83.167[a]	0.02438
$C_3H_7NO_4S$	cysteine	55.02457	56.571[a]	0.02733
$C_6H_{14}N_2O_2$	lysine	95.77799	98.194[a]	0.02461
$C_6H_{14}N_2O_2$	arginine	105.07007	107.420[a]	0.02188
$C_6H_9N_3O_2$	histidine	88.10232	89.599[a]	0.01671
$C_4H_8N_2O_2$	asparagine	71.57414	73.513[a]	0.02637
$C_5H_{10}N_2O_2$	glutamine	83.73184	85.843[a]	0.02459
$C_4H_9NO_3$	threonine	68.95678	71.058[a]	0.02956
$C_9H_{11}NO_3$	tyrosine	109.40427	111.450[a]	0.01835
$C_3H_7NO_3$	serine	56.66986	58.339[a]	0.02861
$C_{11}H_{12}N_2O_2$	tryptophan	126.74291	128.084[a]	0.01047
$C_9H_{11}NO_2$	phenylalanine	104.90618	105.009	0.00098
$C_5H_9NO_2$	proline	71.76826	71.332	-0.00611
$C_5H_9NO_2$	methionine	79.23631	79.214	-0.00028
$C_6H_{13}NO_2$	leucine	89.12115	89.047	-0.00083
$C_6H_{13}NO_2$	isoleucine	89.02978	90.612	0.01746
$C_6H_{13}NO_2$	valine	76.87208	76.772	-0.00130
$C_3H_7NO_2$	alanine	52.57549	52.991	0.00785
$C_2H_5NO_2$	glycine	40.28857	40.280	-0.00021

[a] Crystal

Table 49. Summary results of allotropes of carbon.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_n	diamond	3.74829	3.704	-0.01
C_{60}	fullerene	419.75539	419.73367	-0.00005
C_n	graphite	4.91359	4.89866	-0.00305

Table 50. Summary results of silanes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
SiH	silylidyne	3.07526	3.02008	-0.01827
SiH_2	silylene	6.15052	6.35523	0.03221
SiH_3	silyl	9.22578	9.36494	0.01486
SiH_4	silane	13.57257	13.34577	-0.01699
Si_2H_6	disilane	21.76713	22.05572	0.01308
Si_3H_8	trisilane	31.23322	30.81334	-0.01363

Table 51. Summary results of alkyl silanes and disilanes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_6Si	methylsilane	25.37882	25.99491	0.02370
C_2H_8Si	dimethylsilane	38.45660	38.64819	0.00496
$C_3H_{10}Si$	trimethylsilane	51.53438	51.33567	-0.00387
$C_4H_{12}Si$	tetramethylsilane	64.61216	64.22319	-0.00606
$C_4H_{12}Si$	diethylsilane	62.77200	63.37771	0.00956
$C_6H_{16}Si$	triethylsilane	88.00748	87.46141	-0.00624
$C_8H_{20}Si$	tetraethylsilane	113.24296	112.06547	-0.01051
CH_8Si_2	methyldisilane	34.56739	34.73920	0.00495
$C_2H_{10}Si_2$	1,1-dimethyldisilane	47.36764	47.42283	0.00116
$C_2H_{10}Si_2$	1,2-dimethyldisilane	47.36764	47.42283	0.00116
$C_3H_{12}Si_2$	1,1,1-trimethyldisilane	60.16789	60.10646	-0.00102
$C_3H_{12}Si_2$	1,1,2-trimethyldisilane	60.16789	60.10646	-0.00102
$C_4H_{14}Si_2$	1,1,1,2-tetramethyldisilane	72.96815	72.79442	-0.00239
$C_4H_{14}Si_2$	1,1,2,2-tetramethyldisilane	72.96815	72.79442	-0.00239
$C_5H_{16}Si_2$	1,1,1,2,2-pentamethyldisilane	85.76840	85.47805	-0.00340
$C_6H_{18}Si_2$	hexamethyldisilane	98.56865	98.32646	-0.00246

Table 52. Summary results of silicon oxides, silicic acids, silanols, siloxanes, and disiloxanes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
SiO	silicon oxide	8.30876	8.29905	-0.00117
SiO_2	silicon dioxide	12.94190	12.98073	0.00299
SiH_4O	H_3SiOH	18.67184	19.00701[a]	0.01763
SiH_4O_2	$H_2Si(OH)_2$	25.04264	25.04264 [a]	0.00563
SiH_4O_3	$HSi(OH)_3$	31.41344	31.47012[a]	0.00180
SiH_4O_4	$Si(OH)_4$	37.78423	38.03638	0.00663
$C_3H_{10}SiO$	trimethylsilanol	57.31895	57.30073	-0.00032
C_2H_6SiO	vinylsilanol	37.33784		
CH_6SiO_4	$(HO)_3SiOCH_3$	47.45144	49.28171[a]	0.03714
$C_4H_{12}SiO_4$	tetramethoxysilioxane	83.48783	84.04681	0.00665
$C_6H_{16}SiO_3$	triethoxysilioxane	102.74755	102.57961	-0.00164
$C_8H_{20}SiO_4$	tetraethoxysilioxane	132.89639	133.23177	0.00252
$C_6H_{18}Si_3O_3$	$((CH_3)_2SiO)_3$	123.61510	123.22485	-0.00317
$C_8H_{24}Si_4O_4$	$((CH_3)_2SiO)_4$	164.82014	164.79037	-0.00018
$C_{10}H_{30}Si_5O_5$	$((CH_3)_2SiO)_5$	206.02517	206.35589	0.00160
$C_6H_{18}Si_2O$	hexamethyldisiloxane	105.24639	105.20196	-0.00042

[a] theory

Table 53. Summary results of boranes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
BB	diboron	3.12475	3.10405	-0.00667
B_2H_6	diborane	24.94229	24.89030	-0.00209
B_4H_{10}	tetraborane(10)	44.92160	45.33134	0.00904
B_5H_9	pentaborane(9)	48.25462	48.85411	0.01227
B_5H_{11}	pentaborane(11)	54.00546	53.06086	-0.01780
B_6H_{10}	hexaborane(10)	56.55063	56.74739	0.00347
B_9H_{15}	nonaborane(15)	85.61380	84.95008	-0.00781
$B_{10}H_{14}$	decaborane(14)	89.73467	89.69790	-0.00041

Table 54. Summary results of alkyl boranes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_5B	methylborane	24.60991	24.49350	-0.00475
C_2H_7B	dimethylborane	37.08821	37.17713	0.00239
B_2CH_8	methyldiborane	37.42060	37.58259	0.00431
$B_2C_2H_{10}$	ethyldiborane	49.57830	49.50736	-0.00143
C_3H_9B	trimethylboron	49.56652	49.76102	0.00391
$B_2C_2H_{10}$	1,1-dimethyldiborane	49.89890	50.20118	0.00602
$B_2C_2H_{10}$	1,2-dimethyldiborane	49.89890	50.20118	0.00602
B_4CH_{12}	methyltetraborane	57.39990	57.74604	0.00599
B_5CH_{11}	methylpentaborane	60.73292	61.51585	0.01273
$B_2C_3H_{12}$	trimethyldiborane	62.37721	62.88481	0.00807
$B_4C_2H_{14}$	ethyltetraborane	69.55760	69.99603	0.00626
$B_5C_2H_{13}$	ethylpentaborane	72.89062	73.76585	0.01186
$B_2C_4H_{14}$	1,1-diethyldiborane	74.21430	74.34420	0.00175
$B_2C_4H_{14}$	tetramethyldiborane	74.85551	75.48171	0.00830
$B_5C_3H_{15}$	propylpentaborane	85.04832	85.84239	0.00925
$C_6H_{15}B$	triethylboron	86.03962	86.12941	0.00104
$B_2C_6H_{18}$	triethyldiborane	98.85031	98.59407	-0.00260
$B_{10}CH_{16}$	methyldecaborane	102.21298	101.91775	-0.00290
$C_8H_{17}B$	n-butylboracyclopentane	105.35916	105.69874[a]	0.00321
$B_{10}C_2H_{18}$	ethyldecaborane	114.37068	113.56066	-0.00713
$C_9H_{21}B$	tripropylboron	122.51272	122.59753	0.00069
$C_9H_{21}B$	tri-isopropylboron	122.81539	122.75798	-0.00047
$B_2C_8H_{22}$	tetraethyldiborane	123.48631	123.74017	0.00205
$B_{10}C_3H_{20}$	propyldecaborane	126.52838	125.94075	-0.00467
$C_{12}H_{27}B$	tri-s-butylboron	159.28849	158.50627	-0.00493
$C_{12}H_{27}B$	tributylboron	158.98582	159.03530	0.00031
$C_{12}H_{27}B$	tri-isobutylboron	159.20350	159.34318	0.00088
$C_{18}H_{15}B$	triphenylboron	172.15755	172.09681	-0.00035
$C_{15}H_{33}B$	tri-3-methylbutylboron	195.67660	195.78095	0.00053
$C_{18}H_{33}B$	tricyclohexylboron	217.24711	218.23763	0.00454
$C_{18}H_{39}B$	tri-n-hexylboron	231.93202	231.76340	-0.00073
$C_{21}H_{45}B$	tri-n-heptylboron	268.40512	268.22285	-0.00068
$C_{24}H_{51}B$	tri-s-octylboron	305.18089	304.61292	-0.00186
$C_{24}H_{51}B$	tri-n-octylboron	304.87822	304.68230	-0.00064

[a] Crystal.

Table 55. Summary results of alkoxy boranes and borinic acids.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
BH_3O	hydroxyborane	18.29311	18.22572	-0.00370
BH_3O_2	dihydroxyborane	24.45460	24.43777	-0.00069
BH_3O_3	boric acid	30.61610	30.68431	0.00222
$BC_2H_7O_2$	dimethoxyborane	47.75325	47.72358	-0.00062
$BC_3H_9O_3$	trimethyl borate	65.56408	65.53950	-0.00037
$C_5H_{11}OB$	methoxyboracyclopentane	71.24858	74.47566[a]	0.00345
$C_6H_7O_2B$	phenylborinic acid	77.79659	78.86121[a]	0.01350
$C_6H_{15}O_2B$	di-isoproxyborane	96.97471	97.41737[a]	0.00454
$BC_6H_{15}O_3$	triethyl borate	102.62050	102.50197	-0.00116
$C_8H_{19}OB$	di-n-butylborinic acid	116.19591	116.45117	0.00219
$BC_9H_{21}O_3$	tri-n-propyl borate	139.09360	139.11319	0.00014
$C_{12}H_{27}OB$	n-butyl di-n-butylborinate	164.51278	165.29504[a]	0.00473
$C_{12}H_{27}O_2B$	di-n-butyl n-butylboronate	170.03974	170.86964[a]	0.00486
$BC_{12}H_{27}O_3$	tri-n-butyl borate	175.56670	175.62901	0.00035
$C_{18}H_{15}O_3B_3$	phenylborinic anhydride	204.75082	205.96548[a]	0.00590
$C_{16}H_{36}OB_2$	di-n-butylborinic anhydride	222.84551	223.70232[a]	0.00383
$C_{24}H_{20}OB_2$	diphenylborinic anhydride	240.40782	241.38941[a]	0.00407

[a] Crystal.

Table 56. Summary results of tertiary and quaternary amino boranes and borane amines.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
B_2H_7N	aminodiborane	32.36213	31.99218	-0.01156
$B_2C_2H_{11}N$	n-dimethylaminodiborane	57.21517	57.52855	0.00545
$C_6H_{18}N_3B$	tris(dimethylamino)borane	108.95023	108.64490	-0.00281
$C_8H_{20}NB$	di-n-butylboronamine	117.45425	119.49184 [a]	0.01705
$C_{12}H_{28}NB$	di-n-butylboron-n-butylamine	166.49595	167.83269 [a]	0.00796
$C_2H_{10}NB$	dimethylaminoborane	49.30740	49.52189	0.00433
$BC_3H_{12}N$	trimethylaminoborane	61.37183	61.05205	-0.00524
$BC_3H_{12}N$	ammonia-trimethylborane	62.91857	62.52207	-0.00634
$C_6H_{18}NB$	triethylaminoborane	97.84493	97.42044	-0.00436
$BC_6H_{18}N$	trimethylaminotrimethylborane	98.80674	98.27036	-0.00546

[a] Crystal.

Table 57. Summary results of halidoboranes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
HBF$_2$	difluoroboron	17.55666	17.41845	-0.00793
BF$_3$	boron trifluoride	20.26918	20.09744	-0.00855
BF$_2$HO	difluoroborinic acid	23.71816	23.64784	-0.00297
BFH$_2$O$_2$	fluoroboronic acid	27.16713	27.18135	0.00052
BCH$_3$F$_2$	difluoro-methyl-borane	30.03496	30.33624	0.00993
BC$_2$H$_3$F$_2$	vinyldifluoroborane	36.21893	36.54981	0.00905
BC$_3$H$_9$NF$_3$	trimethylamine-trifluoroborane	69.50941	69.11368	-0.00573
HBCl$_2$	dichloroboron	13.21640	13.25291	0.00276
BCl$_3$	boron trichloride	13.75879	13.80748	0.00353
BCl$_2$F	dichlorofluoroborane	15.92892	15.87507	-0.00339
BClF$_2$	chlorodifluoroborane	18.09905	17.98169	-0.00653
C$_2$H$_5$OCl$_2$B	ethoxydichloroborane	43.37936	43.55732	0.00409
C$_2$H$_4$O$_2$ClB	2-chloro-1,3,2-dioxaborolan	43.68867	43.99361[a]	0.00693
C$_2$H$_6$NCI$_2$B	dimethylaminodichloroborane	45.48927	45.73940	0.00547
BC$_2$ClH$_6$0$_2$	dimethoxychloroborane	48.29565	48.40390	0.00224
C$_3$H$_6$O$_2$ClB	4-methyl-2-chloro-1,3,2-dioxaborolan	55.94726	56.39537[a]	0.00795
BC$_6$H$_5$Cl$_2$	phenylboron dichloride	66.55838	66.97820	0.00627
C$_4$H$_8$O$_2$ClB	4,5-dimethyl-2-chloro-1,3,2-dioxaborolan	68.23418	68.72342[a]	0.00712
C$_4$H$_{10}$O$_2$ClB	diethoxychloroborane	72.99993	73.07735	0.00106
C$_4$H$_{12}$N$_2$ClB	bis(dimethlamino)chloroborane	77.21975	77.38078	0.00208
C$_8$H$_{18}$ClB	di-n-butylchloroborane	110.57681	110.99317	0.00375
C$_{12}$H$_{10}$ClB	diphenylchloroborane	119.35796	119.79335	0.00363

[a] Crystal.

Table 58. Summary results of organoaluminum.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_7Al	dimethylaluminum hydride	34.31171	34.37797[a]	0.00193
C_3H_9Al	trimethyl aluminum	47.10960	46.95319	-0.00333
$C_4H_{11}Al$	diethylaluminum hydride	58.62711	60.10948[b]	0.02466
$C_6H_{15}Al$	triethylaluminum hydride	83.58270	83.58176	-0.00001
$C_6H_{15}Al$	di-n-propylaluminum hydride	82.94251	84.40566[b]	0.01733
$C_9H_{21}Al$	tri-n-propyl aluminum	120.05580	121.06458[b]	0.00833
$C_8H_{19}Al$	di-n-butylaluminum hydride	107.25791	108.71051[b]	0.01336
$C_8H_{19}Al$	di-isobutylaluminum hydride	107.40303	108.77556[b]	0.01262
$C_{12}H_{27}Al$	tri-n-butyl aluminum	156.52890	157.42429[b]	0.00569
$C_{12}H_{27}Al$	tri-isobutyl aluminum	156.74658	157.58908[b]	0.00535

[a] Estimated.
[b] Crystal

Table 59. Summary results of scandium coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
ScF	scandium fluoride	6.34474	6.16925	-0.02845
ScF_2	scandium difluoride	12.11937	12.19556	0.00625
ScF_3	scandium trifluoride	19.28412	19.27994	-0.00022
ScCl	scandium chloride	4.05515	4.00192	-0.01330
ScO	scandium oxide	7.03426	7.08349	0.00695

Table 60. Summary results of titanium coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
TiF	titanium fluoride	6.44997	6.41871	-0.00487
TiF$_2$	titanium difluoride	13.77532	13.66390	-0.00815
TiF$_3$	titanium trifluoride	19.63961	19.64671	0.00036
TiF$_4$	titanium tetrafluoride	24.66085	24.23470	-0.01758
TiCl	titanium chloride	4.56209	4.56198	-0.00003
TiCl$_2$	titanium dichoride	10.02025	9.87408	-0.01517
TiCl$_3$	titanium trichloride	14.28674	14.22984	-0.00400
TiCl$_4$	titanium tetrachloride	17.94949	17.82402	-0.00704
TiBr	titanium bromide	3.77936	3.78466	0.00140
TiBr$_2$	titanium dibromide	8.91650	8.93012	0.00153
TiBr$_3$	titanium tribromide	12.07765	12.02246	-0.00459
TiBr$_4$	titanium tetrabromide	14.90122	14.93239	0.00209
TiI	titanium iodide	3.16446	3.15504	-0.00299
TiI$_2$	titanium diiodide	7.35550	7.29291	-0.00858
TiI$_3$	titanium triiodide	9.74119	9.71935	-0.00225
TiI$_4$	titanium tetraiodide	12.10014	12.14569	0.00375
TiO	titanium oxide	7.02729	7.00341	-0.00341
TiO$_2$	titanium dioxide	13.23528	13.21050	-0.00188
TiOF	titanium fluoride oxide	12.78285	12.77353	-0.00073
TiOF$_2$	titanium difluoride oxide	18.94807	18.66983	-0.01490
TiOCl	titanium chloride oxide	11.10501	11.25669	0.01347
TiOCl$_2$	titanium dichloride oxide	15.59238	15.54295	-0.00318

Table 61. Summary results of vanadium coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
VF$_5$	vanadium pentafluoride	24.06031	24.24139	0.00747
VCl$_4$	vanadium tetrachloride	15.84635	15.80570	-0.00257
VN	vanadium nitride	4.85655	4.81931	-0.00775
VO	vanadium oxide	6.37803	6.60264	0.03402
VO$_2$	vanadium dioxide	12.75606	12.89729	0.01095
VOCl$_3$	vanadium trichloride oxide	18.26279	18.87469	0.03242
V(CO)$_6$	vanadium hexacarbonyl	75.26791	75.63369	0.00484
V(C$_6$H$_6$))$_2$	dibenzene vanadium	119.80633	121.20193[a]	0.01151

[a] Liquid.

Table 62. Summary results of chromium coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CrF_2	chromium difluoride	10.91988	10.92685	0.00064
$CrCl_2$	chromium dichloride	7.98449	7.96513	-0.00243
CrO	chromium oxide	4.73854	4.75515	0.00349
CrO_2	chromium dioxide	10.02583	10.04924	0.00233
CrO_3	chromium trioxide	14.83000	14.85404	0.00162
CrO_2Cl_2	chromium dichloride dioxide	17.46158	17.30608	-0.00899
$Cr(CO)_6$	chromium hexacarbonyl	74.22588	74.61872	0.00526
$Cr(C_6H_6)_2$	dibenzene chromium	117.93345	117.97971	0.00039
$Cr((CH_3)_3C_6H_3)_2$	di-(1,2,4-trimethylbenzene) chromium	191.27849	192.42933[a]	0.00598

[a] Liquid.

Table 63. Summary results of manganese coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
MnF	manganese fluoride	4.03858	3.97567	-0.01582
$MnCl$	manganese chloride	3.74528	3.73801	-0.00194
$Mn_2(CO)_{10}$	dimanganese decacarbonyl	123.78299	122.70895	-0.00875

Table 64. Summary results of iron coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
FeF	iron fluoride	4.65726	4.63464	-0.00488
FeF_2	iron difluoride	10.03188	9.98015	-0.00518
FeF_3	iron trifluoride	15.31508	15.25194	-0.00414
$FeCl$	iron chloride	2.96772	2.97466	0.00233
$FeCl_2$	iron dichoride	8.07880	8.28632	0.02504
$FeCl_3$	iron trichloride	10.82348	10.70065	-0.01148
FeO	iron oxide	4.09983	4.20895	0.02593
$Fe(CO)_5$	iron pentacarbonyl	61.75623	61.91846	0.00262
$Fe(C_5H_5)_2$	bis-cylopentadienyl iron (ferrocene)	98.90760	98.95272	0.00046

Table 65. Summary results of cobalt coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CoF_2	cobalt difluoride	9.45115	9.75552	0.03120
CoCl	cobalt chloride	3.66504	3.68049	0.00420
CoI_2	cobalt dichloride	7.98467	7.92106	-0.00803
$CoCl_3$	cobalt trichloride	9.83521	9.87205	0.00373
$CoH(CO)_4$	cobalt tetracarbonyl hydride	50.33217	50.36087	0.00057

Table 66. Summary results of nickel coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
NiCl	nickel chloride	3.84184	3.82934	-0.00327
$NiCl_2$	nickel dichloride	7.76628	7.74066	-0.00331
$Ni(CO)_4$	nickel tetracarbonyl	50.79297	50.77632	-0.00033
$Ni(C_5H_5)_2$	bis-cylopentadienyl nickel (nickelocene)	97.73062	97.84649	0.00118

Table 67. Summary results of copper coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CuF	copper fluoride	4.39399	4.44620	0.01174
CuF_2	copper difluoride	7.91246	7.89040	-0.00280
CuCl	copper chloride	3.91240	3.80870	-0.02723
CuO	copper oxide	2.93219	2.90931	-0.00787

Table 68. Summary results of zinc coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
ZnCl	zinc chloride	2.56175	2.56529	0.00138
$ZnCl_2$	zinc dichloride	6.68749	6.63675	-0.00764
$Zn(CH_3)_2$	dimethylzinc	29.35815	29.21367	-0.00495
$(CH_3CH_2)_2Zn$	diethylzinc	53.67355	53.00987	-0.01252
$(CH_3CH_2CH_2)_2Zn$	di-n-propylzinc	77.98895	77.67464	-0.00405
$(CH_3CH_2CH_2CH_2)_2Zn$	di-n-butylzinc	102.30435	101.95782	-0.00340

Table 69. Summary results of germanium compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_8H_{20}Ge$	tetraethylgermanium	109.99686	110.18166	0.00168
$C_{12}H_{28}Ge$	tetra-n-propylgermanium	158.62766	158.63092	0.00002
$C_{12}H_{30}Ge_2$	hexaethyldigermanium	167.88982	167.89836	0.00005

Table 70. Summary results of tin compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$SnCl_4$	tin tetrachloride	12.95756	13.03704	0.00610
CH_3Cl_3Sn	methyltin trichloride	24.69530	25.69118[a]	0.03876
$C_2H_6Cl_2Sn$	dimethyltin dichloride	36.43304	37.12369	0.01860
C_3H_9ClSn	trimethylin chloride	48.17077	49.00689	0.01706
$SnBr_4$	tin tetrabromide	10.98655	11.01994	0.00303
C_3H_9BrSn	trimethyltin bromide	47.67802	48.35363	0.01397
$C_{12}H_{10}Br_2Sn$	diphenyltin dibromide	117.17489	117.36647[a]	0.00163
$C_{12}H_{27}BrSn$	tri-n-butyltin bromide	157.09732	157.26555[a]	0.00107
$C_{18}H_{15}BrSn$	triphenyltin bromide	170.26905	169.91511[a]	-0.00208
SnI_4	tin tetraiodide	9.71697	9.73306	0.00165
C_3H_9ISn	trimethyltin iodide	47.36062	47.69852	0.00708
$C_{18}H_{15}SnI$	triphenyltin iodide	169.95165	167.87948[a]	-0.01234
SnO	tin oxide	5.61858	5.54770	-0.01278
SnH_4	stannane	10.54137	10.47181	-0.00664
C_2H_8Sn	dimethylstannane	35.22494	35.14201	-0.00236
$C_3H_{10}Sn$	trimethylstannane	47.56673	47.77353	0.00433
$C_4H_{12}Sn$	diethylstannane	59.54034	59.50337	-0.00062
$C_4H_{12}Sn$	tetramethyltin	59.90851	60.13973	0.00384
$C_5H_{12}Sn$	trimethylvinyltin	66.08296	66.43260	0.00526
$C_5H_{14}Sn$	trimethylethyltin	72.06621	72.19922	0.00184
$C_6H_{16}Sn$	trimethylisopropyltin	84.32480	84.32346	-0.00002
$C_8H_{12}Sn$	tetravinyltin	84.64438	86.53803[a]	0.02188
$C_6H_{18}Sn_2$	hexamethyldistannane	91.96311	91.75569	-0.00226
$C_7H_{18}Sn$	trimethyl-t-butyltin	96.81417	96.47805	-0.00348
$C_9H_{14}Sn$	trimethylphenyltin	100.77219	100.42716	-0.00344
$C_8H_{18}Sn$	triethylvinyltin	102.56558	102.83906[a]	-0.00266
$C_8H_{20}Sn$	tetraethyltin	108.53931	108.43751	-0.00094
$C_{10}H_{16}Sn$	trimethylbenzyltin	112.23920	112.61211	0.00331
$C_{10}H_{14}O_2Sn$	trimethyltin benzoate	117.28149	119.31199[a]	0.01702
$C_{10}H_{20}Sn$	tetra-allyltin	133.53558	139.20655[a]	0.04074
$C_{12}H_{28}Sn$	tetra-n-propyltin	157.17011	157.01253	-0.00100
$C_{12}H_{28}Sn$	tetraisopropyltin	157.57367	156.9952	-0.00366
$C_{12}H_{30}Sn_2$	hexaethyldistannane	164.90931	164.76131[a]	-0.00090
$C_{19}H_{18}Sn$	triphenylmethyltin	182.49954	180.97881[a]	-0.00840
$C_{20}H_{20}Sn$	triphenylethyltin	194.65724	192.92526[a]	-0.00898
$C_{16}H_{36}Sn$	tetra-n-butyltin	205.80091	205.60055	-0.00097
$C_{16}H_{36}Sn$	tetraisobutyltin	206.09115	206.73234	0.00310
$C_{21}H_{24}Sn_2$	triphenyl-trimethyldistannane	214.55414	212.72973[a]	-0.00858
$C_{24}H_{20}Sn$	tetraphenyltin	223.36322	221.61425	-0.00789
$C_{24}H_{44}Sn$	tetracyclohexyltin	283.70927	284.57603	0.00305
$C_{36}H_{30}Sn_2$	hexaphenyldistannane	337.14517	333.27041	-0.01163

[a] Crystal.

Table 71. Summary results of lead compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_4H_{12}Pb$	tetramethyl-lead	57.55366	57.43264	-0.00211
$C_8H_{20}Pb$	tetraethyl-lead	106.18446	105.49164	-0.00657

Table 72. Summary results of alkyl arsines.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_9As	trimethylarsine	44.73978	45.63114	0.01953
$C_6H_{15}As$	triethylarsine	81.21288	81.01084	-0.00249
$C_{18}H_{15}As$	triphenylarsine	167.33081	166.49257	-0.00503

Table 73. Summary results of alkyl stibines.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_9Sb	trimethylstibine	44.73078	45.02378	0.00651
$C_6H_{15}Sb$	triethylstibine	81.20388	80.69402	-0.00632
$C_{18}H_{15}Sb$	triphenylstibine	167.32181	165.81583	-0.00908

Table 74. Summary results of alkyl bismuths.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_9Bi	trimethylbismuth	42.07387	42.79068	0.01675
$C_6H_{15}Bi$	triethylbismuth	78.54697	78.39153	-0.00198
$C_{18}H_{15}Bi$	triphenylbismuth	164.66490	163.75184	-0.00558

Table 75. The results (in eV) of Millsian 1.0, the results with 3-21G and 6-31G* basis sets generated from a pre-computed Spartan database, and the experimental values.

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
Acid Anhydrides											
Acetic Anhydride	56.9481	62.1278	9.1%	37.2288	-34.6%	4.3505	-92.4%	41.0447	-27.9%	56.9409	-0.01%
Propanoic Anhydride	81.4007	63.9229	-21.5%	56.1520	-31.0%	5.4793	-93.4%	60.5175	-25.7%	81.2563	-0.18%
Acid Halides											
Acetyl Chloride	27.9897	130.8487	367.5%	20.5457	-26.6%	50.8018	81.4%	19.8545	-29.1%	28.0217	0.11%
Alcohols											
1-Butanol	57.7361	18.0161	-68.8%	42.8966	-25.7%	16.9111	-70.7%	44.8972	-22.2%	57.7210	-0.03%
1-Decanol	130.6761	23.7172	-81.9%	99.1702	-24.1%	46.4250	-64.5%	103.1056	-21.1%	130.6670	-0.01%
1-Dodecanol	154.9836	25.5514	-83.5%	117.9542	-23.9%	56.3020	-63.7%	122.5255	-20.9%	154.9830	0.00%
1-Heptanol	94.2139	20.8614	-77.9%	71.0522	-24.6%	31.6673	-66.4%	74.0006	-21.5%	94.1941	-0.02%
1-Hexadecanol	203.6027	29.3631	-85.6%	155.4789	-23.6%	75.9560	-62.7%	161.3382	-20.8%	203.6130	0.01%
1-Hexanol	82.0540	19.9117	-75.7%	61.6592	-24.9%	26.7490	-67.4%	64.3181	-21.6%	82.0364	-0.02%
1-Nonanol	118.5214	22.7347	-80.8%	89.8071	-24.2%	41.5365	-65.0%	93.4228	-21.2%	118.5090	-0.01%
1-Octanol	106.3583	21.8289	-79.5%	80.4402	-24.4%	36.5475	-65.6%	83.7123	-21.3%	106.3520	-0.01%
1-Pentanol	69.8868	18.9619	-72.9%	52.2935	-25.2%	21.8312	-68.8%	54.6088	-21.9%	69.8787	-0.01%
1-Propanol	45.5845	17.0550	-62.6%	33.5321	-26.4%	12.0056	-73.7%	35.2174	-22.7%	45.5633	-0.05%
2-Butanol	57.9216	17.8139	-69.2%	43.0987	-25.6%	17.0482	-70.6%	45.0343	-22.2%	57.8785	-0.07%
2-Ethyl-1-hexanol	106.4588	21.8545	-79.5%	80.4146	-24.5%	36.4125	-65.8%	83.5773	-21.5%	106.4240	-0.03%
2-Hexanol	82.2364	19.7086	-76.0%	61.8623	-24.8%	26.8836	-67.3%	64.4527	-21.6%	82.1939	-0.05%
2-Methyl-1-butanol	69.9572	18.8745	-73.0%	52.3809	-25.1%	21.7981	-68.8%	54.5757	-22.0%	69.9513	-0.01%
2-Methyl-1-propanol	57.8284	17.9029	-69.0%	43.0098	-25.6%	16.9336	-70.8%	44.9197	-22.3%	57.7936	-0.06%
2-Methyl-2-butanol	70.2464	18.6290	-73.5%	52.6263	-25.1%	22.0035	-68.6%	54.7811	-22.0%	70.3112	0.09%
2-Methyl-2-Propanol	58.1258	17.7016	-69.5%	43.2111	-25.7%	17.1331	-70.5%	45.1193	-22.4%	58.1535	0.05%
2-Pentanol	70.0567	18.7609	-73.2%	52.4945	-25.1%	21.9647	-68.7%	54.7423	-21.9%	70.0362	-0.03%
2-Propanol	45.7658	16.8987	-63.1%	33.6884	-26.4%	12.1401	-73.5%	35.3519	-22.8%	45.7209	-0.10%
3-Methyl-2-butanol	70.0826	18.7263	-73.3%	52.5291	-25.0%	21.9118	-68.9%	54.6894	-22.0%	69.9608	-0.17%
3-Pentanol	69.9796	18.7314	-73.2%	52.5240	-24.9%	21.9500	-68.6%	54.7276	-21.8%	69.9796	0.00%
Ethanol	33.4276	16.1205	-51.8%	24.1239	-27.8%	7.0850	-78.9%	25.5053	-23.7%	33.4056	-0.07%
Methanol	21.1309	15.3306	-27.4%	14.5711	-31.0%	2.0134	-90.6%	15.6423	-26.0%	21.1104	-0.10%
Aldehydes											
2-Ethylhexanal	101.2592	26.3268	-74.0%	75.7638	-25.2%	32.1677	-68.2%	79.2629	-21.7%	101.2340	-0.02%
Ethanal	28.1980	20.7163	-26.5%	19.3424	-31.4%	2.7065	-90.4%	21.0500	-25.3%	28.1871	-0.04%
Butanal	52.4910	22.5260	-57.1%	38.2010	-27.2%	12.5748	-76.0%	40.5113	-22.8%	52.5025	0.02%
Formaldehyde	15.6550	20.1562	28.8%	9.5870	-38.8%	2.6182	-83.3%	10.9611	-30.0%	15.6463	-0.06%
Heptanal	88.9420	25.3662	-71.5%	66.3617	-25.4%	27.3318	-69.2%	69.6155	-21.7%	88.9756	0.04%
Isobutanal	52.6039	22.4584	-57.3%	38.2686	-27.3%	12.5785	-76.1%	40.5150	-23.0%	52.6034	0.00%
Octanal	101.1790	26.3354	-74.0%	75.7553	-25.1%	32.2346	-68.2%	79.3298	-21.6%	101.1330	-0.05%
Pentanal	64.6820	23.4735	-63.7%	47.5962	-26.4%	17.4936	-73.0%	50.1943	-22.4%	64.6602	-0.03%

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
Propanal	40.3450	21.5720	-46.5%	28.8295	-28.5%	7.6678	-81.0%	30.8028	-23.7%	40.3448	0.00%
Alkanes (Branched)											
2,2,3,3-Tetramethylbutane	102.4326	3.4929	-96.6%	79.3458	-22.5%	43.2442	-57.8%	81.5912	-20.3%	102.4160	-0.02%
2,2,3,3-Tetramethylpentane	114.4941	4.5551	-96.0%	88.5990	-22.6%	48.0214	-58.0%	91.1598	-20.4%	114.5740	0.07%
2,2,3,4-Tetramethylpentane	114.4920	4.5568	-96.0%	88.5974	-22.6%	48.0849	-58.0%	91.2234	-20.3%	114.5200	0.02%
2,2,3-Trimethylbutane	90.2623	2.4223	-97.3%	70.0636	-22.4%	38.5475	-57.3%	72.0931	-20.1%	90.2229	-0.04%
2,2,3-Trimethylpentane	102.3704	3.4359	-96.6%	79.4027	-22.4%	43.3804	-57.6%	81.7274	-20.2%	102.3810	0.01%
2,2,4,4-Tetramethylpentane	114.5407	4.4871	-96.1%	88.6671	-22.6%	48.1654	-57.9%	91.3039	-20.3%	114.5730	0.03%
2,2,4-Trimethylpentane	102.4119	3.3749	-96.7%	79.4638	-22.4%	43.4677	-57.6%	81.8148	-20.1%	102.4090	0.00%
2,2-Dimethylbutane	78.1241	1.3714	-98.2%	60.7990	-22.2%	33.7872	-56.8%	62.5684	-19.9%	78.0210	-0.13%
2,2-Dimethylhexane	102.4171	3.2878	-96.8%	79.5509	-22.3%	43.6073	-57.5%	81.9543	-20.0%	102.3360	-0.08%
2,2-Dimethylpentane	90.2758	2.3249	-97.4%	70.1610	-22.3%	38.6957	-57.2%	72.2413	-20.0%	90.1787	-0.11%
2,3,3,4-Tetramethylpentane	114.4837	4.5717	-96.0%	88.5824	-22.6%	48.0428	-58.0%	91.1813	-20.4%	114.5830	0.09%
2,3,3-Trimethylpentane	102.3321	3.4683	-96.6%	79.3704	-22.4%	43.3457	-57.6%	81.6928	-20.2%	102.3810	0.05%
2,3,4-Trimethylpentane	102.3424	3.4656	-96.6%	79.3731	-22.4%	43.3944	-57.6%	81.7414	-20.1%	102.2920	-0.05%
2,3,5-Trimethylhexane	114.5511	4.3467	-96.2%	88.8074	-22.5%	48.3834	-57.8%	91.5219	-20.1%	114.5410	-0.01%
2,3-Dimethylbutane	78.0433	1.4478	-98.1%	60.7226	-22.2%	33.7473	-56.8%	62.5286	-19.9%	77.9958	-0.06%
2,3-Dimethylhexane	102.3062	3.4115	-96.7%	79.4272	-22.4%	43.5053	-57.5%	81.8523	-20.0%	102.3110	0.00%
2,4-Dimethylhexane	102.3621	3.3544	-96.7%	79.4842	-22.3%	43.5581	-57.4%	81.9051	-20.0%	102.4030	0.04%
2,4-Dimethylpentane	90.2333	2.3495	-97.4%	70.1364	-22.3%	38.7135	-57.1%	72.2591	-19.9%	90.2448	0.01%
2,5-Dimethylhexane	102.3963	3.3074	-96.8%	79.5312	-22.3%	43.6267	-57.4%	81.9738	-19.9%	102.4030	0.01%
2-Methylheptane	102.3217	3.3141	-96.8%	79.5246	-22.3%	43.6639	-57.3%	82.0110	-19.8%	102.3300	0.01%
2-Methylhexane	90.1597	2.3562	-97.4%	70.1297	-22.2%	38.7555	-57.0%	72.3010	-19.8%	90.1723	0.01%
2-Methylnonane	126.6800	5.2099	-95.9%	98.2869	-22.4%	53.5009	-57.8%	101.4037	-20.0%	126.6450	-0.03%
2-Methylpentane	78.0070	1.4085	-98.2%	60.7619	-22.1%	33.8369	-56.6%	62.6182	-19.7%	78.0146	0.01%
3,3-Diethylpentane	114.4547	4.5227	-96.0%	88.6314	-22.6%	48.1812	-57.9%	91.3197	-20.2%	114.4940	0.03%
3,3-Dimethylhexane	102.3694	3.3681	-96.7%	79.4706	-22.4%	43.5026	-57.5%	81.8496	-20.0%	102.3360	-0.03%
3,3-Dimethylpentane	90.2270	2.4068	-97.3%	70.0791	-22.3%	38.5998	-57.2%	72.1454	-20.0%	90.1787	-0.05%
3,4-Dimethylhexane	102.2958	3.4599	-96.6%	79.3787	-22.4%	43.4429	-57.5%	81.7899	-20.0%	102.3110	0.01%
3-Ethyl-2-methylpentane	102.2771	3.4664	-96.6%	79.3722	-22.4%	43.4297	-57.5%	81.7767	-20.0%	102.3110	0.03%
3-Ethyl-3-methylpentane	102.3165	3.4686	-96.6%	79.3701	-22.4%	43.3886	-57.6%	81.7356	-20.1%	102.3360	0.02%
3-Ethylhexane	102.2740	3.4537	-96.6%	79.3850	-22.4%	43.5109	-57.4%	81.8579	-20.0%	102.3300	0.05%
3-Ethylpentane	90.1079	2.4848	-97.2%	70.0011	-22.3%	38.6095	-57.1%	72.1551	-19.9%	90.1723	0.07%
3-Methylheptane	102.2927	3.3953	-96.7%	79.4433	-22.3%	43.5713	-57.4%	81.9183	-19.9%	102.3300	0.04%
3-Methylhexane	90.1265	2.4377	-97.3%	70.0482	-22.3%	38.6627	-57.1%	72.2083	-19.9%	90.1723	0.05%
3-Methylpentane	77.9790	1.4558	-98.1%	60.7146	-22.1%	33.7795	-56.7%	62.5607	-19.8%	78.0146	0.05%
4-Methylheptane	102.2865	3.3978	-96.7%	79.4408	-22.3%	43.5669	-57.4%	81.9139	-19.9%	102.3300	0.04%
5-Methylnonane	126.6634	5.2931	-95.8%	98.2038	-22.5%	53.4041	-57.8%	101.3068	-20.0%	126.6450	-0.01%
Isobutane	53.6954	0.5284	-99.0%	42.0405	-21.7%	24.0536	-55.2%	43.2519	-19.4%	53.6992	0.01%
Methylbutane	65.8429	0.3316	-99.5%	51.4961	-21.8%	28.9227	-56.1%	52.9125	-19.6%	65.8569	0.02%
Dimethylpropane	65.9921	0.4585	-99.3%	51.3692	-22.2%	28.9766	-56.2%	52.9664	-19.7%	65.8633	-0.20%

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
Alkanes (Straight Chain)											
Butane	53.6073	0.4744	-99.1%	41.9866	-21.7%	24.0368	-55.1%	43.2351	-19.3%	53.6266	0.04%
Decane	126.5691	5.2224	-95.9%	98.2745	-22.4%	53.5402	-57.7%	101.4429	-19.9%	126.5730	0.00%
Dodecane	150.8755	7.0779	-95.3%	117.0372	-22.4%	63.4172	-58.0%	120.8629	-19.9%	150.8880	0.01%
Ethane	29.2822	2.3732	-91.9%	23.2090	-20.7%	14.2050	-51.4%	23.8349	-18.6%	29.3112	0.10%
Heptane	90.0882	2.3742	-97.4%	70.1117	-22.2%	38.7904	-56.9%	72.3360	-19.7%	90.0997	0.01%
Hexane	77.9272	1.4236	-98.2%	60.7468	-22.0%	33.8723	-56.5%	62.6536	-19.6%	77.9420	0.02%
Nonane	114.4019	4.2742	-96.3%	88.8800	-22.3%	48.6217	-57.5%	91.7602	-19.8%	114.4150	0.01%
Octadecane	223.8518	12.8455	-94.3%	173.3243	-22.6%	92.8481	-58.5%	179.0682	-20.0%	223.8350	-0.01%
Octane	102.2512	3.3268	-96.7%	79.5118	-22.2%	43.7018	-57.3%	82.0489	-19.8%	102.2570	0.01%
Pentane	65.7734	0.4744	-99.3%	51.3533	-21.9%	28.9550	-56.0%	52.9448	-19.5%	65.7843	0.02%
Propane	41.4339	1.4194	-96.6%	32.5888	-21.3%	19.1171	-53.8%	33.5512	-19.0%	41.4689	0.08%
Undecane	138.7363	6.2000	-95.5%	107.6696	-22.4%	58.4287	-57.9%	111.1529	-19.9%	138.7310	0.00%
Alkene Halides											
2-Chloropropene	35.0548	114.2854	226.0%	28.0640	-19.9%	40.1160	14.4%	26.5568	-24.2%	35.0298	-0.07%
Chloroethene	22.5052	113.3698	403.7%	18.6341	-17.2%	45.0677	100.4%	16.8109	-25.3%	22.4670	-0.17%
Alkenes											
1-Butene	47.7848	4.7041	-90.2%	36.6224	-23.4%	18.7744	-60.8%	37.9231	-20.6%	47.7180	-0.14%
1-Decene	120.7424	10.3763	-91.4%	92.9149	-23.0%	48.3007	-60.0%	96.1339	-20.4%	120.6640	-0.06%
1-Dodecene	145.0716	12.3321	-91.5%	111.6773	-23.0%	58.0777	-60.0%	115.5266	-20.4%	144.9800	-0.06%
1-Heptene	84.2708	7.5426	-91.0%	64.7849	-23.1%	33.5351	-60.3%	67.0310	-20.5%	84.1911	-0.09%
1-Hexadecene	193.7177	16.0438	-91.7%	149.2021	-23.0%	77.8317	-59.9%	154.3393	-20.3%	193.6100	-0.06%
1-Hexene	72.1295	6.5949	-90.9%	55.3898	-23.2%	28.6163	-60.4%	57.3208	-20.5%	72.0334	-0.13%
1-Octene	96.4142	8.5004	-91.2%	74.1525	-23.1%	38.4437	-60.2%	76.7138	-20.4%	96.3488	-0.07%
1-Pentene	59.9509	5.6470	-90.6%	46.0222	-23.2%	23.6976	-60.5%	47.6105	-20.6%	59.8757	-0.13%
2,3,3-Trimethyl-1-butene	84.5113	7.4935	-91.1%	64.8339	-23.3%	33.4409	-60.4%	66.9368	-20.8%	84.5127	0.00%
2,3-Dimethyl-1-butene	72.3254	6.5172	-91.0%	55.4675	-23.3%	28.6498	-60.4%	57.3543	-20.7%	72.3194	-0.01%
2,3-Dimethyl-2-butene	72.3845	6.5754	-90.9%	55.4093	-23.5%	28.6535	-60.3%	57.3579	-20.8%	72.4974	0.16%
2,4,4-Trimethyl-1-pentene	96.7168	8.4182	-91.3%	74.2347	-23.2%	38.3856	-60.4%	76.6558	-20.7%	96.6129	-0.11%
2,4,4-Trimethyl-2-pentene	96.6588	8.4963	-91.2%	74.1567	-23.3%	38.3444	-60.3%	76.6146	-20.7%	96.6758	0.02%
2,4-Dimethyl-1-Pentene	84.4937	7.4162	-91.2%	64.9112	-23.2%	33.6065	-60.3%	67.1024	-20.6%	84.4488	-0.05%
2,4-Dimethyl-2-pentene	84.5445	7.3884	-91.3%	64.9390	-23.2%	33.6626	-60.1%	67.1586	-20.6%	84.6306	0.10%
2-Ethyl-1-butene	72.2591	6.5167	-91.0%	55.4680	-23.2%	28.6938	-60.3%	57.3982	-20.6%	72.2185	-0.06%
2-Ethyl-3-methyl-1-butene	84.4491	7.4992	-91.1%	64.8282	-23.2%	33.5017	-60.3%	66.9976	-20.7%	84.4771	0.03%
2-Methyl-1-butene	60.0971	5.5722	-90.7%	46.0970	-23.3%	23.7738	-60.5%	47.6867	-20.7%	60.0608	-0.06%
2-Methyl-1-pentene	72.2943	6.5167	-91.0%	55.4680	-23.3%	28.6938	-60.4%	57.3982	-20.6%	72.2185	-0.10%
2-Methyl-2-butene	60.1644	5.5536	-90.8%	46.1156	-23.4%	23.8264	-60.3%	47.7394	-20.7%	60.2143	0.08%
2-Methyl-2-pentene	72.3721	6.4960	-91.0%	55.4887	-23.3%	28.7403	-60.3%	57.4447	-20.6%	72.3720	0.00%
3,3-Dimethyl-1-butene	72.3037	6.5111	-91.0%	55.4736	-23.3%	28.5681	-60.5%	57.2725	-20.8%	72.3179	0.02%
3-Ethyl-2-methyl-1-pentene	96.6111	8.4298	-91.3%	74.2231	-23.2%	38.4339	-60.2%	76.7041	-20.6%	96.6348	0.02%

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
3-Methyl-1-butene	60.0173	5.5963	-90.7%	46.0729	-23.2%	23.7023	-60.5%	47.6153	-20.7%	59.9766	-0.07%
3-Methyl-1-pentene	72.1917	6.5422	-90.9%	55.4425	-23.2%	28.6034	-60.4%	57.3078	-20.6%	72.1343	-0.08%
3-Methyl-trans-2-pentene	72.3327	6.5206	-91.0%	55.4641	-23.3%	28.7009	-60.3%	57.4053	-20.6%	72.3720	0.05%
4,4-Dimethyl-1-Pentene	84.4709	7.4524	-91.2%	64.8750	-23.2%	33.4800	-60.5%	66.9759	-20.7%	84.2701	-0.24%
4-Methyl-1-pentene	72.2104	6.5436	-90.9%	55.4411	-23.2%	28.6112	-60.5%	57.3156	-20.6%	72.1060	-0.14%
4-Methyl-trans-2-pentene	72.3161	6.5283	-91.0%	55.4564	-23.3%	28.6553	-60.3%	57.3597	-20.7%	72.3474	0.04%
5-Methyl-1-hexene	84.3061	7.5303	-91.1%	64.7972	-23.1%	33.4944	-60.3%	66.9903	-20.5%	84.2637	-0.05%
Ethylene	23.3498	2.9090	-87.5%	17.7520	-24.0%	8.8120	-62.4%	18.3786	-21.3%	23.2829	-0.29%
Isobutene	47.9610	4.5994	-90.4%	36.7271	-23.4%	18.8984	-60.7%	38.0471	-20.7%	47.9031	-0.12%
Propylene	35.6321	3.6906	-89.6%	27.3204	-23.3%	13.9280	-61.0%	28.2852	-20.6%	35.5603	-0.20%
trans-2,2-Dimethyl-3-hexene	96.6878	8.5610	-91.1%	74.0920	-23.4%	38.2670	-60.4%	76.5372	-20.8%	96.6984	0.01%
trans-2-Butene	47.9040	4.6874	-90.2%	36.6391	-23.5%	18.8206	-60.7%	37.9693	-20.7%	47.9311	0.06%
trans-2-Hexene	72.2373	6.5741	-90.9%	55.4106	-23.3%	28.6573	-60.3%	57.3618	-20.6%	72.2465	0.01%
trans-2-Pentene	60.0629	5.6321	-90.6%	46.0371	-23.4%	23.7340	-60.5%	47.6470	-20.7%	60.0888	0.04%
trans-3-Hexene (cis)	72.2425	6.5858	-90.9%	55.3989	-23.3%	28.6344	-60.4%	57.3388	-20.6%	72.2465	0.01%
trans-3-Methyl-3-hexene	84.4211	7.4716	-91.1%	64.8558	-23.2%	33.6127	-60.1%	67.1086	-20.5%	84.5297	0.13%
trans-4,4-Dimethyl-2-pentene	84.5455	7.6158	-91.0%	64.7116	-23.5%	33.3600	-60.5%	66.8559	-20.9%	84.5407	-0.01%
Alkenes (Cyclic & Conjugated)											
1,3-Butadiene	42.1270	9.7379	-76.9%	31.4301	-25.4%	13.6692	-67.6%	32.7411	-22.3%	42.0916	-0.08%
1,3-Pentadiene	54.4248	10.5829	-80.6%	40.9006	-24.8%	18.7166	-65.6%	42.5799	-21.8%	54.4077	-0.03%
1,4-Pentadiene	54.1181	10.8333	-80.0%	40.6502	-24.9%	18.4263	-66.0%	42.2897	-21.9%	54.0375	-0.15%
Alkynes											
1-Butyne	41.5549	10.1367	-75.6%	31.0313	-25.3%	13.1086	-68.4%	32.1804	-22.6%	41.5870	0.08%
1-Nonyne	102.3537	14.8764	-85.5%	77.9336	-23.9%	37.7048	-63.1%	80.7168	-21.1%	102.3750	0.02%
2-Butyne	41.7570	9.8951	-76.3%	31.2729	-25.1%	13.3870	-68.0%	32.4588	-22.3%	41.7276	-0.07%
Acetylene	17.0174	8.5194	-49.9%	11.9668	-29.7%	2.9603	-82.3%	12.4610	-26.8%	17.0848	0.40%
Propyne	29.4043	9.1963	-68.7%	21.6289	-26.4%	8.1899	-72.1%	22.4702	-23.6%	29.4293	0.08%
Aluminum (Alkyl)											
Di-isobutylaluminum hydride	108.7756	57.9771	-46.7%	84.0203	-22.8%	23.0542	-79.8%	84.9770	-21.9%	107.4030	-1.26%
Di-n-butylaluminum hydride	108.7105	58.0399	-46.6%	83.9575	-22.8%	23.0568	-79.9%	84.9796	-21.8%	107.2580	-1.34%
Di-n-propylaluminum hydride	84.4057	56.2451	-33.4%	65.1323	-22.8%	13.1138	-86.0%	65.4936	-22.4%	82.9425	-1.73%
Diethylaluminum hydride	60.1095	54.2871	-9.7%	46.3703	-22.9%	3.3935	-96.7%	46.1576	-23.2%	58.6271	-2.47%
Tri-n-butylaluminum hydride	157.5891	61.4845	-61.0%	121.8530	-22.7%	42.8355	-73.3%	123.9170	-21.4%	156.5290	-0.67%
Tri-n-propylaluminum hydride	121.0646	58.6567	-51.5%	93.7008	-22.6%	28.0423	-77.5%	94.7865	-21.7%	120.0560	-0.83%
Triethylaluminum hydride	83.5818	55.8994	-33.1%	65.4780	-21.7%	13.2587	-84.1%	65.6386	-21.5%	83.5826	0.00%
Trimethylaluminum hydride	46.9532	52.5282	11.9%	37.8392	-19.4%	0.9576	-97.6%	37.0550	-21.1%	47.1096	0.33%

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
Amides											
2,2-Dimethylpropanamide	72.7180	32.9962	-54.6%	51.9839	-28.5%	15.9102	-78.2%	54.8747	-24.5%	72.6792	-0.05%
2-Methylpropanamide	60.4555	32.1104	-46.9%	42.5541	-29.6%	11.0779	-81.6%	45.2510	-25.1%	60.5151	0.10%
Acetamide	36.1035	30.3860	-15.8%	23.6203	-34.6%	N/A	N/A	N/A	N/A	36.1522	0.14%
Butanamide	60.4493	32.1665	-46.8%	42.4980	-29.7%	11.0784	-81.6%	45.2515	-25.1%	60.4676	0.03%
Formamide	23.6968	29.7290	25.5%	13.9345	-41.2%	N/A	N/A	N/A	N/A	23.6871	-0.04%
Hexanamide	84.7795	34.0741	-59.8%	61.2587	-27.7%	20.9092	-75.3%	64.6480	-23.7%	84.7830	0.00%
N,N-Dimethylacetamide	59.8896	32.6470	-45.5%	42.0175	-29.8%	N/A	N/A	N/A	N/A	60.1445	0.43%
N,N-Dimethylformamide	47.5742	31.8634	-33.0%	32.4584	-31.8%	N/A	N/A	N/A	N/A	47.6795	-0.22%
N-Butylacetamide	84.5899	34.1695	-59.6%	61.1633	-27.7%	20.8343	-75.3%	64.5731	-23.7%	84.6365	0.06%
Octanamide	109.0715	35.9309	-67.1%	80.0301	-26.6%	30.7764	-71.8%	84.0682	-22.9%	109.0980	0.02%
Pentanamide	72.4807	33.1143	-54.3%	51.8658	-28.4%	15.9962	-77.8%	54.9608	-24.2%	72.6253	0.20%
Propanamide	48.2644	31.2241	-35.3%	33.0977	-31.4%	6.1611	-87.2%	35.5427	-26.4%	48.3099	0.09%
Amines											
Butylamine	60.4152	10.5351	-82.6%	44.8874	-25.7%	21.4343	-64.6%	46.8964	-22.4%	60.3561	-0.10%
Dibutylamine	108.8716	14.4354	-86.7%	82.3137	-24.4%	41.0091	-62.3%	85.5928	-21.4%	108.8600	-0.01%
Diethylamine	60.2111	10.6627	-82.3%	44.7699	-25.6%	21.3364	-64.5%	46.8085	-22.3%	60.2293	0.03%
Diisobutylamine	109.1058	14.2636	-86.9%	82.4854	-24.4%	41.0161	-62.5%	85.5997	-21.5%	109.0050	-0.09%
Diisopropylamine	84.8460	12.4192	-85.4%	63.6716	-25.0%	31.1855	-63.3%	66.2134	-22.0%	84.7464	-0.12%
Dimethylamine	35.7647	8.8915	-75.1%	25.8728	-27.7%	11.3549	-68.2%	27.2341	-23.9%	35.7689	0.01%
Dipropylamine	84.5579	12.5439	-85.2%	63.5469	-24.8%	31.1759	-63.1%	66.2038	-21.7%	84.5447	-0.02%
Ethylamine	36.0622	8.6358	-76.1%	26.1285	-27.5%	11.5982	-67.9%	27.4774	-23.8%	36.0407	-0.06%
Isobutylamine	60.4857	10.4417	-82.7%	44.9809	-25.6%	21.4409	-64.6%	46.9030	-22.5%	60.4286	-0.09%
Methylamine	23.8566	7.7803	-67.4%	16.6549	-30.2%	6.5916	-72.3%	17.6929	-25.8%	23.8830	0.11%
Propylamine	48.2428	9.5840	-80.1%	35.5230	-26.4%	16.5181	-65.8%	37.1888	-22.9%	48.1984	-0.09%
sec-Butylamine	60.5469	10.4509	-82.7%	44.9717	-25.7%	21.4883	-64.6%	46.9504	-22.5%	60.4569	-0.15%
t-Butylamine	60.7168	10.3024	-83.0%	45.1201	-25.7%	21.5589	-64.4%	47.0210	-22.6%	60.7886	0.12%
Triethylamine	84.3164	12.8192	-84.8%	63.2716	-25.0%	30.8642	-63.4%	65.8921	-21.9%	84.3064	-0.01%
Trimethylamine	47.7609	9.9560	-79.2%	35.1511	-26.4%	16.1571	-66.1%	36.8278	-22.9%	47.8334	0.15%
Tripropylamine	120.8636	15.6323	-87.1%	91.4895	-24.3%	45.6011	-62.3%	95.0062	-21.4%	120.7800	-0.07%
Amino Acids											
Alanine	52.9910	49.4457	-6.7%	34.3037	-35.3%	0.5808	-99.7%	37.6158	-29.0%	52.5755	-0.78%
Arginine	107.4200	88.3093	-17.8%	67.9838	-36.7%	2.8453	-99.5%	74.0192	-31.1%	105.0700	-2.19%
Asparagine	73.5130	82.8495	12.7%	44.3479	-39.7%	8.4619	-90.9%	49.4538	-32.7%	71.5741	-2.64%
Aspartic Acid	70.8430	90.3945	27.6%	42.3230	-40.3%	12.8407	-84.1%	47.6561	-32.7%	68.9811	-2.63%
Cysteine	56.5710	N/A	N/A	N/A	N/A	43.1131	-24.5%	38.4481	-32.0%	55.0246	-2.73%
Glutamic Acid	83.1670	91.2410	9.7%	51.8491	-37.7%	7.9160	-92.7%	57.4023	-31.0%	81.1388	-2.44%
Glutamine	85.8430	83.6503	-2.6%	53.9198	-37.2%	3.4694	-98.4%	59.2677	-31.0%	83.7318	-2.46%
Glycine	40.2800	48.5934	20.6%	24.8034	-38.4%	5.5007	-86.3%	27.8944	-30.7%	40.2886	0.02%
Histidine	89.5990	87.1120	-2.8%	54.9541	-38.7%	4.0173	-97.1%	60.8280	-32.1%	88.1023	-1.67%
Isoleucine	90.6120	52.1983	-42.4%	62.5349	-31.0%	14.1414	-85.9%	66.6953	-26.4%	89.0297	-1.75%
Leucine	89.0470	52.1702	-41.4%	62.5630	-29.7%	14.2063	-84.0%	66.7602	-25.0%	89.1211	0.08%
Lysine	98.1940	63.1298	-35.7%	65.5010	-33.3%	11.7051	-90.3%	70.4555	-28.2%	95.7780	-2.46%

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
Methionine	79.2140	N/A	N/A	N/A	N/A	33.3208	-57.9%	57.8561	-27.0%	79.2363	0.03%
Phenylalanine	105.0090	72.6915	-30.8%	72.3371	-31.1%	10.9245	-89.7%	77.5554	-26.1%	104.9060	-0.10%
Proline	71.3320	55.7869	-21.8%	48.3952	-32.2%	4.6564	-92.9%	52.2919	-26.7%	71.7682	0.61%
Serine	58.3390	67.7342	16.1%	35.4257	-39.3%	7.5786	-89.6%	39.4158	-32.4%	56.6699	-2.86%
Threonine	71.0580	68.5162	-3.6%	45.0165	-36.6%	2.5692	-99.3%	49.2195	-30.7%	68.9851	-2.92%
Tryptophan	128.0840	94.0026	-26.6%	85.2577	-33.4%	9.4578	-93.7%	91.7617	-28.4%	126.6110	-1.15%
Tyrosine	111.4500	90.8131	-18.5%	73.6265	-33.9%	4.0735	-98.1%	79.4930	-28.7%	109.4040	-1.84%
Valine	76.7720	51.2007	-33.3%	53.1871	-30.7%	9.2863	-87.8%	57.0186	-25.7%	76.8720	0.13%
Antimony (Alkyl)											
Triethylstibine	80.6940	N/A	N/A	60.5563	-25.0%	N/A	N/A	N/A	N/A	81.2038	0.63%
Trimethylstibine	45.0238	N/A	N/A	32.7262	-27.3%	N/A	N/A	N/A	N/A	44.7307	-0.65%
Triphenylstibine	165.8158	N/A	N/A	117.9350	-28.9%	N/A	N/A	N/A	N/A	167.3220	0.91%
Aromatics											
1,2,3-Trichlorobenzene	55.0767	351.5382	538.3%	44.4924	-19.2%	146.9640	166.7%	38.9900	-29.2%	55.1377	0.11%
1,3,5-Trichlorobenzene	55.2549	351.3246	535.8%	44.7060	-19.1%	N/A	N/A	N/A	N/A	55.2954	0.07%
2,4-Dinitrophenol	77.6420	148.3752	91.1%	37.6802	-51.5%	38.1149	-50.9%	46.7391	-39.8%	77.6131	-0.04%
2-Chlorobenzoic Acid	73.0815	170.8918	133.8%	50.8067	-30.5%	50.8208	-30.5%	52.2333	-28.5%	73.0619	-0.03%
2-Nitroaniline	72.4242	85.1441	17.6%	42.7912	-40.9%	10.0542	-86.1%	48.4632	-33.1%	72.4748	0.07%
3-Chlorobenzoic Acid	73.2608	170.5946	132.9%	51.1039	-30.2%	50.5018	-31.1%	52.5524	-28.3%	73.2682	0.01%
3-Nitroaniline	72.4812	85.3756	17.8%	42.5597	-41.3%	10.1669	-86.0%	48.3505	-33.3%	72.4748	-0.01%
4-Chlorobenzoic Acid	73.2474	170.5763	132.9%	51.1493	-30.2%	50.4792	-31.1%	52.5750	-28.2%	73.2682	0.03%
4-Nitroaniline	72.4760	85.1926	17.5%	42.7427	-41.0%	9.9983	-86.2%	48.5192	-33.1%	72.4748	0.00%
Aniline-2-Carboxylic Acid	80.9414	70.4183	-13.0%	53.8921	-33.4%	1.2030	-98.6%	58.2181	-28.1%	80.9086	-0.04%
Aniline-3-Carboxylic Acid	80.8129	70.7117	-12.5%	53.5987	-33.7%	1.0810	-98.5%	58.0961	-28.1%	80.9086	0.12%
Aniline-4-Carboxylic Acid	80.9487	70.5553	-12.8%	53.7551	-33.6%	1.2017	-98.6%	58.2168	-28.1%	80.9086	-0.05%
Aniline	64.3740	29.8989	-53.6%	45.5036	-29.3%	13.2841	-79.3%	48.0590	-25.3%	64.3993	0.04%
Anisole	73.3553	38.5829	-47.4%	52.6152	-28.3%	13.4216	-81.7%	55.5019	-24.3%	73.3901	0.05%
Benzene	57.2634	19.1281	-66.6%	42.3268	-26.1%	15.6644	-72.6%	44.1655	-22.9%	57.2601	-0.01%
Benzoic Acid	73.7624	60.1205	-18.5%	50.3195	-31.8%	3.4161	-95.4%	54.2346	-26.5%	73.7694	0.01%
Chlorobenzene	56.5815	129.7011	129.2%	43.0494	-23.9%	38.2133	-32.5%	42.5606	-24.8%	56.5526	-0.05%
Hexachlorobenzene	52.4774	683.4705	1202.4%	45.8449	-12.6%	296.7383	464.6%	45.6224	-13.1%	52.5713	0.18%
m-Dichlorobenzene	55.8519	240.2862	330.2%	43.9588	-21.3%	92.2361	65.2%	40.9823	-26.6%	55.8452	-0.01%
Nitrobenzene	65.2172	74.8101	14.7%	39.2548	-39.8%	62.2090	-4.6%	9.9154	-84.8%	65.1875	-0.05%
Phenol	61.7042	37.4424	-39.3%	43.4401	-29.6%	8.7615	-85.7%	46.0776	-25.3%	61.7582	0.09%
Salicylic Acid	78.4260	77.9221	-0.6%	51.9084	-33.8%	3.2331	-96.1%	56.3632	-28.1%	78.2675	-0.20%
Toluene	69.5456	20.1808	-71.0%	51.6268	-25.8%	20.6345	-70.4%	53.9370	-22.4%	69.4843	-0.09%
Aromatics (Heterocyclic)											
Furan	41.6920	32.0318	-23.2%	28.3510	-32.0%	2.6698	-93.7%	30.4798	-26.9%	41.6623	-0.07%
Imidazole	39.7411	33.8677	-14.8%	24.6298	-38.0%	0.5642	-98.5%	27.3053	-31.3%	39.7634	0.06%
Pyrazine	46.5138	39.4914	-15.1%	29.1631	-37.3%	0.9304	-97.9%	32.3861	-30.4%	46.5760	0.13%
Pyridine	51.8793	29.2881	-43.5%	35.7716	-31.0%	8.3663	-83.8%	38.3497	-26.1%	51.9180	0.07%

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
Pyrimidine	46.5179	39.2557	-15.6%	29.3988	-36.8%	1.2164	-97.3%	32.6721	-29.8%	46.5760	0.12%
Pyrrole	44.7853	24.0901	-46.2%	30.8026	-31.2%	7.4813	-83.2%	32.7401	-26.9%	44.8109	0.06%
Thiophene	40.4302	106.3195	163.0%	30.4333	-24.7%	32.8829	-18.7%	29.5539	-26.9%	40.4250	-0.01%
Arsenic (Alkyl)											
Triethylarsine	81.0108	N/A	N/A	66.7984	-17.5%	N/A	N/A	115.6857	42.8%	81.2128	0.25%
Trimethylarsine	45.6311	N/A	N/A	38.8412	-14.9%	N/A	N/A	86.8467	90.3%	44.7397	-1.95%
Boranes (Alkoxy)											
Boric Acid	30.6843	45.5185	48.3%	683.9415	2129.0%	8.1749	-73.5%	21.9639	-28.4%	30.6161	-0.22%
Dihydroxyborane	24.4378	29.5531	20.9%	680.5064	2684.7%	3.2697	-86.6%	18.0813	-26.0%	24.4546	0.07%
Dimethyloxyborane	47.7236	31.9818	-33.0%	698.7360	1364.1%	5.9664	-87.4%	36.9003	-22.7%	47.7532	0.06%
Phenylborinic acid	78.8612	52.2311	-33.8%	719.1447	811.9%	8.5646	-90.4%	58.3871	-26.0%	77.7966	-1.35%
Tri-n-butyl borate	175.6290	57.5321	-67.2%	795.8845	353.2%	49.9574	-71.6%	137.4923	-21.7%	175.5670	-0.04%
Tri-n-propyl borate	139.1132	54.6624	-60.7%	767.7632	451.9%	35.2531	-74.7%	108.4508	-22.0%	139.0940	-0.01%
Triethyl borate	102.5020	51.7649	-49.5%	739.6970	621.6%	20.8320	-79.6%	79.6925	-22.3%	102.6200	0.12%
Trimethyl borate	65.5395	49.1740	-25.0%	711.2969	985.3%	5.5777	-91.5%	50.1009	-23.6%	65.5640	0.04%
Boranes (Alkyl)											
Tri-isopropylboron	122.7580	5.0290	-95.9%	759.1980	518.5%	51.2874	-58.2%	98.1244	-20.1%	122.8150	0.05%
Triethylboron	86.1294	2.0741	-97.6%	731.1792	748.9%	36.7976	-57.3%	69.2875	-19.6%	86.0396	-0.10%
Trimethylborane	49.7610	1.0765	-97.8%	703.3188	1313.4%	22.3937	-55.2%	40.5263	-18.6%	49.5665	-0.39%
Triphenylboron	172.0968	66.0412	-61.6%	789.0992	358.5%	41.9484	-75.6%	131.0982	-23.8%	172.1580	0.04%
Boron Chlorides											
Boron trichloride	13.8075	324.7150	2251.7%	680.2961	4827.0%	150.7397	995.2%	9.6108	-30.4%	13.7588	-0.35%
Dichloroboron	13.2529	215.6264	1527.0%	678.2262	5017.6%	98.2622	643.2%	10.0616	-24.1%	13.2164	-0.28%
Phenylborondichloride	66.9782	238.3500	255.9%	716.8889	970.3%	86.4038	29.2%	50.5704	-24.5%	66.5584	-0.63%
Boron Fluorides											
Boron trifluoride	20.0974	71.0456	253.5%	678.2240	3274.7%	23.9797	19.2%	15.5465	-22.6%	20.2692	0.85%
Difluoroboron	17.4185	46.4944	166.9%	676.7682	3785.4%	13.6717	-21.3%	13.9433	-20.0%	17.5567	0.79%
Difluoromethylborane	30.3362	46.5958	53.6%	686.9922	2164.6%	8.3556	-73.2%	24.0609	-20.7%	30.0349	-0.99%
Vinyldifluoroborane	36.5498	52.6156	44.0%	691.1295	1790.9%	8.6342	-77.1%	28.4969	-22.0%	36.2189	-0.91%
Bromides											
Bromoform	12.8770	N/A	N/A	20.4274	58.6%	N/A	N/A	N/A	N/A	12.8770	0.00%
Bromomethane CH3Br	15.7321	N/A	N/A	16.0988	2.3%	N/A	N/A	71.2954	353.2%	15.6755	-0.36%
Tetrabromomethane	11.2593	N/A	N/A	23.5616	109.3%	N/A	N/A	242.2493	2051.5%	11.2593	0.00%
Bromides (Alkyl)											
1-Bromododecane	149.5735	N/A	N/A	119.7434	-19.9%	N/A	N/A	178.1153	19.1%	149.6160	0.03%
1-Bromoheptane	88.7830	N/A	N/A	72.6331	-18.2%	N/A	N/A	129.4287	45.8%	88.8279	0.05%
1-Bromohexadecane	198.1915	N/A	N/A	157.1050	-20.7%	N/A	N/A	N/A	N/A	198.2470	0.03%
1-Bromohexane	76.6345	N/A	N/A	63.1566	-17.6%	N/A	N/A	119.8000	56.3%	76.6702	0.05%

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1-Bromooctane	100.9523	N/A	N/A	82.1099	-18.7%	N/A	N/A	139.3294	38.0%	100.9860	0.03%
1-Bromopropane	40.1598	N/A	N/A	34.9956	-12.9%	N/A	N/A	90.6387	125.7%	40.1971	0.09%
2,3-Dibromo-2-methylbutane	63.4772	N/A	N/A	56.4482	-11.1%	N/A	N/A	167.1594	163.3%	63.5395	0.10%
2-Bromopropane	40.2883	N/A	N/A	35.0723	-12.9%	N/A	N/A	90.6910	125.1%	40.2980	0.02%
Bromoethane	27.9532	N/A	N/A	25.7675	-7.8%	N/A	N/A	80.9999	189.8%	28.0394	0.31%
Carboxylic Acids											
2,2-Dimethylpropanoic Acid	69.9892	40.3886	-42.3%	50.0715	-28.5%	11.6334	-83.0%	53.1392	-24.1%	70.3167	0.47%
3-Methyl-butanoic Acid	70.1830	40.5198	-42.3%	49.9403	-28.8%	11.6676	-83.5%	53.1733	-24.2%	70.1048	-0.11%
Acetic Acid	33.5370	37.8472	12.9%	21.6392	-35.5%	3.1142	-90.7%	24.0171	-28.4%	33.5591	0.07%
Butanoic Acid	57.8830	39.6450	-31.5%	40.4997	-30.0%	6.7552	-88.3%	43.4694	-24.9%	57.8745	-0.01%
Decanoic Acid	130.7952	45.3050	-65.4%	96.7943	-26.0%	36.2903	-72.2%	101.6790	-22.3%	130.8210	0.02%
Dodecanoic Acid	155.1762	47.2609	-69.5%	115.5567	-25.5%	46.0673	-70.3%	121.0717	-22.0%	155.1360	-0.03%
Arachidic Acid	252.5139	54.7843	-78.3%	190.6062	-24.5%	85.4753	-66.2%	198.6971	-21.3%	252.3980	-0.05%
Formic Acid	21.0360	37.3056	77.3%	11.8381	-43.7%	8.4040	-60.1%	13.9630	-33.6%	21.0195	-0.08%
Fumaric Acid	56.0830	84.9492	51.5%	33.6922	-39.9%	15.8391	-71.5%	38.3643	-31.6%	56.2967	0.38%
Heptanoic Acid	94.3474	42.4747	-55.0%	68.6337	-27.3%	21.5244	-77.2%	72.5759	-23.1%	94.3476	0.00%
Hexadecanoic Acid	203.9476	51.0725	-75.0%	153.0815	-24.9%	65.7213	-67.8%	159.8844	-21.6%	203.7670	-0.09%
Hexanoic Acid	82.1491	41.4989	-49.5%	59.2640	-27.9%	16.6336	-79.7%	62.8637	-23.5%	82.1899	0.05%
Maleic Acid	56.1200	85.3677	52.1%	33.2737	-40.7%	16.1206	-71.1%	38.0828	-32.1%	56.2967	0.31%
Nonanoic Acid	118.6663	44.4278	-62.6%	87.4261	-26.3%	31.3017	-73.6%	91.9689	-22.5%	118.6630	0.00%
Octanoic Acid	106.4815	43.4605	-59.2%	78.0206	-26.7%	26.4131	-75.2%	82.2861	-22.7%	106.5050	0.02%
Pentadecanoic Acid	191.6063	50.0946	-73.9%	143.7139	-25.0%	60.8328	-68.3%	150.1745	-21.6%	191.6090	0.00%
Pentanoic Acid	69.9954	40.5905	-42.0%	49.8696	-28.8%	11.6749	-83.3%	53.1806	-24.0%	70.0322	0.05%
Propanoic Acid	45.7270	38.7038	-15.4%	31.0981	-32.0%	1.8277	-96.0%	33.7505	-26.2%	45.7168	-0.02%
Octadecanoic Acid	228.2976	52.9284	-76.8%	171.8439	-24.7%	75.5982	-66.9%	179.3043	-21.5%	228.0820	-0.09%
Tetradecanoic Acid	179.6049	49.1167	-72.7%	134.3191	-25.2%	55.9443	-68.9%	140.4917	-21.8%	179.4520	-0.09%
Chlorides											
Trichloromethane	14.5230	329.0074	2165.4%	15.4919	6.7%	153.2462	957.3%	8.6605	-40.4%	14.4915	-0.22%
Chloromethane	16.3118	107.1976	557.2%	14.6392	-10.3%	44.6616	174.3%	12.4651	-23.6%	16.2630	-0.30%
Dichloromethane	15.4495	217.9086	1310.5%	15.1867	-1.7%	98.7520	541.9%	10.6375	-31.1%	15.3725	-0.50%
Tetrachloromethane	13.4483	440.0158	3171.9%	15.6691	16.5%	207.6964	1446.2%	6.3460	-52.8%	13.4318	-0.12%
Chlorides (Alkyl)											
1-Chloro-2-methylpropane	52.9533	109.8903	107.5%	42.9103	-19.0%	29.8120	-43.7%	41.6792	-21.3%	52.9986	0.09%
1-Chloro-3-methylbutane	65.1112	110.8825	70.3%	52.2908	-19.7%	24.9438	-61.6%	51.3416	-21.1%	65.1563	0.07%
1-Chlorobutane	52.9025	109.9185	107.8%	42.8821	-18.9%	29.7859	-43.7%	41.7052	-21.2%	52.9260	0.04%
1-Chlorododecane	150.2019	117.5382	-21.7%	117.9353	-21.5%	9.5271	-93.7%	119.3084	-20.6%	150.1880	-0.01%
1-Chlorooctadecane	223.1750	123.2057	-44.8%	174.1137	-22.0%	39.0583	-82.5%	177.4596	-20.5%	223.1340	-0.02%
1-Chlorooctane	101.5641	113.7268	12.0%	80.4103	-20.8%	10.1272	-90.0%	80.4954	-20.7%	101.5570	-0.01%
1-Chloropentane	65.0615	110.8955	70.4%	52.2778	-19.6%	24.8962	-61.7%	51.3892	-21.0%	65.0837	0.03%
1-Chloropropane	40.7229	108.9402	167.5%	33.5148	-17.7%	34.6738	-14.8%	31.9958	-21.4%	40.7683	0.11%
2-Chloro-2-	65.3444	110.7170	69.4%	52.4563	-19.7%	24.8428	-62.0%	51.4426	-21.3%	65.3682	0.04%

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
methylbutane											
2-Chloro-2-methylpropane	53.1907	109.6945	106.2%	43.1061	-19.0%	29.6623	-44.2%	41.8289	-21.4%	53.2105	0.04%
2-Chloro-3-methylbutane	65.1672	110.8032	70.0%	52.3701	-19.6%	24.9014	-61.8%	51.3840	-21.2%	65.1658	0.00%
2-Chlorobutane	52.9720	109.8207	107.3%	42.9799	-18.9%	29.7266	-43.8%	41.7646	-21.2%	53.0269	0.10%
2-Chlorohexane	77.3126	111.7766	44.6%	61.7422	-20.1%	19.9516	-74.2%	61.1553	-20.9%	77.3423	0.04%
2-Chloropropane	40.8576	108.8429	166.4%	33.6122	-17.7%	34.5988	-15.3%	32.0708	-21.5%	40.8692	0.03%
Chloroethane	28.6106	108.0822	277.8%	24.1001	-15.8%	39.6731	38.7%	22.2751	-22.1%	28.6106	0.00%
Disulfides											
Di-t-butyl disulfide	107.9187	188.9011	75.0%	85.5874	-20.7%	41.8390	-61.2%	83.2556	-22.9%	107.9960	0.07%
Diethyl disulfide	58.8727	185.2462	214.7%	47.8242	-18.8%	61.4027	4.3%	44.6148	-24.2%	58.7967	-0.13%
Dimethyl disulfide	34.4128	183.3664	432.8%	28.9857	-15.8%	71.2297	106.8%	25.1721	-26.9%	34.4813	0.20%
Dipropyl disulfide	83.1687	187.0662	124.9%	66.5135	-20.0%	51.4991	-38.1%	64.1158	-22.9%	83.1121	-0.07%
DNA Base Pairs											
Adenine	70.7981	80.2156	13.3%	40.2258	-43.2%	8.9530	-87.3%	45.9075	-35.2%	70.8542	0.08%
Cytosine	60.5806	66.8320	10.3%	35.1706	-41.9%	6.9925	-90.0%	39.4976	-34.8%	59.5338	-1.73%
Guanine	76.8821	97.7527	27.1%	42.0792	-45.3%	15.3397	-80.0%	48.2986	-37.2%	76.8821	0.00%
Thymine	69.0879	74.3132	7.6%	43.4550	-37.1%	5.6920	-91.7%	48.1009	-30.4%	69.1021	0.02%
Esters											
Butyl acetate	81.8735	41.6166	-49.2%	59.1462	-27.8%	16.5005	-79.8%	62.7305	-23.4%	81.9542	0.10%
Butyl pentanoate	118.4891	44.4403	-62.5%	87.4136	-26.2%	31.2013	-73.7%	91.8685	-22.5%	118.4270	-0.05%
Ethyl 2,2-dimethylpropanoate	94.3454	42.2991	-55.2%	68.8365	-27.0%	21.3816	-77.3%	72.4331	-23.2%	94.3964	0.05%
Ethyl 3-methylbutanoate	94.2521	42.4332	-55.0%	68.7024	-27.1%	21.4170	-77.3%	72.4685	-23.1%	94.1845	-0.07%
Ethyl acetate	57.5484	39.7767	-30.9%	40.3680	-29.9%	6.6256	-88.3%	43.3399	-24.7%	57.6388	0.16%
Ethyl pentanoate	94.0334	42.5018	-54.8%	68.6338	-27.0%	21.4247	-77.2%	72.4762	-22.9%	94.1119	0.08%
Ethyl propanoate	69.7000	40.6237	-41.7%	49.8365	-28.5%	11.5776	-83.3%	53.0833	-23.8%	69.7965	0.14%
Isobutyl isobutanoate	106.3633	43.2947	-59.3%	78.1864	-26.5%	26.3099	-75.2%	82.1829	-22.7%	106.4430	0.07%
Isobutyl pentanoate	118.5761	44.3451	-62.6%	87.5087	-26.2%	31.2151	-73.7%	91.8823	-22.5%	118.5000	-0.06%
Isopropyl pentanoate	106.3841	43.3099	-59.3%	78.1712	-26.5%	26.4149	-75.2%	82.2879	-22.7%	106.3700	-0.01%
Isopropyl acetate	69.8887	40.5441	-42.0%	49.9161	-28.6%	11.6507	-83.3%	53.1565	-23.9%	69.8974	0.01%
Methyl 2,2-dimethylpropanoate	81.9346	41.4606	-49.4%	59.3023	-27.6%	16.3542	-80.0%	62.5842	-23.6%	82.0060	0.09%
Methyl acetate	45.2880	38.9560	-14.0%	30.8459	-31.9%	1.5726	-96.6%	33.4954	-26.0%	45.2485	-0.09%
Methyl decanoate	142.5229	46.4495	-67.4%	106.0226	-25.6%	40.9419	-71.3%	111.1520	-22.0%	142.5100	-0.01%
Methyl dodecanoate	166.8418	48.3053	-71.0%	124.7850	-25.2%	50.8189	-69.5%	130.5448	-21.8%	166.8250	-0.01%
Methyl formate	32.7620	38.3904	17.2%	21.0960	-35.6%	3.6919	-88.9%	23.4394	-28.5%	32.7107	-0.16%
Methyl heptanoate	106.0794	43.6160	-58.9%	77.8651	-26.6%	28.5979	-73.1%	84.4708	-20.4%	106.0370	-0.04%
Methyl hexanoate	93.8910	42.6462	-54.6%	68.4894	-27.1%	21.2874	-77.3%	72.3389	-23.0%	93.8792	-0.01%
Methyl nonanoate	130.3733	45.4716	-65.1%	96.6277	-25.9%	36.0533	-72.4%	101.4420	-22.2%	130.3520	-0.02%
Methyl octanoate	118.2165	44.5921	-62.3%	87.2617	-26.2%	31.0647	-73.7%	91.7320	-22.4%	118.1950	-0.02%
Methyl pentadecanoate	203.3559	51.2391	-74.8%	152.9150	-24.8%	65.4843	-67.8%	159.6475	-21.5%	203.2990	-0.03%
Methyl pentanoate	81.7260	41.6676	-49.0%	59.0953	-27.7%	16.3950	-79.9%	62.6250	-23.4%	81.7215	-0.01%
Methyl tetradecanoate	191.1700	50.2612	-73.7%	143.5473	-24.9%	60.5958	-68.3%	149.9375	-21.6%	191.1410	-0.02%

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
Methyl tridecanoate	178.9997	49.2833	-72.5%	134.1526	-25.1%	55.7073	-68.9%	140.2547	-21.6%	178.9830	-0.01%
Methyl undecanoate	154.6767	47.4274	-69.3%	115.3902	-25.4%	45.8303	-70.4%	120.8348	-21.9%	154.6680	-0.01%
Propyl formate	57.7463	40.1287	-30.5%	40.0160	-30.7%	6.2873	-89.1%	43.0015	-25.5%	57.7636	0.03%
Propyl pentanoate	106.2669	43.4596	-59.1%	78.0215	-26.6%	26.3142	-75.2%	82.1872	-22.7%	106.2700	0.00%
sec-Butyl pentanoate	118.6238	44.2541	-62.7%	87.5997	-26.2%	31.3011	-73.7%	91.9683	-22.5%	118.5280	-0.08%
t-Butyl acetate	82.1968	41.3383	-49.7%	59.4246	-27.7%	16.5663	-79.8%	62.7963	-23.6%	82.2387	0.05%

Ethers

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
Di-t-butyl ether	106.4246	21.6820	-79.6%	80.5871	-24.3%	36.3704	-65.7%	83.5353	-21.5%	106.6560	0.22%
Dibutyl ether	106.1220	21.8040	-79.5%	80.4652	-24.2%	36.5349	-65.5%	83.6997	-21.1%	106.1800	0.05%
Diethyl ether	57.4998	18.0280	-68.6%	42.8846	-25.4%	16.9014	-70.5%	44.8875	-21.9%	57.5492	0.09%
Diisopropyl ether	82.0882	19.6834	-76.0%	61.8875	-24.6%	26.8569	-67.3%	64.4260	-21.5%	82.0664	-0.03%
Dimethyl ether	32.9022	16.3942	-50.2%	23.8502	-27.5%	6.7816	-79.5%	25.2020	-23.4%	32.8449	-0.17%
Dipropyl ether	81.8166	19.8778	-75.7%	61.6931	-24.6%	26.7440	-67.3%	64.3130	-21.4%	81.8646	0.06%
Ethyl methyl ether	45.1834	17.1925	-61.9%	33.3946	-26.1%	11.8501	-73.8%	35.0620	-22.4%	45.1971	0.03%
Isopropyl methyl ether	57.4988	18.0321	-68.6%	42.8806	-25.4%	16.8172	-70.8%	44.8033	-22.1%	57.4557	-0.07%
Methyl propyl ether	57.3547	18.1373	-68.4%	42.7754	-25.4%	16.7568	-70.8%	44.7429	-22.0%	57.3548	0.00%
t-Butyl ethyl ether	82.0332	19.7189	-76.0%	61.8520	-24.6%	26.7740	-67.3%	64.3430	-21.6%	82.1027	0.08%
t-Butyl isobutyl ether	106.4972	21.5071	-79.8%	80.7621	-24.2%	36.5913	-65.6%	83.7562	-21.4%	106.4910	-0.01%

Fluorides

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
Difluoromethane	18.2795	50.5360	176.5%	11.9965	-34.4%	15.5081	-15.1%	13.1726	-27.9%	18.3701	0.50%
Trifluoromethane	19.3624	76.7759	296.5%	11.7636	-39.2%	27.2536	40.9%	13.3383	-31.1%	19.2840	-0.40%
Tetrafluoromethane	21.0163	102.9024	389.6%	11.5841	-44.9%	38.9858	85.2%	13.4574	-36.0%	21.0799	0.30%

Fluorides (Alkyl)

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
1-Fluoropropane	41.8845	25.5026	-39.1%	31.6639	-24.4%	6.6683	-84.1%	33.0036	-21.2%	41.8674	-0.04%
2-Fluoropropane	41.9633	25.3449	-39.6%	31.8216	-24.2%	6.8411	-83.7%	33.1763	-20.9%	41.9683	0.01%

Germanium (Alkyl)

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
Hexaethyldigermanium	167.8984	N/A	N/A	137.2331	-18.3%	N/A	N/A	N/A	N/A	167.8890	-0.01%
Tetra-n-propylgermanium	158.6309	N/A	N/A	127.1642	-19.8%	N/A	N/A	175.1482	10.4%	158.6270	0.00%
Tetraethylgermanium	110.1817	N/A	N/A	89.4700	-18.8%	N/A	N/A	136.3247	23.7%	109.9970	-0.17%

Iodides

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
Diiodomethane	12.9209	N/A	N/A	3.1585	-75.6%	N/A	N/A	N/A	N/A	12.9461	0.20%
Iodoform	10.4050	N/A	N/A	0.6586	-93.7%	N/A	N/A	N/A	N/A	10.3589	-0.44%
Iodomethane	15.1630	N/A	N/A	9.2532	-39.0%	N/A	N/A	N/A	N/A	15.2029	0.26%

Iodides (Alkyl)

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
1-Iodoethane	27.3430	N/A	N/A	18.7398	-31.5%	N/A	N/A	N/A	N/A	27.3606	0.06%
1-Iodopropane	39.5160	N/A	N/A	27.9706	-29.2%	N/A	N/A	N/A	N/A	39.5183	0.01%
2-Iodo-2-methylpropane	51.8990	N/A	N/A	37.5040	-27.7%	N/A	N/A	N/A	N/A	51.9605	0.12%
2-Iodopropane	39.6230	N/A	N/A	27.9793	-29.4%	N/A	N/A	N/A	N/A	39.6192	-0.01%

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
Ketones											
2,2,4-Trimethyl-3-pentanone	101.6603	25.9258	-74.5%	76.1648	-25.1%	32.3144	-68.2%	79.4096	-21.9%	101.7110	0.05%
2,2-Dimethyl-3-pentanone	89.4579	24.8961	-72.2%	66.8318	-25.3%	30.2568	-66.2%	72.5405	-18.9%	89.4519	-0.01%
2,4-Dimethyl-3-pentanone	89.4340	24.9030	-72.2%	66.8249	-25.3%	27.5833	-69.1%	69.8670	-21.9%	89.5172	0.09%
2,6-Dimethyl-4-heptanone	113.8068	26.8027	-76.4%	85.6334	-24.8%	37.4121	-67.1%	89.3016	-21.5%	113.7760	-0.03%
2-Butanone	52.8400	22.1902	-58.0%	38.5368	-27.1%	12.8781	-75.6%	40.8146	-22.8%	52.8424	0.00%
2-Hexanone	77.1518	24.0841	-68.8%	57.3283	-25.7%	22.7118	-70.6%	60.2040	-22.0%	77.1578	0.01%
2-Methyl-3-pentanone	77.2254	23.9757	-69.0%	57.4367	-25.6%	22.7052	-70.6%	60.1974	-22.0%	77.2587	0.04%
2-Nonanone	113.6316	26.9722	-76.3%	85.4639	-24.8%	37.4220	-67.1%	89.3115	-21.4%	113.6310	0.00%
2-Pentanone	64.9970	23.1360	-64.4%	47.9337	-26.3%	17.7939	-72.6%	50.4946	-22.3%	65.0001	0.00%
3,3-Dimethyl-2-butanone	77.2730	24.0133	-68.9%	57.3991	-25.7%	22.6064	-70.7%	60.0987	-22.2%	77.2943	0.03%
3-Heptanone	89.2869	24.9596	-72.0%	66.7683	-25.2%	27.6531	-69.0%	69.9368	-21.7%	89.3155	0.03%
3-Hexanone	77.1383	24.0112	-68.9%	57.4012	-25.6%	22.7355	-70.5%	60.2277	-21.9%	77.1578	0.03%
3-Methyl-2-butanone	65.0364	23.1068	-64.5%	47.9629	-26.3%	17.7570	-72.6%	50.4577	-22.4%	65.1010	0.10%
3-Pentanone	64.9877	23.0655	-64.5%	48.0042	-26.1%	17.8204	-72.6%	50.5212	-22.3%	65.0001	0.02%
4-Heptanone	89.2993	24.9576	-72.1%	66.7703	-25.2%	27.6544	-69.0%	69.9381	-21.7%	89.3155	0.02%
5-Nonanone	113.6752	26.9050	-76.3%	85.5311	-24.8%	37.4432	-67.1%	89.3326	-21.4%	113.6310	-0.04%
Acetone	40.6720	21.3138	-47.6%	29.0876	-28.5%	7.9401	-80.5%	31.0751	-23.6%	40.6847	0.03%
Nitrates											
Ethyl Nitrate	40.3958	72.7415	80.1%	20.0830	-50.3%	17.2537	-57.4%	24.9293	-38.3%	40.3430	-0.13%
Isopropyl Nitrate	52.7247	73.5202	39.4%	29.6397	-43.8%	12.2511	-76.9%	34.7433	-34.1%	52.6016	-0.23%
Methyl Nitrate	28.1167	71.9582	155.9%	10.5236	-62.6%	22.3304	-20.5%	15.0611	-46.4%	28.1853	0.24%
Propyl Nitrate	52.5496	73.6884	40.2%	29.4715	-43.9%	12.3552	-76.6%	34.6392	-34.1%	52.5007	-0.09%
Nitriles											
2,2-Dimethylpropanenitrile	62.3956	19.8863	-68.1%	45.5176	-27.0%	17.6032	-71.7%	47.7131	-23.5%	62.4782	0.13%
2-Methylpropanenitrile	50.1828	19.0334	-62.1%	36.0450	-28.2%	12.6813	-74.8%	38.0170	-24.2%	50.1369	-0.09%
Acetonitrile	25.7655	17.1981	-33.3%	17.2221	-33.2%	2.8223	-89.2%	18.5750	-27.9%	25.7206	-0.17%
Butanenitrile	50.0771	19.0732	-61.9%	36.0051	-28.1%	12.6769	-74.7%	38.0125	-24.1%	50.0360	-0.08%
Decanenitrile	123.0524	24.7751	-79.9%	92.3080	-25.0%	42.1739	-65.8%	96.2340	-21.8%	122.9820	-0.06%
Heptanenitrile	86.5860	21.9123	-74.7%	64.1770	-25.9%	27.4373	-68.4%	67.1302	-22.5%	86.5091	-0.09%
Octanenitrile	98.7345	22.8596	-76.8%	73.5452	-25.5%	32.3564	-67.3%	76.8135	-22.2%	98.6668	-0.07%
Pentanenitrile	62.2630	20.0334	-67.8%	45.3705	-27.1%	17.5918	-71.8%	47.7017	-23.4%	62.1937	-0.11%
Propanenitrile	37.9431	18.1413	-52.2%	26.5943	-29.9%	7.7457	-79.7%	28.2898	-25.4%	37.8783	-0.17%
Tetradecanenitrile	171.7025	28.5866	-83.4%	129.8330	-24.4%	61.8283	-64.0%	135.0198	-21.4%	171.6130	-0.05%
Nitrites											
Methyl nitrite	24.9548	51.8341	107.7%	11.2472	-54.9%	14.2215	-43.1%	14.3821	-42.4%	24.9233	-0.13%
Nitros											
1-Nitrobutane	61.6005	55.1890	-10.4%	38.8760	-36.9%	0.6324	-98.9%	43.5933	-29.2%	61.6224	0.04%
1-Nitropentane	73.7801	56.1098	-24.0%	48.2780	-34.6%	5.5755	-92.4%	53.3078	-27.7%	73.7801	0.00%

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
1-Nitropropane	49.4509	54.2424	9.7%	29.5071	-40.3%	4.2900	-91.3%	33.9066	-31.4%	49.4647	0.03%
2-Nitroisobutane	61.9446	54.8272	-11.5%	39.2378	-36.7%	0.7433	-98.9%	43.7042	-29.4%	61.9069	-0.06%
2-Nitropropane	49.6022	54.0610	9.0%	29.6885	-40.1%	4.1953	-91.6%	34.0013	-31.5%	49.5656	-0.07%
Nitroethane	37.2920	53.3117	43.0%	20.0850	-46.1%	9.2118	-75.3%	24.1833	-35.2%	37.3070	0.04%
Nitromethane	25.1072	52.5109	109.1%	10.5704	-57.9%	14.2479	-43.2%	14.3558	-42.8%	25.1493	0.17%
Phosphates											
Tri-n-butylphosphate	178.0774	150.8505	-15.3%	131.8525	-26.0%	7.1087	-95.9%	134.7033	-24.4%	178.2650	0.11%
Triethylphosphate	104.4040	145.1636	39.0%	75.6207	-27.6%	22.2846	-78.0%	76.5628	-26.7%	105.3190	0.88%
Tri-isopropylphosphate	141.4228	147.3611	4.2%	104.3870	-26.2%	7.1421	-94.5%	106.0697	-25.0%	142.0950	0.48%
Phosphine Oxides											
Trimethylphosphine Oxide	52.9119	91.1759	72.3%	40.4188	-23.6%	18.6849	-64.6%	39.4919	-25.4%	53.0043	0.17%
Phosphines											
Triethylphosphine	82.2824	77.6546	-5.6%	65.5135	-20.4%	1.6000	-98.1%	65.3362	-20.6%	82.2824	0.00%
Trimethylphosphine	46.8733	74.6125	59.2%	37.5918	-19.8%	12.9331	-74.1%	36.4659	-22.2%	45.8093	-2.27%
Triphenylphosphine	167.4659	142.2898	-15.0%	122.8370	-26.6%	6.1010	-95.8%	126.4600	-24.5%	168.4000	0.56%
Phosphites											
Triethylphosphite	97.9795	129.6340	32.3%	71.7327	-26.8%	17.3831	-82.1%	72.6865	-25.8%	98.1240	0.15%
Triisopropylphosphite	135.0070	131.6300	-2.5%	100.7277	-25.4%	2.1443	-98.5%	102.2625	-24.3%	134.9000	-0.08%
Trimethylphosphite	60.9433	127.2626	108.8%	43.1403	-29.2%	32.6238	-46.4%	43.1085	-29.3%	61.0676	0.20%
Silanes											
Disilane	22.0557	118.2799	436.3%	20.3729	-7.6%	39.9784	82.3%	17.3921	-21.1%	21.7671	-1.31%
Silicon tetrahydride	13.3458	57.2157	328.7%	12.2135	-8.5%	18.0076	34.3%	10.7125	-19.7%	13.5726	1.70%
Trisilane	30.8133	179.3183	482.0%	28.6080	-7.2%	61.9579	99.7%	24.1131	-21.7%	31.2332	1.36%
Silanes (Alkyl)											
1,1,1,2,2-Pentamethyldisilane	85.4781	120.5926	41.1%	69.7422	-18.4%	13.9495	-83.4%	67.4013	-21.1%	85.7683	0.34%
1,1,1-Trimethyldisilane	60.1065	119.5917	99.0%	50.0248	-16.8%	24.2915	-59.5%	47.4163	-21.1%	60.1679	0.10%
1,1,2,2-Tetramethyldisilane	72.7944	120.1183	65.0%	59.8709	-17.8%	19.1309	-73.5%	57.3983	-21.2%	72.9681	0.24%
1,1,2-Trimethyldisilane	60.1065	119.6315	99.0%	49.9850	-16.8%	24.3118	-59.5%	47.3959	-21.1%	60.1679	0.10%
1,1-Dimethyldisilane	47.4228	119.2321	151.4%	40.1390	-15.4%	29.5888	-37.7%	37.3975	-21.1%	47.3676	-0.12%
1,2-Dimethyldisilane	47.4228	119.2495	151.5%	40.1216	-15.4%	29.5969	-37.6%	37.3894	-21.2%	47.3676	-0.12%
Diethylsilane	63.3777	60.1568	-5.1%	50.5589	-20.2%	2.1355	-97.6%	49.9643	-21.2%	62.7720	-0.96%
Dimethylsilane	38.6482	58.0728	50.3%	32.0247	-17.1%	7.5049	-81.0%	30.8082	-20.3%	38.4566	-0.50%
Hexamethyldisilane	98.3265	121.1303	23.2%	79.5772	-19.1%	8.8661	-90.8%	77.2789	-21.4%	98.5686	0.25%
Methylsilane	25.9949	57.6400	121.7%	22.1047	-15.0%	12.7467	-52.2%	20.7649	-20.1%	25.3788	-2.37%
Tetraethylsilane	112.0655	63.1479	-43.7%	88.9043	-20.7%	22.1608	-79.4%	89.1483	-20.4%	113.2430	1.05%
Tetramethylsilane	64.2232	58.8720	-8.3%	51.8437	-19.3%	3.0466	-94.7%	50.8754	-20.8%	64.6121	0.61%
Triethylsilane	87.4614	61.7029	-29.5%	69.7311	-20.3%	12.1105	-85.6%	69.5550	-20.5%	88.0074	0.62%
Trimethylsilane	51.3357	58.5147	14.0%	41.9283	-18.3%	2.2717	-95.2%	40.8356	-20.5%	51.5343	0.39%

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
Siloxanes											
H3SiOH	19.0070	73.5492	287.0%	15.2805	-19.6%	23.5614	24.4%	13.9465	-26.6%	18.6718	-1.76%
Hexamethyldisiloxane	105.2020	134.5360	27.9%	85.5620	-18.7%	12.3287	-88.2%	82.5941	-21.5%	105.2460	0.04%
Tetraethoxysiloxane	133.2318	129.1227	-3.1%	100.6186	-24.5%	0.2327	-100.1%	101.9659	-23.5%	132.8960	-0.25%
Tetramethoxysilioxane	84.0468	126.0056	49.9%	62.3993	-25.8%	20.5035	-76.1%	62.5364	-25.6%	83.4878	-0.67%
Triethoxysilioxane	102.5796	111.2787	8.5%	78.3539	-23.6%	4.7894	-95.2%	79.0157	-23.0%	102.7480	0.16%
Trimethylsilanol	57.3007	74.4781	30.0%	45.3826	-20.8%	7.5944	-86.7%	44.2907	-22.7%	57.3189	0.03%
Simple Molecules											
Ammonia	4.6016	6.5694	42.8%	7.5367	63.8%	1.9248	-58.5%	8.2455	79.2%	4.5791	-0.49%
Carbon Dioxide	16.6711	41.1178	146.6%	7.8674	-52.8%	11.9221	-28.5%	10.3681	-37.8%	16.6621	-0.05%
Chlorine	2.5141	217.8118	8563.5%	5.0379	100.4%	104.7654	4053.8%	0.0974	-96.1%	2.5224	0.33%
Dihydrogen Carbide	4.3306	5.4991	27.0%	4.8300	11.5%	0.5015	-87.6%	5.2848	22.0%	4.3697	0.90%
Flourine	1.6060	53.5542	3234.6%	1.3645	-15.0%	25.4309	1469.1%	1.5416	-4.0%	1.6217	0.98%
Methane	4.4900	3.3766	-24.8%	13.8806	209.1%	9.3167	107.5%	14.1633	215.4%	4.4900	0.00%
Water H2O	5.0991	14.1930	178.3%	5.3905	5.7%	2.6315	-48.3%	6.2223	22.0%	5.1059	0.13%
Sugars											
D-ribose	83.4980	96.2874	15.3%	52.4014	-37.2%	10.3504	-89.7%	57.5187	-31.1%	81.5103	-2.38%
Sulfates											
Diethyl sulfate	73.3456	165.1439	125.2%	49.8151	-32.1%	47.7830	-34.9%	50.0282	-31.8%	73.3007	-0.06%
Dimethyl sulfate	48.7345	168.4497	245.6%	25.7910	-47.1%	57.9016	18.8%	30.2667	-37.9%	48.7019	-0.07%
Dipropyl sulfate	97.6085	166.9494	71.0%	68.6278	-29.7%	37.8941	-61.2%	69.4329	-28.9%	97.6161	0.01%
Sulfides											
Butyl ethyl sulfide	80.2875	94.4346	17.6%	63.5263	-20.9%	9.0083	-88.8%	63.2075	-21.3%	80.2875	0.00%
Butyl methyl sulfide	68.1298	93.4409	37.2%	54.1744	-20.5%	13.8583	-79.7%	53.5361	-21.4%	68.1298	0.00%
Di-t-butyl-sulfide	104.9082	96.3610	-8.1%	82.2181	-21.6%	0.5693	-99.5%	82.3009	-21.5%	104.9080	0.00%
Dibutyl sulfide	104.6029	96.2744	-8.0%	82.3047	-21.3%	N/A	N/A	N/A	N/A	104.6030	0.00%
Diethyl sulfide	55.9721	92.4891	65.2%	44.7535	-20.0%	100.4109	79.4%	37.8380	-32.4%	55.9721	0.00%
Diisobutyl sulfide	104.7480	96.2103	-8.2%	82.3688	-21.4%	0.8691	-99.2%	82.6007	-21.1%	104.7480	0.00%
Diisopentyl sulfide	129.0634	98.1911	-23.9%	101.1063	-21.7%	10.5987	-91.8%	101.9733	-21.0%	129.0630	0.00%
Diisopropyl sulfide	80.4893	94.3617	17.2%	63.5991	-21.0%	8.9924	-88.8%	63.2234	-21.5%	80.4892	0.00%
Dimethyl sulfide	31.6567	90.6283	186.3%	25.9961	-17.9%	28.6323	-9.6%	24.4249	-22.8%	31.6567	0.00%
Dipentyl sulfide	128.9183	98.2142	-23.8%	101.0832	-21.6%	10.6820	-91.7%	102.0294	-20.9%	128.9180	0.00%
Ethyl isopropyl sulfide	68.2307	93.4375	36.9%	54.1778	-20.6%	13.8887	-79.6%	53.5057	-21.6%	68.2306	0.00%
Ethyl methyl sulfide	43.8144	91.5924	109.0%	35.4048	-19.2%	23.7254	-45.9%	34.1532	-22.1%	43.8144	0.00%
Ethyl propyl sulfide	68.1298	93.4559	37.2%	54.1594	-20.5%	13.8944	-79.6%	53.5000	-21.5%	68.1298	0.00%
Isopropyl methyl sulfide	56.0730	92.4674	64.9%	44.7753	-20.1%	18.7801	-66.5%	43.7928	-21.9%	56.0729	0.00%
Methyl propyl sulfide	55.9721	92.4631	65.2%	44.7795	-20.0%	18.7469	-66.5%	43.8261	-21.7%	55.9721	0.00%
t-Butyl methyl sulfide	68.2825	93.3773	36.8%	54.2381	-20.6%	13.9020	-79.6%	53.4923	-21.7%	68.2824	0.00%
Sulfites											

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Dibutyl sulfite	117.1912	151.0859	28.9%	85.6919	-26.9%	21.1152	-82.0%	86.9498	-25.8%	117.1800	-0.01%
Diethyl sulfite	68.6478	147.7653	115.3%	47.6760	-30.5%	40.9394	-40.4%	47.9941	-30.1%	68.5494	-0.14%
Dimethyl sulfite	44.0418	146.1923	231.9%	28.6307	-35.0%	51.1529	16.2%	28.2376	-35.9%	43.9506	-0.21%
Sulfones											
Dimethyl sulfone	40.3161	127.9014	217.2%	27.5311	-31.7%	43.8739	8.8%	26.7389	-33.7%	40.2759	-0.10%
Sulfoxides											
Diethyl sulfoxide	59.8905	111.9273	86.9%	44.7331	-25.3%	27.0118	-54.9%	44.3389	-26.0%	59.8399	-0.08%
Dimethyl sulfoxide	35.4348	110.1795	210.9%	25.8626	-27.0%	1125.4243	3068.3%	1063.5893	2901.5%	35.5245	0.25%
Dipropyl sulfoxide	84.2944	113.8292	35.0%	63.5494	-24.6%	17.2114	-79.7%	63.7823	-24.3%	84.1553	-0.16%
Thiols											
1-Butanethiol	56.0892	92.4483	64.8%	44.7943	-20.1%	18.7158	-66.6%	43.8572	-21.8%	56.0757	-0.02%
1-Decanethiol	129.0478	98.2146	-23.9%	101.0828	-21.7%	10.7172	-91.7%	102.0918	-20.9%	129.0220	-0.02%
1-Heptanethiol	92.5701	95.2810	2.9%	72.9526	-21.2%	3.9485	-95.8%	72.9616	-21.2%	92.5488	-0.02%
1-Hexanethiol	80.4163	94.4032	17.4%	63.5576	-21.0%	8.9373	-88.9%	63.2786	-21.3%	80.3911	-0.03%
1-Pentanethiol	68.2636	93.4256	36.9%	54.1898	-20.6%	13.8263	-79.8%	53.5681	-21.5%	68.2334	-0.04%
1-Propanethiol	43.9334	91.5706	108.4%	35.4265	-19.4%	23.7045	-46.1%	34.1742	-22.2%	43.9180	-0.03%
2,2-Dimethyl-1-propanethiol	68.4605	93.3337	36.3%	54.2816	-20.7%	13.8874	-80.1%	53.5070	-21.8%	68.1644	-0.43%
2-Butanethiol	56.1766	92.4201	64.5%	44.8226	-20.2%	18.7382	-66.6%	43.8347	-22.0%	56.1766	0.00%
2-Methyl-1-butanethiol	68.3144	93.4576	36.8%	54.1578	-20.7%	13.9253	-79.6%	53.4691	-21.7%	68.3060	-0.01%
2-Methyl-1-propanethiol	56.1856	92.4438	64.5%	44.7988	-20.3%	18.7649	-66.6%	43.8080	-22.0%	56.1483	-0.07%
2-Methyl-2-butanethiol	68.5180	93.3642	36.3%	54.2512	-20.8%	13.9075	-79.7%	53.4869	-21.9%	68.5179	0.00%
2-Methyl-2-propanethiol	56.3130	92.3383	64.0%	44.9043	-20.3%	18.7199	-66.7%	43.8530	-22.1%	56.3602	0.08%
2-Propanethiol	44.0204	91.5368	107.9%	35.4603	-19.4%	23.7058	-46.1%	34.1728	-22.4%	44.0189	0.00%
3-Methyl-2-butanethiol	68.3807	93.4167	36.6%	54.1987	-20.7%	13.9220	-79.7%	53.4724	-21.8%	68.3155	-0.10%
Dihydrogen Sulfide	7.6048	88.6455	1065.6%	7.2607	-4.5%	38.3673	406.9%	5.0742	-33.3%	7.5606	-0.58%
Ethanethiol	31.7620	90.6107	185.3%	26.0137	-18.1%	28.6033	-9.9%	24.4539	-23.0%	31.7603	-0.01%
Methanethiol	19.5751	89.6681	358.1%	16.6108	-15.1%	33.5268	71.2%	14.7089	-24.9%	19.6026	0.14%
Tin											
Diethylstannane	59.5034	N/A	N/A	44.7874	-24.7%	N/A	N/A	N/A	N/A	59.5403	0.06%
Dimethylstannane	35.1420	N/A	N/A	26.3660	-25.0%	N/A	N/A	N/A	N/A	35.2249	0.24%
Dimethyltin dichloride	37.1237	N/A	N/A	32.3360	-12.9%	N/A	N/A	N/A	N/A	36.4330	-1.86%
Hexaethyldistannane	164.7613	N/A	N/A	124.6357	-24.4%	N/A	N/A	N/A	N/A	164.9090	0.09%
Hexamethyldistannane	91.7557	N/A	N/A	67.9087	-26.0%	N/A	N/A	N/A	N/A	91.9630	0.23%
Hexaphenyldistannane	333.2704	N/A	N/A	237.9203	-28.6%	N/A	N/A	N/A	N/A	337.1450	1.16%
Methyltin trichloride	25.6912	N/A	N/A	25.0342	-2.6%	N/A	N/A	N/A	N/A	24.6953	-3.88%
Stannane	10.4718	N/A	N/A	6.6015	-37.0%	N/A	N/A	N/A	N/A	10.5414	0.66%
Tetra-allyltin	139.2066	N/A	N/A	99.5932	-28.5%	N/A	N/A	N/A	N/A	133.5360	-4.07%
Tetra-n-butyltin	205.6006	N/A	N/A	158.0889	-23.1%	N/A	N/A	N/A	N/A	205.8010	0.10%
Tetra-n-propyltin	157.0125	N/A	N/A	120.7008	-23.1%	N/A	N/A	N/A	N/A	157.1700	0.10%
Tetracyclohexyltin	284.5760	N/A	N/A	215.4928	-24.3%	N/A	N/A	N/A	N/A	283.6790	-0.32%

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
Tetraethyltin	108.4375	N/A	N/A	82.9803	-23.5%	N/A	N/A	N/A	N/A	108.5390	0.09%
Tetraisobutyltin	206.7323	N/A	N/A	158.2173	-23.5%	N/A	N/A	N/A	N/A	206.0910	-0.31%
Tetraisopropyltin	156.9995	N/A	N/A	120.3223	-23.4%	N/A	N/A	N/A	N/A	157.5740	0.37%
Tetramethyltin	60.1397	N/A	N/A	45.8712	-23.7%	N/A	N/A	N/A	N/A	59.9085	-0.38%
Tetraphenyltin	221.6143	N/A	N/A	159.5224	-28.0%	N/A	N/A	N/A	N/A	223.3630	0.79%
Tetravinyltin	86.5380	N/A	N/A	61.8558	-28.5%	N/A	N/A	N/A	N/A	84.6444	-2.19%
Tin Tetrachloride SnCl4	13.0370	N/A	N/A	17.4750	34.0%	N/A	N/A	N/A	N/A	12.9576	-0.61%
Tri-n-butyltin bromide	157.2655	N/A	N/A	125.2630	-20.3%	N/A	N/A	N/A	N/A	157.0970	-0.11%
Triethylvinyltin	102.8391	N/A	N/A	77.6216	-24.5%	N/A	N/A	N/A	N/A	102.5660	-0.27%
Trimethyl-t-butyltin	96.4781	N/A	N/A	73.8559	-23.4%	N/A	N/A	N/A	N/A	96.8141	0.35%
Trimethylethyltin	72.1992	N/A	N/A	55.2136	-23.5%	N/A	N/A	N/A	N/A	72.0662	-0.18%
Trimethylisopropyltin	84.3235	N/A	N/A	64.3641	-23.7%	N/A	N/A	N/A	N/A	84.3247	0.00%
Trimethylstannane	47.7735	N/A	N/A	35.9595	-24.7%	N/A	N/A	N/A	N/A	47.5667	-0.43%
Trimethyltin bromide	48.3536	N/A	N/A	40.9941	-15.2%	N/A	N/A	N/A	N/A	47.6780	-1.40%
Trimethyltin chloride	49.0069	N/A	N/A	39.0919	-20.2%	N/A	N/A	N/A	N/A	48.1707	-1.71%
Trimethyltin iodide	47.6985	N/A	N/A	34.2650	-28.2%	N/A	N/A	N/A	N/A	47.3606	-0.71%
Trimethylvinyltin	66.4326	N/A	N/A	49.8383	-25.0%	N/A	N/A	N/A	N/A	66.0925	-0.51%
Triphenylethyltin	192.9253	N/A	N/A	140.5451	-27.2%	N/A	N/A	N/A	N/A	194.6570	0.90%
Triphenylmethyltin	180.9788	N/A	N/A	131.1760	-27.5%	N/A	N/A	N/A	N/A	182.5000	0.84%
Triphenyltin Bromide	169.9151	N/A	N/A	125.9869	-25.9%	N/A	N/A	N/A	N/A	170.2690	0.21%
Triphenyltin iodide	167.8795	N/A	N/A	119.2231	-29.0%	N/A	N/A	N/A	N/A	169.9520	1.23%
Triphenyltrimethyldistannane	212.7297	N/A	N/A	153.0165	-28.1%	N/A	N/A	N/A	N/A	214.5540	0.86%

Urea

Molecule	Exp Tot E	3-21G Tot E (Eq. 100)	Rel error	3-21G Tot E (Eq. 101)	Rel error	6-31G* Tot E (Eq. 100)	Rel error	6-31G* Tot E (Eq. 101)	Rel error	Millsian Tot E	Rel error
Urea	31.3930	39.5924	26.1%	18.0087	-42.6%	N/A	N/A	N/A	N/A	31.3592	-0.11%

Figure Captions

Figure 1. A bound electron is a constant two-dimensional spherical surface of charge (zero thickness, total charge $= \theta = \pi$, and total mass$=m_e$), called *an electron orbitsphere.* The corresponding uniform current-density function having angular momentum components of $\mathbf{L}_{xy} = \dfrac{\hbar}{4}$ and $\mathbf{L}_z = \dfrac{\hbar}{2}$ give rise to the phenomenon of electron spin.

Figures 2A-B. The bound electron exists as a spherical two-dimensional supercurrent (electron *orbitsphere*), an extended distribution of charge and current completely surrounding the nucleus. Unlike a spinning sphere, there is a complex pattern of motion on its surface (indicated by vectors) that generates two orthogonal components of angular momentum (Figure 1) that give rise to the phenomenon of electron spin. (A) A great-circle representation of the z-axis view of the total current pattern of the $Y_0^0(\phi,\theta)$ orbitsphere comprising 144 great circle current elements. (B) A representation of the $\left(-\dfrac{1}{\sqrt{2}}\mathbf{i}_x, \dfrac{1}{\sqrt{2}}\mathbf{i}_y, \mathbf{i}_z \right)$-axis view of the total uniform current-density pattern of the $Y_0^0(\phi,\theta)$ orbitsphere with 144 vectors overlaid on the continuous bound-electron current density giving the direction of the current of each great circle element (nucleus not to scale).

Figure 3. The orbital function modulates the constant (spin) function, (shown for $t = 0$; three-dimensional view).

Figures 4A-B. Prolate spheroidal H_2 MO, an equipotential minimum energy two-dimensional surface of charge and current that is stable to radiation. (A) External surface showing the charge density that is proportional to the distance from the origin to the tangent to the surface with the maximum density of the MO closest to the nuclei, an energy minimum. (B) Prolate spheroid parameters of molecules and molecular ions where a is the semimajor axis, $2a$ is the total length of the molecule or molecular ion along the principal axis, $b = c$ is the semiminor axis, $2b = 2c$ is the total width of the molecule or molecular ion along the minor axis, c' is the distance from the origin to a focus (nucleus), $2c'$ is the internuclear distance, and the protons are at the foci.

Figure 5. C_4H_{10} MO comprising a linear combination of $C-H$-bond MOs and $C-C$-bond MOs of the two methyl and two methylene groups. (A) Color scale, translucent view of the charge-density of the $C-C$-bond and $C-H$-bond MOs and the $C_{\text{butane}} 2sp^3$ HOs. Each $C-C$-bond MO comprises a H_2-type ellipsoidal MO bridging two $C_{\text{butane}} 2sp^3$ HOs. For each $C-H$ and the $C-C$ bond, the ellipsoidal surface of the H_2-type ellipsoidal MO that transitions to the $C_{\text{butane}} 2sp^3$ HO, the $C_{\text{butane}} 2sp^3$ HO shell, inner most $C1s$ shell, and the nuclei (red, not to scale), are shown. (B)-(C) Opaque view and translucent view high-lighting the $C-C$-bond MOs of the charge-density of the C_4H_{10} MO.

Figure 6. $C_{18}H_{38}$ MO comprising a linear combination of $C-H$-bond MOs and $C-C$-bond MOs of the two methyl and sixteen methylene groups. (A) Opaque view of the charge-density of the $C-C$-bond and $C-H$-bond MOs. Each $C-C$-bond MO comprises a H_2-type ellipsoidal MO bridging two $C_{\text{octadecane}} 2sp^3$ HOs. (B) Translucent view high-lighting the $C-C$-

bond MOs of the charge-density of the $C_{18}H_{38}$ MO. For each $C-H$ and the $C-C$ bond, the ellipsoidal surface of the H_2-type ellipsoidal MO that transitions to the $C_{octadecane}2sp^3$ HO, the $C_{octadecane}2sp^3$ HO shell, inner most $C1s$ shell, and the nuclei (red, not to scale), are shown.

Figure 7. Opaque pentagonal view of the charge-density of the C_{60} MO high-lighting the twenty hexagonal and twelve pentagonal units joined together such that no two pentagons share an edge. The six-six ring edges are $C=C$ bonds and the five-five ring edges are $C-C$-bonds such that each hexagon is comprised of alternating $C=C$-bond MOs and $C-C$-bond MOs and each pentagon is comprised of only $C-C$-bond MOs.

Figure 8. C_{60} MO comprising a hollow cage of sixty carbon atoms bound with the linear combination of sixty sets of $C-C$-bond MOs bridged by 30 sets of $C=C$-bond MOs. A $C=C$ group is bound to two $C-C$ groups at each vertex carbon atom of C_{60}. Color scale, translucent pentagonal view of the charge-density of the C_{60}-bond MO with each $C2sp^3$ HO shown transparently. For each $C-C$ and $C=C$ bond, the ellipsoidal surface of the H_2-type ellipsoidal MO that transitions to the $C2sp^3$ HO, the $C2sp^3$ HO shell, inner most $C1s$ shell, and the nuclei (red, not to scale), are shown.

Figure 9. Color scale, translucent view of the charge-density of benzoic acid.

Figure 10. Color scale, translucent view of the charge-density of adenine.

Figure 11. Color scale, translucent view of the charge-density of phenylborinic anhydride.

Figure 12. Color scale, opaque view of the charge-density of $\left(C_6H_5\right)_3 SnSn\left(C_6H_5\right)_3$.

Figure 13. Color scale, opaque view of the charge-density of representative polypeptide phenylalanine-leucine-glutami ne-aspartic acid (phe-leu-gln-asp). Using the amino-acid functional groups, proteins of any length and complexity may be rendered.

Figure 14. Color scale rendering of the charge-density of the representative DNA fragment $\begin{array}{c}\text{ACTGACTGACTG}\\\text{TGACTGACTGAC}\end{array}$. Using the nucleotide functional groups, DNA or RNA of any length and complexity may be rendered.

Figures 15A-B. Comparison of the rendering of the simple alkane butane (C_4H_{10}) using the two basis sets with an arbitrary cutoff of the all-space density at 95%. (A) C_4H_{10} rendered using the Spartan with the 3-21G basis set. (B) C_4H_{10} rendered using the Spartan with the 3-31G* basis set. Neither shows any resemblance to butane in that they are not even symmetrical, nor do the density patterns from the two basis sets show any resemblance to each other. The results are not even internally consistent in addition to giving large errors in predicted energies.
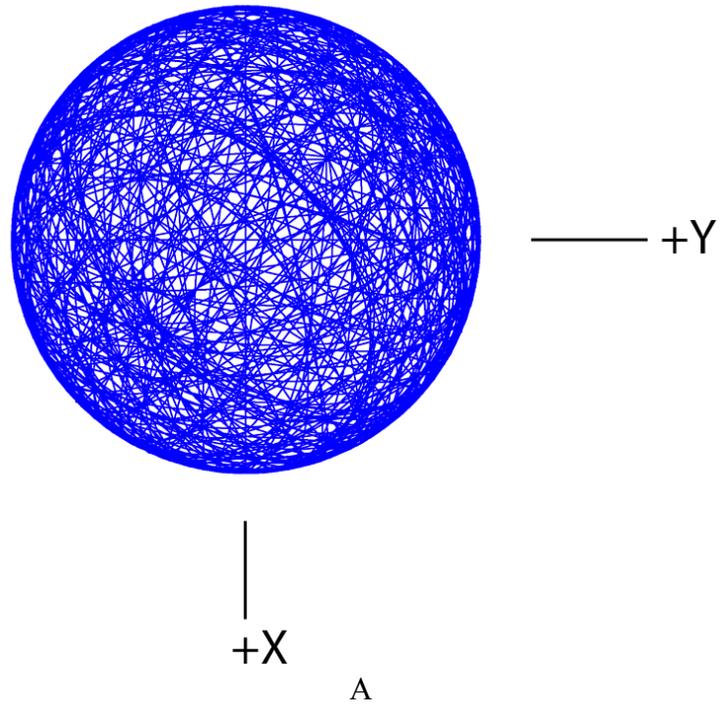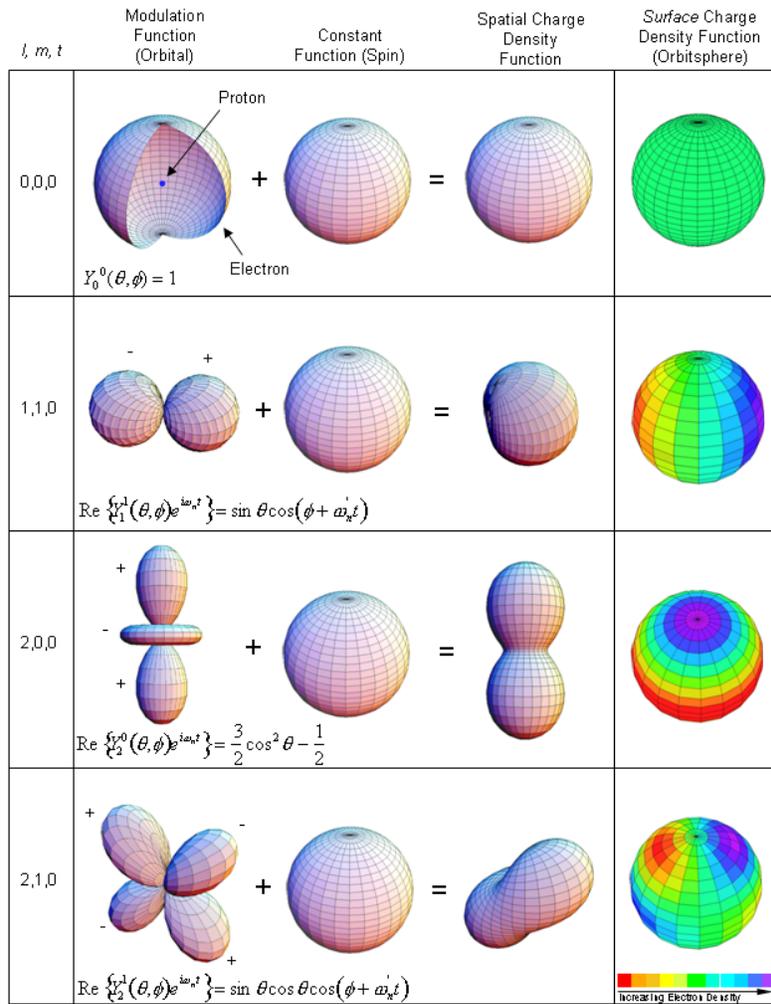
Fig. 1

Fig. 2

+Y

+X

A

B

Fig. 3

l, m, t	Modulation Function (Orbital)	Constant Function (Spin)	Spatial Charge Density Function	Surface Charge Density Function (Orbitsphere)
0,0,0	Proton / Electron $Y_0^0(\theta,\phi) = 1$	+	=	
1,1,0	− + $\mathrm{Re}\left\{Y_1^1(\theta,\phi)e^{i\omega_n t}\right\} = \sin\theta\cos\left(\phi + \omega_n' t\right)$	+	=	
2,0,0	+ − + $\mathrm{Re}\left\{Y_2^0(\theta,\phi)e^{i\omega_n t}\right\} = \frac{3}{2}\cos^2\theta - \frac{1}{2}$	+	=	
2,1,0	+ − − + $\mathrm{Re}\left\{Y_2^1(\theta,\phi)e^{i\omega_n t}\right\} = \sin\theta\cos\theta\cos\left(\phi + \omega_n' t\right)$	+	=	

Increasing Electron Density

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Fig. 4A-B

Increasing Electron Density
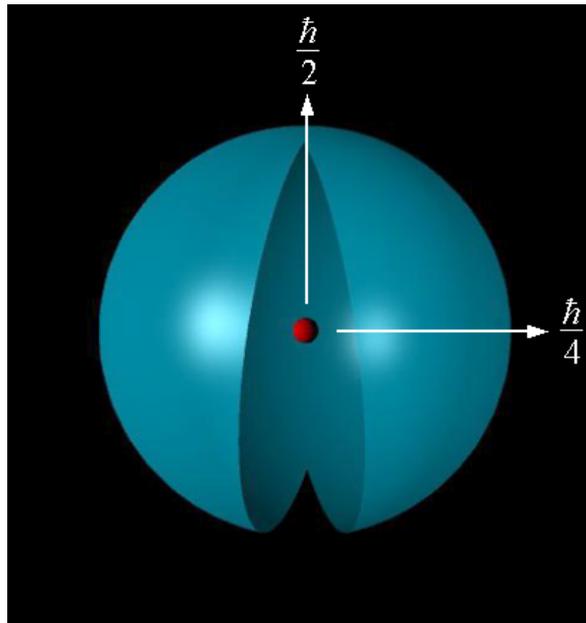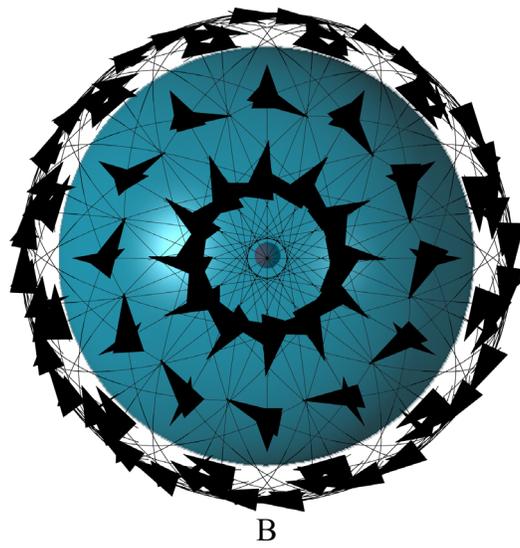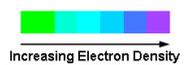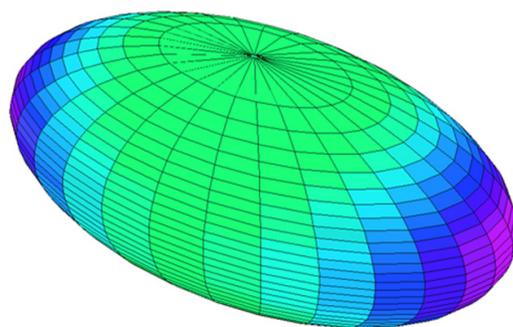
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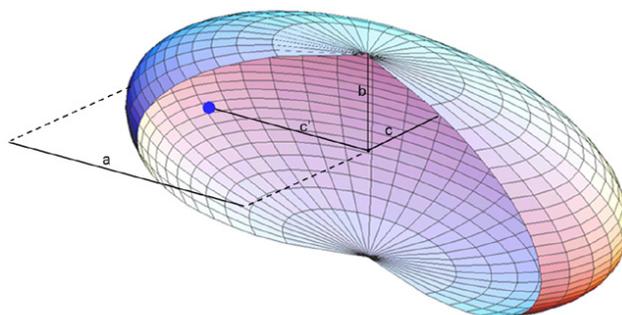
B

Fig. 5
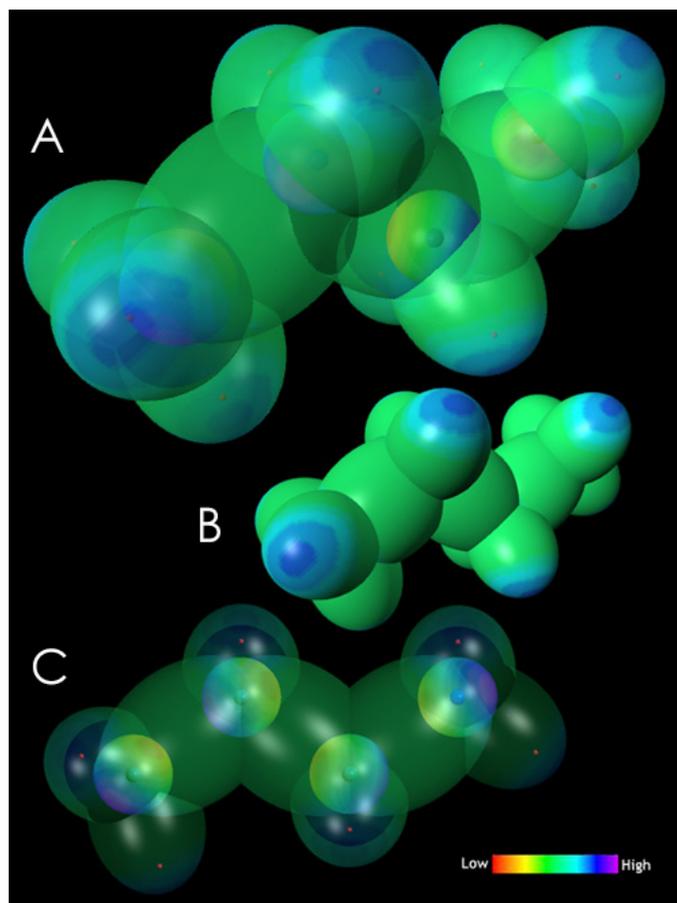
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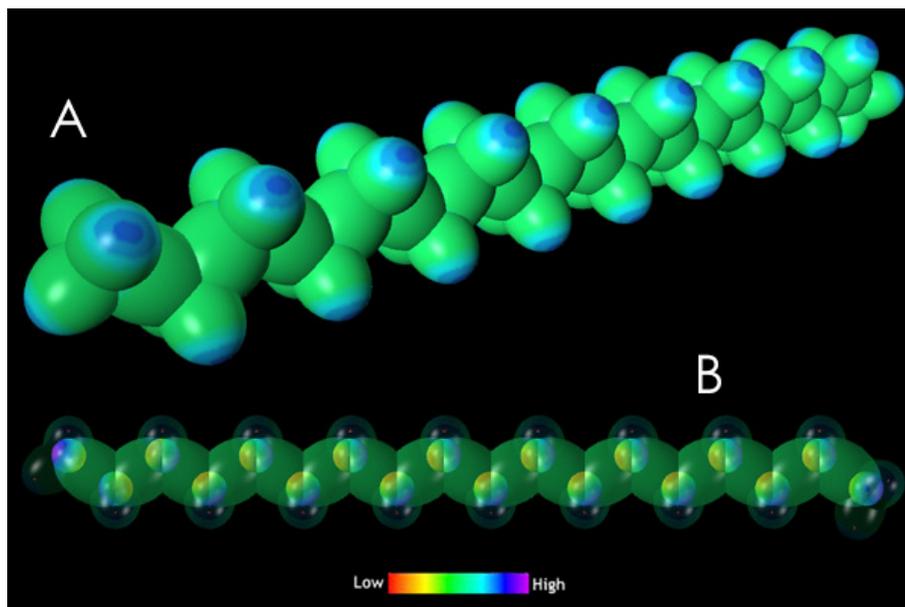
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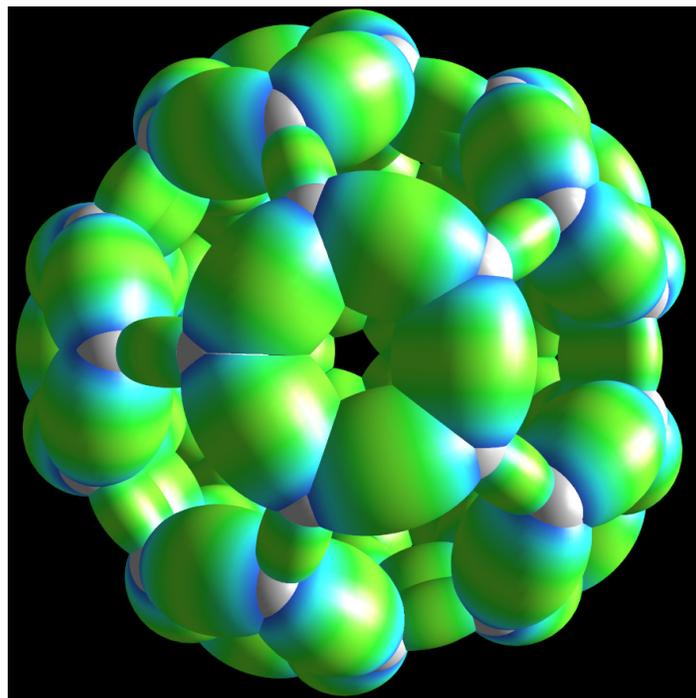
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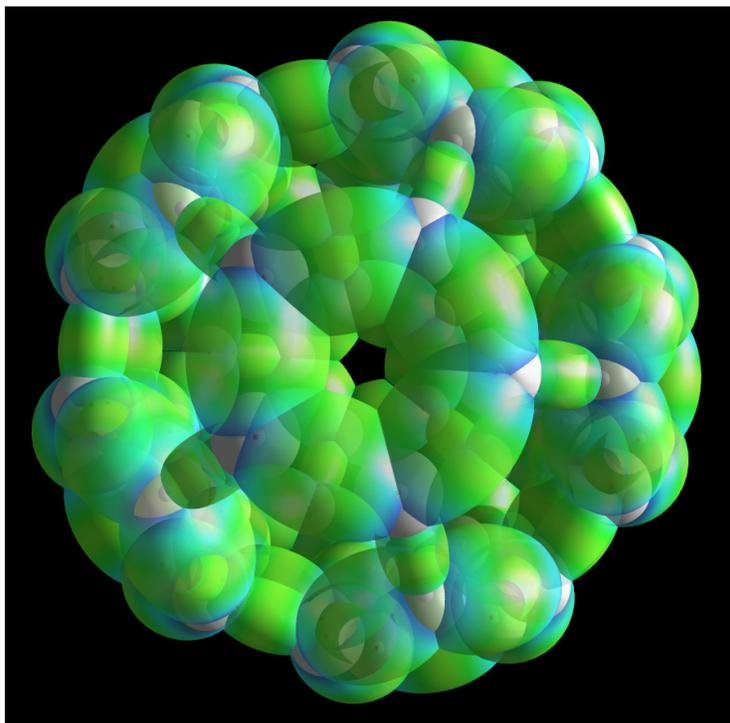
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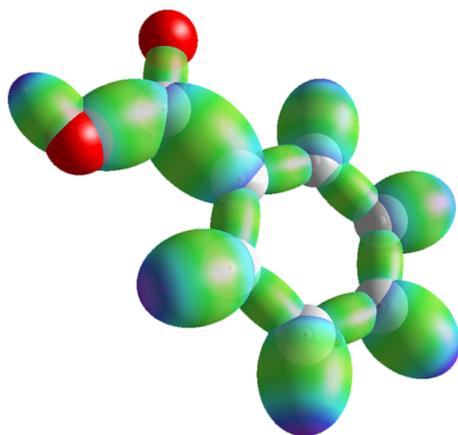
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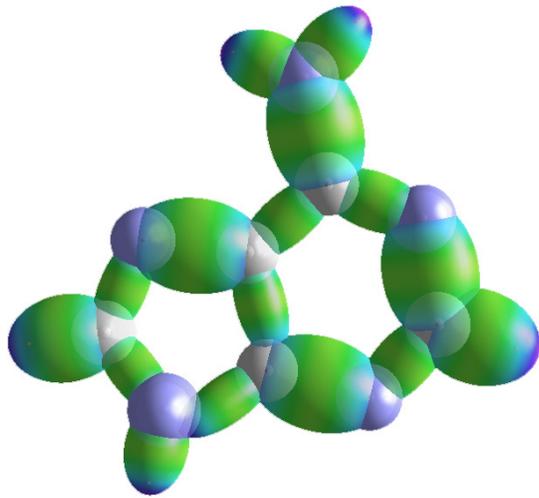
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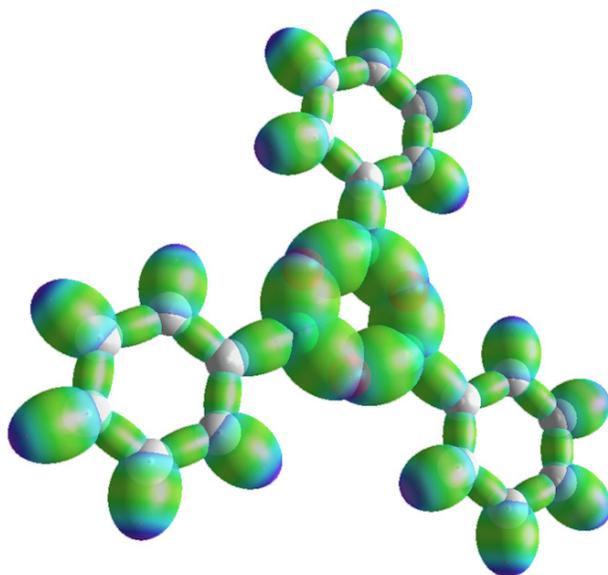
Fig. 12

Fig. 13

Fig. 14

Fig. 15A-B

A

B