

Total bond energies of exact classical solutions of molecules generated by MILLSIAN 1.0 compared to those computed using modern 3–21 G and 6–31 G* basis sets

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Abstract: Mills 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 precomputed database using 3–21 G and 6–31 G* 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 experimental values. In contrast, the 3–21 G and 6–31 G* 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. © 2010 Physics Essays Publication. [DOI: 10.4006/1.3310832]

Résumé: Mills a déterminé la structure de l'électron liée utilisant les lois classiques et par la suite a développé une théorie de l'unification fondée sur ces lois intitulée la Théorie de la grande unification de la physique classique. Les résultats correspondent aux observations des phénomènes de base de la physique et la chimie allant de l'échelle des quarks à celle du cosmos. MILLSIAN 1.0 est un logiciel d'application de modélisation moléculaire de la Théorie de la grande unification de la physique classique. Il détermine les structures atomiques et moléculaires en appliquant les lois classiques de la physique (lois de Newton et Maxwell) à l'échelle atomique. Les groupes fonctionnels de toutes les classes majeures de liaison chimique comprenant ceux impliqués dans la plupart des molécules organiques ont été exactement déterminés par les solutions de forme fermée. L'utilisation des groupes fonctionnels comme éléments constitutifs ou indépendants, peut potentiellement résoudre un nombre infini de molécules. Par conséquent, le logiciel MILLSIAN visualise la structure tridimensionnelle exacte et calcule les caractéristiques physiques de presque toute molécule sans égard à sa longueur ou complexité. Même les protéines et l'ADN (les molécules qui comportent les informations génétiques) peuvent être calculés sur un PC normal de manière interactive en temps réel. Les logiciels précédents utilisant les méthodes quantiques traditionnelles doivent, par contre dépendre d'approximations et nécessitent des ordinateurs puissants pour même les systèmes les plus simples. Les énergies des solutions classiques exactes des molécules telles que générées par MILLSIAN 1.0 et celles du programme moderne de mécanique quantique, la base de données précalculée SPARTAN qui utilise les bases minimales 3–21 G et 6–31 G* au niveau de la théorie Hartree–Fock ont été comparées aux valeurs expérimentales. Les résultats MILLSIENS tombaient régulièrement à l'intérieur de la déviation relative moyenne d'environ 0,1% des valeurs expérimentales. Au contraire, les résultats 3–21 G and 6–31 G* s'écartaient sur une grande plage d'erreur relative, notamment entre >30%–150% dont un important pourcentage d'échecs catastrophiques suivant le type de groupe fonctionnel et de bases minimales.

Key words: Classical Physics; Molecular Modeling; Functional Groups; Organic Molecules; Biomolecules.

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 theories, 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 non-radiation 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 quantum mechanics (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: “ $\Psi \rightarrow 0$ as $r \rightarrow \infty$,” 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 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, Jackson²⁰ gave 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

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

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

$$\begin{aligned} G(\mathbf{x}', \mathbf{x}) &= \frac{e^{-ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} \\ &= ik \sum_{\ell=0}^{\infty} j_{\ell}(kr_{<}) h_{\ell}^{(1)}(kr_{>}) \\ &\quad \times \sum_{m=-\ell}^{\ell} Y_{\ell,m}^*(\theta', \phi') Y_{\ell,m}(\theta, \phi). \end{aligned} \quad (2)$$

Jackson²⁰ further gave the general multipole field solution to Maxwell's equations in a source-free region of empty space with the assumption of a time dependence $e^{i\omega t}$:

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

$$\mathbf{E} = \sum_{\ell,m} \left[\frac{i}{k} a_E(\ell,m) \nabla \times f_\ell(kr) \mathbf{X}_{\ell,m} + a_M(\ell,m) g_\ell(kr) \mathbf{X}_{\ell,m} \right], \quad (3)$$

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

$$g_\ell(kr) = A_\ell^{(1)} h_\ell^{(1)} + A_\ell^{(2)} h_\ell^{(2)}. \quad (4)$$

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

$$\mathbf{X}_{\ell,m}(\theta, \phi) = \frac{1}{\sqrt{\ell(\ell+1)}} \mathbf{L} Y_{\ell,m}(\theta, \phi), \quad (5)$$

where

$$\mathbf{L} = \frac{1}{i} (\mathbf{r} \times \nabla) \quad (6)$$

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 gave the result of the electric and magnetic coefficients from the sources as

$$a_E(\ell, m) = \frac{4\pi k^2}{i\sqrt{\ell(\ell+1)}} \int Y_\ell^{m*} \left\{ \rho \frac{\partial}{\partial r} [r j_\ell(kr)] + \frac{ik}{c} (\mathbf{r} \cdot \mathbf{J}) j_\ell(kr) - ik \nabla \cdot (r \times \mathbf{M}) j_\ell(kr) \right\} d^3x \quad (7)$$

and

$$a_M(\ell, m) = \frac{-4\pi k^2}{\sqrt{\ell(\ell+1)}} \int j_\ell(kr) Y_\ell^{m*} \mathbf{L} \cdot \left(\frac{\mathbf{J}}{c} + \nabla \times \mathbf{M} \right) d^3x, \quad (8)$$

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

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 Gauss' law which for a point charge or a two-dimensional spherical shell at a distance r from the nucleus the potential is

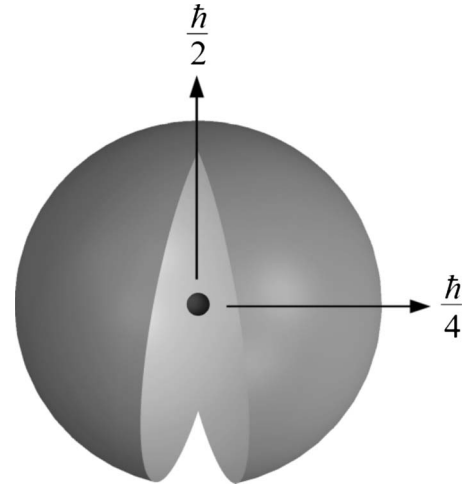


FIG. 1. A bound electron is a constant two-dimensional spherical surface of charge (zero thickness, total charge $= -e$, and total mass $= m_e$), called an *electron orbitsphere*. The corresponding uniform current-density function having angular momentum components of $\mathbf{L}_{xy} = \hbar/4$ and $\mathbf{L}_z = \hbar/2$ following Larmor excitation in a magnetic field gives rise to the phenomenon of electron spin.

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}. \quad (9)$$

Thus, consideration of conservation of energy would require that the electron radius must be fixed. Additional 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 II of Ref. 1), and exact electroneutrality of the hydrogen atom wherein the electric field is given by

$$\mathbf{n} \cdot (\mathbf{E}_1 - \mathbf{E}_2) = \frac{\sigma_s}{\epsilon_0}, \quad (10)$$

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

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

where r_n is an allowed radius. This function defines the charge density on a spherical shell of a fixed radius (see Fig. 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

$$2\pi r_n = \lambda_n. \quad (12)$$

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

$$\nu_n = \frac{h}{m_e \lambda_n} = \frac{h}{m_e 2\pi r_n} = \frac{\hbar}{m_e r_n}, \quad (13)$$

$$\omega_n = \frac{\hbar}{m_e r_n^2}. \quad (14)$$

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 [$f(r)=(1/r^2)\delta(r-r_n)$], 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 ensure that the function is positive definite, the form of the angular solution must be a superposition:

$$Y_0^0(\theta, \phi) + Y_\ell^m(\theta, \phi). \quad (15)$$

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

$$\ell = 0,$$

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

$$\ell \neq 0,$$

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

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 $\text{Re}\{Y_\ell^m(\theta, \phi)e^{im\omega_n t}\} = P_\ell^m(\cos \theta)\cos(m\phi + m\omega_n t)$.

The Fourier transform of the electron charge-density function is a solution of the four-dimensional wave equation in frequency space ($\mathbf{k}, \omega$ -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.

$$\begin{aligned} K(s, \Theta, \Phi, \omega) &= 4\pi\omega_n \frac{\sin(2s_n r_n)}{2s_n r_n} \otimes 2\pi \sum_{\nu=1}^{\infty} \frac{(-1)^{\nu-1} (\pi \sin \Theta)^{2(\nu-1)}}{(v-1)!(v-1)!} \frac{\Gamma(\frac{1}{2})\Gamma(v+\frac{1}{2})}{(\pi \cos \Theta)^{2\nu+1} 2^{\nu+1}} \frac{2\nu!}{(v-1)!} s^{-2\nu} \\ &\otimes 2\pi \sum_{\nu=1}^{\infty} \frac{(-1)^{\nu-1} (\pi \sin \Phi)^{2(\nu-1)}}{(v-1)!(v-1)!} \frac{\Gamma(\frac{1}{2})\Gamma(v+\frac{1}{2})}{(\pi \cos \Phi)^{2\nu+1} 2^{\nu+1}} \frac{2\nu!}{(v-1)!} s^{-2\nu} \frac{1}{4\pi} [\delta(\omega - \omega_n) + \delta(\omega + \omega_n)]. \end{aligned} \quad (18)$$

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

$$\mathbf{s}_n \cdot \mathbf{v}_n = \mathbf{s}_n \cdot \mathbf{c} = \omega_n, \quad (19)$$

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

$$r_n = \lambda_n. \quad (20)$$

Substitution of Eq. (20) into the sinc function results in the vanishing of the entire Fourier transform of the current-density function. Thus, spacetime harmonics of $\omega_n/c=k$ or $(\omega_n/c)\sqrt{\epsilon/\epsilon_0}=k$ 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 Refs. 22 and 23). Nonradiation is also shown directly using Maxwell's equations 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 macrospherical wave in the far field.

In Chap. 1 of Ref. 1, the uniform current-density function $Y_0^0(\theta, \phi)$ [Eqs. (16) and (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

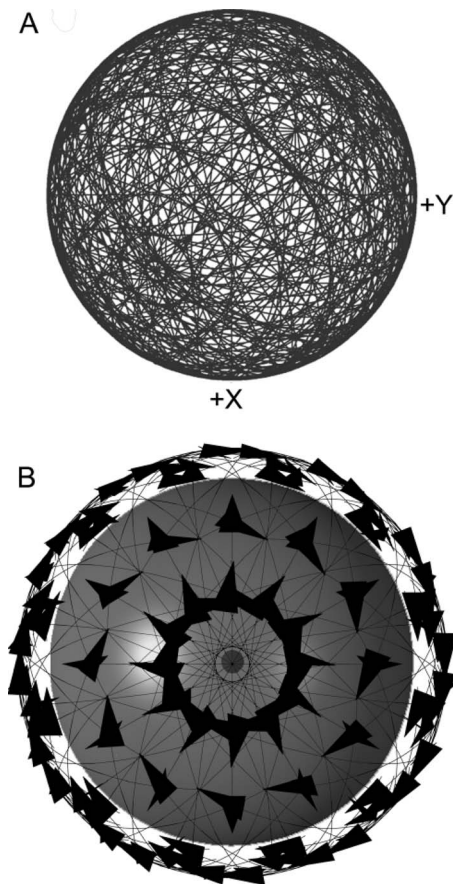


FIG. 2. The bound electron exists as a spherical two-dimensional supercurrent (electron *orbitsphere*), an extended distribution of charge and current completely surrounding the nucleus. Unlike a spinning sphere, there is a complex pattern of motion on its surface (indicated by vectors) that generates two orthogonal components of angular momentum (Fig. 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 $(-1/\sqrt{2}\mathbf{i}_x, 1/\sqrt{2}\mathbf{i}_y, \mathbf{i}_z)$ -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).

rotations of two orthogonal great circle current loops that serve as basis elements about each of the $(-\mathbf{i}_x, \mathbf{i}_y, 0\mathbf{i}_z)$ and $(-1/\sqrt{2}\mathbf{i}_x, 1/\sqrt{2}\mathbf{i}_y, \mathbf{i}_z)$ -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 $\mathbf{L}_{xy} = \pm \hbar/4$ ($\pm$ designates both the positive and negative vector directions along an axis in the xy -plane and Larmor excitation selects one of these components) and $\mathbf{L}_z = \hbar/2$. 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 Fig. 2(A). As the number of great circles goes to infinity, the current distribution becomes continuous and is exactly uniform following normalization. A representation of the $(-1/\sqrt{2}\mathbf{i}_x, 1/\sqrt{2}\mathbf{i}_y, \mathbf{i}_z)$ -axis view of the total uniform current-density pattern of the $Y_0^0(\theta, \phi)$ 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 Fig. 2(B). This super-

conducting 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 pointlike (behaves like a point at the origin). The free electron is continuous with the bound electron as it is ionized and is also pointlike, 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 Fig. 1 for the charge function and Fig. 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 velocities, 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 1 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 Fig. 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 previously¹⁻¹² 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 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

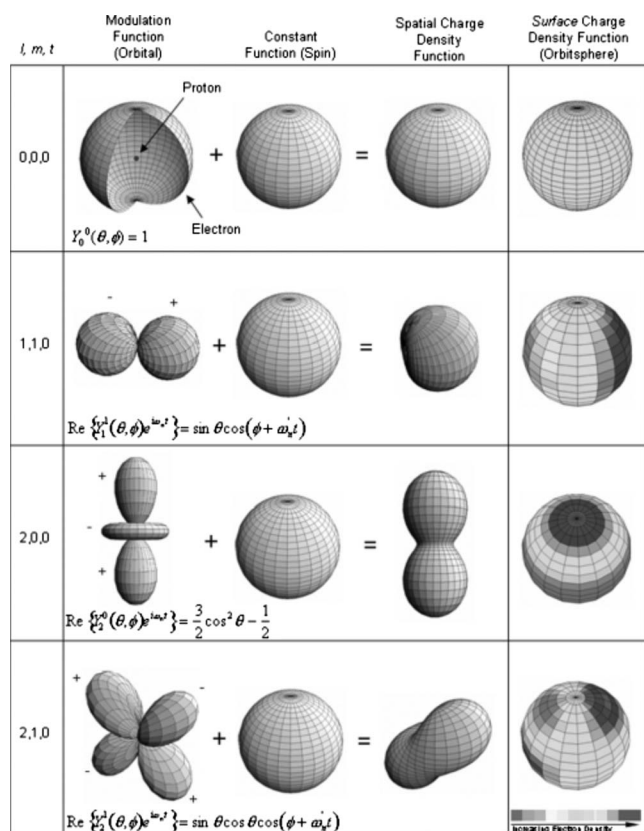


FIG. 3. The orbital function modulates the constant (spin) function, (shown for $t=0$; three-dimensional view).

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 non-physical, unpredictable, 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 non-radiative 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 1–21 electron atoms are available from the internet²⁴. For 400 atoms and ions, the agreement between the predicted and experimental results is 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 molecular ion 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 arises 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 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 Fig. 4 for H_2 which is direct evidence that molecular orbitals (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'

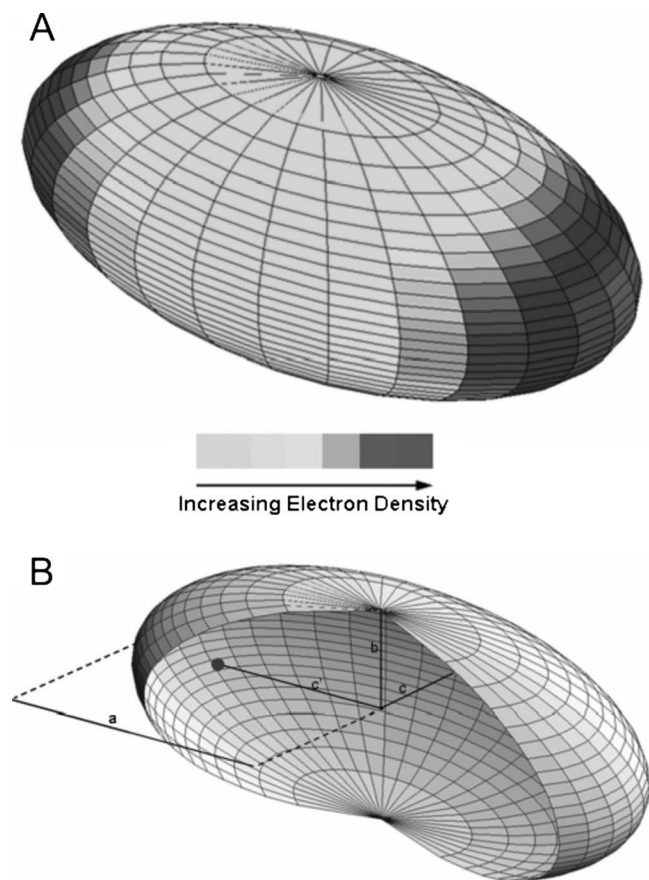


FIG. 4. Prolate spheroidal H_2 MO, an equipotential minimum-energy two-dimensional surface of charge and current that is stable to radiation. (A) External surface showing the charge density that is proportional to the distance from the origin to the tangent to the surface with the maximum density of 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.

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 non-physical 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 momenta, lack of physical relativistic invariance, and the electron is unbounded such that the edge of

TABLE I. Partial list of organic functional groups solved by classical physics.

Continuous-chain alkanes	<i>N,N</i> -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	Imidazole
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	

molecules 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 I.

The two basic equations that solve 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 are 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 II. 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}

$$\begin{aligned} &(\eta - \xi)R_{\xi}\frac{\partial}{\partial\xi}\left(R_{\xi}\frac{\partial\phi}{\partial\xi}\right) + (\xi - \eta)R_{\eta}\frac{\partial}{\partial\eta}\left(R_{\eta}\frac{\partial\phi}{\partial\eta}\right) \\ &+ (\xi - \eta)R_{\xi}\frac{\partial}{\partial\xi}\left(R_{\xi}\frac{\partial\phi}{\partial\xi}\right) = 0. \end{aligned} \quad (21)$$

1. The geometrical parameters of the hydrogen molecule

As shown in Fig. 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

$$\frac{\hbar^2}{m_e a^2 b^2} D = \frac{e^2}{8\pi\epsilon_0 a b^2} D + \frac{\hbar^2}{2m_e a^2 b^2} D, \quad (22)$$

where

$$D = \mathbf{r}(t) \cdot \mathbf{i}_{\xi} \quad (23)$$

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

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

when the semimajor axis, a , is

TABLE II. Partial list of additional molecules and compositions of matter solved by classical physics.

Solid molecular bond of the three allotropes of carbon
Diamond
Graphite
Fullerene (C_{60})
Dipole-dipole bonding
Hydrogen bonding
Van der Waals bonding
Solid ionic bond of alkali-hydrides and halides
Alkali-hydride crystal structures
Lithium hydride
Sodium hydride
Potassium hydride
Rubidium and cesium hydride
Potassium hydrino hydride
Solid metallic bond of alkali metals
Alkali metal crystal structures
Lithium metal
Sodium metal
Potassium metal
Rubidium and cesium metals
Alkyl aluminum hydrides
Silicon groups and molecules
Silanes
Alkyl silanes and disilanes
Solid semiconductor bond of silicon
Insulator-type semiconductor bond
Conductor-type semiconductor bond
Boron molecules
Boranes
Bridging bonds of boranes
Alkoxy boranes
Alkyl boranes
Alkyl borinic acids
Tertiary aminoboranes
Quaternary aminoboranes
Borane amines
Halido boranes
Organometallic molecular functional groups and molecules
Alkyl aluminum hydrides
Bridging bonds of organoaluminum hydrides
Organogermanium and digermanium
Organolead
Organoarsenic
Organoantimony
Organobismuth
Organic ions
1° amino
2° amino
Carboxylate
Phosphate
Nitrate
Sulfate
Silicate
Proteins
Amino acids
Peptide bonds
DNA
Bases
2-deoxyribose

TABLE II. (Continued.)

Ribose
Phosphate backbone
Water
Condensed noble gases

$$a = a_o. \quad (25)$$

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

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

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

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

The eccentricity, e , is

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

2. The energies of the hydrogen molecule

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

$$V_e = \frac{-2e^2}{8\pi\epsilon_o\sqrt{a^2-b^2}} \ln \frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} = -67.836 \text{ eV}. \quad (29)$$

The potential energy of the two protons is

$$V_p = \frac{e^2}{8\pi\epsilon_o\sqrt{a^2-b^2}} = 19.242 \text{ eV}. \quad (30)$$

The kinetic energy of the electrons is

$$T = \frac{\hbar^2}{2m_e a \sqrt{a^2-b^2}} \ln \frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} = 33.918 \text{ eV}. \quad (31)$$

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

$$V_m = \frac{-\hbar^2}{4m_e a \sqrt{a^2-b^2}} \ln \frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}} = -16.959 \text{ eV}. \quad (32)$$

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

$$\begin{aligned} \bar{E}_{\text{osc}} &= \bar{E}_D + \bar{E}_{\text{Kvib}} \\ &= (V_e + T + V_m + V_p) \sqrt{\frac{2\bar{E}_K}{Mc^2}} + \frac{1}{2}\hbar \sqrt{\frac{k}{\mu}}. \end{aligned} \quad (33)$$

The total energy is

$$E_T = V_e + T + V_m + V_p + \bar{E}_{\text{osc}}, \quad (34)$$

$$\begin{aligned} E_T &= -\frac{e^2}{8\pi\epsilon_o a_o} \left[\left(2\sqrt{2} - \sqrt{2} + \frac{\sqrt{2}}{2} \right) \ln \frac{\sqrt{2}+1}{\sqrt{2}-1} - \sqrt{2} \right] \\ &\quad \times \left[1 + \sqrt{\frac{2\hbar \sqrt{\frac{e^2}{4\pi\epsilon_o a_o^3}}}{m_e c^2}} \right] - \frac{1}{2}\hbar \sqrt{\frac{k}{\mu}} \\ &= -31.689 \text{ eV}. \end{aligned} \quad (35)$$

The energy of two hydrogen atoms is

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

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)].

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

The experimental energy is $E_D = 4.478 \text{ eV}$. The calculated and experimental parameters of H_2 , D_2 , H_2^+ , and D_2^+ from Ref. 5 and Chap. 11 of Ref. 1 are given in Table III.

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 I 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 functional 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 nonorganic functional groups given in Table II 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 Molecules, and Organometallic Molecular Functional Groups and Molecules sections.

Consider the case wherein at least two atomic orbitals hybridize as a linear combination of electrons at the same

TABLE III. The Maxwellian closed-form calculated and experimental parameters of H₂, D₂, H₂⁺, and D₂⁺.

Parameter	Calc.	Exp.
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	$9.274 \times 10^{-24} \text{ JT}^{-1} (\mu_B)$	$9.274 \times 10^{-24} \text{ JT}^{-1} (\mu_B)$
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 $2a_o$	1.055 9 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	0.014 8 eV	0.015 09 eV
D ₂ $J=1$ to $J=0$ rotational energy ^a	0.007 41 eV	0.007 55 eV
H ₂ ⁺ $J=1$ to $J=0$ rotational energy	0.007 40 eV	0.007 39 eV
D ₂ ⁺ $J=1$ to $J=0$ rotational energy ^a	0.003 70 eV	0.0037 23 eV

^aNot corrected for the slight reduction in internuclear distance due to $\bar{E}_{\text{osc}}$.

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 (HOs) 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 H₂-type-ellipsoidal MO due to the equivalent of two point charges of at the foci is given by

$$k' = \frac{C_1 C_2 2e^2}{4\pi\epsilon_0}, \quad (38)$$

where C_1 is the fraction of the H₂-type-ellipsoidal MO basis function of a chemical bond of the molecule or molecular ion which are 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

$$c' = a \sqrt{\frac{\hbar^2 4\pi\epsilon_0}{m_e e^2 2C_1 C_2 a}} = \sqrt{\frac{aa_0}{2C_1 C_2}}. \quad (39)$$

The internuclear distance is

$$2c' = 2 \sqrt{\frac{aa_0}{2C_1 C_2}}. \quad (40)$$

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

$$b = \sqrt{a^2 - c'^2}. \quad (41)$$

And, the eccentricity, e , is

$$e = \frac{c'}{a}. \quad (42)$$

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

$$V_e = n_1 c_1 c_2 \frac{-2e^2}{8\pi\epsilon_0 \sqrt{a^2 - b^2}} \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}}. \quad (43)$$

The potential energy of the two nuclei is

$$V_p = n_1 \frac{e^2}{8\pi\epsilon_0 \sqrt{a^2 - b^2}}. \quad (44)$$

The kinetic energy of the electrons is

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

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

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

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

$$E_T(H_2MO) = V_e + T + V_m + V_p, \quad (47)$$

$$\begin{aligned} E_T(H_2MO) &= -\frac{n_1 e^2}{8\pi\epsilon_0 \sqrt{a^2 - b^2}} \\ &\times \left[c_1 c_2 \left(2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} - 1 \right] \\ &= -\frac{n_1 e^2}{8\pi\epsilon_0 c'} \left[c_1 c_2 \left(2 - \frac{a_0}{a} \right) \ln \frac{a + c'}{a - c'} - 1 \right] \end{aligned} \quad (48)$$

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 a MO which are 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 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 atomic orbital (AO) of the bonding atoms, the factor c_2 of a H_2 -type-ellipsoidal MO may given by (i) 1, (ii) the ratio of the Coulombic or valence energy of the AO or HO of at least one atom of the bond and 13.605 804 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 the 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 previously¹ are:

- 0.936 127, the ratio of the ionization energy of N 14.534 14 and 13.605 804 eV, the Coulombic energy between the electron and proton of H;
- 0.917 71, the ratio of 14.825 75 eV, $-E_{\text{Coulomb}}(C, 2sp^3)$, and 13.605 804 eV;
- 0.874 95, the ratio of 15.550 33 eV, $-E_{\text{Coulomb}}(C_{\text{ethane}}, 2sp^3)$, and 13.605 804 eV;
- 0.852 52, the ratio of 15.959 55 eV, $-E_{\text{Coulomb}}(C_{\text{ethylene}}, 2sp^3)$, and 13.605 804 eV;
- 0.852 52, the ratio of 15.959 55 eV, $-E_{\text{Coulomb}}(C_{\text{benzene}}, 2sp^3)$, and 13.605 804 eV; and
- 0.863 59, the ratio of 15.550 33 eV, $-E_{\text{Coulomb}}(C_{\text{alkane}}, 2sp^3)$, and 13.605 804 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 $E_T(\text{atom}, msp^3)$ (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.

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

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

$$r_{msp^3} = \sum_{q=Z-n}^{Z-1} \frac{-(Z-q)e^2}{8\pi\epsilon_0 E_T(\text{atom}, msp^3)}. \quad (50)$$

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

$$E_{\text{Coulomb}}(\text{atom}, msp^3) = \frac{-e^2}{8\pi\epsilon_0 r_{msp^3}}. \quad (51)$$

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 $E(\text{magnetic})$ at the initial radius r of the AO electron:

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

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

$$E(\text{atom}, msp^3) = \frac{-e^2}{8\pi\epsilon_0 r_{msp^3}} + \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 r^3}. \quad (53)$$

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 $E(\text{atom}, msp^3)$ 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, $E(\text{atom}, msp^3)$ is the sum of the first ionization energy of the atom and the hybridization energy. An example of $E(\text{atom}, msp^3)$ for $E(C, 2sp^3)$ 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 $E(C, 2sp^3) = -14.63489$ 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 $E_T(\text{mol. atom}, msp^3)$ (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:

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

where IP_m is the m th ionization energy (positive) of the atom and the sum of $-IP_1$ plus the hybridization energy is $E(\text{atom}, msp^3)$. 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

$$\begin{aligned} r_{msp^3} &= \left(\sum_{q=Z-n}^{Z-1} (Z-q) - Q \right) \frac{-e^2}{8\pi\epsilon_0 E_T(\text{mol. atom}, msp^3)} \\ &= \left(\sum_{q=Z-n}^{Z-1} (Z-q) - s(0.25) \right) \\ &\quad \times \frac{-e^2}{8\pi\epsilon_0 E_T(\text{mol. atom}, msp^3)} \end{aligned} \quad (55)$$

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

$$E_{\text{Coulomb}}(\text{mol. atom}, msp^3) = \frac{-e^2}{8\pi\epsilon_0 r_{msp^3}}. \quad (56)$$

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

$$E(\text{mol. atom}, msp^3) = \frac{-e^2}{8\pi\epsilon_0 r_{msp^3}} + \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 r^3} \quad (57)$$

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

$$E_T(\text{atom-atom}, msp^3) = E(\text{mol. atom}, msp^3) - E(\text{atom}, msp^3). \quad (58)$$

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

$$\begin{aligned} r_{2sp^3} &= \sum_{n=2}^5 \frac{(Z-n)e^2}{8\pi\epsilon_0 (e148.25751 \text{ eV})} \\ &= \frac{10e^2}{8\pi\epsilon_0 (e148.25751 \text{ eV})} \\ &= 0.91771a_0, \end{aligned} \quad (59)$$

$$\begin{aligned} E_{\text{Coulomb}}(C, 2sp^3) &= \frac{-e^2}{8\pi\epsilon_0 r_{2sp^3}} \\ &= \frac{-e^2}{8\pi\epsilon_0 0.91771a_0} \\ &= -14.82575 \text{ eV}, \end{aligned} \quad (60)$$

$$\begin{aligned} E(\text{magnetic}) &= \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 (r_3)^3} \\ &= \frac{8\pi\mu_0 \mu_B^2}{(0.84317a_0)^3} \\ &= 0.19086 \text{ eV}, \end{aligned} \quad (61)$$

$$\begin{aligned} E(C, 2sp^3) &= \frac{-e^2}{8\pi\epsilon_0 r_{2sp^3}} + \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 (r_3)^3} \\ &= -14.82575 \text{ eV} + 0.19086 \text{ eV} \\ &= -14.63489 \text{ eV}. \end{aligned} \quad (62)$$

In Eq. (55),

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

Equations (14.147) and (54) give

$$\begin{aligned} E_T(\text{mol. atom}, msp^3) &= E_T(C_{\text{ethane}}, 2sp^3) \\ &= -151.61569 \text{ eV}. \end{aligned} \quad (64)$$

Using Eqs. (55)–(65), the final values of r_{C2sp^3} , $E_{\text{Coulomb}}(C2sp^3)$, and $E(C2sp^3)$, and the resulting $E_T(C-C, C2sp^3)$ of the MO due to charge donation from the HO to the MO where C–C refers to the bond order of the carbon-carbon bond for different values of the parameter s are given in Table IV.

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

MO	Bond order (BO)	s_1	s_2	$r_{C2sp^3}(a_0)$ final	$E_{\text{Coulomb}}(C2sp^3)$ final (eV)	$E(C2sp^3)$ final (eV)	$E_T(C-C, C2sp^3)$ (eV)
I		1	0	0.874 95	-15.550 33	-15.359 46	-0.724 57
II		2	0	0.852 52	-15.959 55	-15.768 68	-1.133 79
III		3	0	0.830 08	-16.390 89	-16.200 02	-1.565 13
IV		4	0	0.807 65	-16.846 19	-16.655 32	-2.020 43

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 HO or AOs, the energy $E(\text{mol. atom}, msp^3)$ of the outer electron of the atom msp^3 shell of each bonding atom must be the average of $E(\text{mol. atom}, msp^3)$ for two different values of s :

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

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

$$E_T(\text{atom-atom}, msp^3) = \frac{E_T(\text{atom-atom}(s_1), msp^3) + E_T(\text{atom-atom}(s_2), msp^3)}{2}. \quad (66)$$

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, $E_T(\text{atom-atom}, msp^3)$ of the C-H-bond MO is given by $0.5E_T(C=C, 2sp^3)$ [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 a 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 IV. 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, $E_T(\text{atom-atom}, msp^3)$, 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:

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

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 $E_{\text{Coulomb}}(\text{atom}, msp^3)$ and $E_T(\text{atom-atom}, msp^3)$, the energy change of each atom msp^3 shell with the formation of each atom-atom-bond MO:

$$r_{msp^3} = \frac{-e^2}{8\pi\epsilon_0 a_0 (E_{\text{Coulomb}}(\text{atom}, msp^3) + E_T(\text{atom-atom}, msp^3))}, \quad (68)$$

where $E_{\text{Coulomb}}(C2sp^3) = -14.825\,751$ eV. The Coulombic energy $E_{\text{Coulomb}}(\text{mol. atom}, msp^3)$ 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 HO, the energy change for the promotion to the unpaired state is the magnetic energy $E(\text{magnetic})$ [Eq. (52)] at the initial radius r of the AO electron. Then, the energy $E(\text{mol. atom}, msp^3)$ of the outer electron of the atom msp^3 shell is given by the sum of $E_{\text{Coulomb}}(\text{mol. atom}, msp^3)$ and $E(\text{magnetic})$ [Eq. (57)]. $E_T(\text{atom-atom}, msp^3)$, the energy change of each atom msp^3 shell with the formation of the atom-atom-bond MO is given by the difference between $E(\text{mol. atom}, msp^3)$ and $E(\text{atom}, msp^3)$ given by Eq. (58). Using Eq. (60) for $E_{\text{Coulomb}}(C, 2sp^3)$ in Eq. (68), the single bond order energies given by Eqs. (55)–(64) and shown in

TABLE V. The final values of r_{C2sp^3} , $E_{\text{Coulomb}}(C2sp^3)$, and $E(C2sp^3)$ and the resulting $E_T(C-C, C2sp^3)$ 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 $E_T[\text{atom-atom}(s_n), msp^3]$ given in Table IV.

MO bond order (BO)	s_1	c_{s_1}	s_2	c_{s_2}	s_3	c_{s_3}	$r_{C2sp^3}(a_0)$ final	$E_{\text{Coulomb}}(C2sp^3)$ final (eV)	$E(C2sp^3)$ final (eV)	$E_T(C-C, C2sp^3)$ final (eV)
1/2I	1	0.5	0	0	0	0	0.895 82	-15.188 04	-14.997 17	-0.362 28
1/2II	2	0.5	0	0	0	0	0.883 92	-15.392 65	-15.201 78	-0.566 89
1/2I+1/4II	1	0.5	2	0.25	0	0	0.879 41	-15.471 49	-15.280 62	-0.645 73
1/4II+1/4(I+II)	2	0.25	1	0.25	2	0.25	0.873 63	-15.573 79	-15.382 93	-0.748 04
3/4II	2	0.75	0	0	0	0	0.867 93	-15.676 10	-15.485 23	-0.850 34
1/2I+1/2II	1	0.5	2	0.5	0	0	0.863 59	-15.754 93	-15.564 07	-0.929 18
1/2I+1/2III	1	0.5	3	0.5	0	0	0.851 93	-15.970 60	-15.779 74	-1.144 85
1/2I+1/2IV	1	0.5	4	0.5	0	0	0.839 95	-16.198 26	-16.007 39	-1.372 50
1/2II+1/2III	2	0.5	3	0.5	0	0	0.841 15	-16.175 21	-15.984 35	-1.349 46
1/2II+1/2IV	2	0.5	4	0.5	0	0	0.829 48	-16.402 86	-16.212 00	-1.577 11
I+1/2(I+II)	1	1	1	0.5	2	0.5	0.825 62	-16.479 51	-16.288 65	-1.653 76
1/2III+1/2IV	3	0.5	4	0.5	0	0	0.818 71	-16.618 53	-16.427 67	-1.792 78
1/2IV+1/2IV	4	0.5	4	0.5	0	0	0.807 65	-16.846 19	-16.655 32	-2.020 43
1/2(I+II)+II	1	0.5	2	0.5	2	1	0.805 61	-16.888 73	-16.697 86	-2.062 97

Table IV, 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 V.

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 $r_{\text{mol } 2sp^3}$ of the $C2sp^3$ HO of a carbon atom of a given molecule is calculated using Eq. (14.514) by considering $\Sigma E_{T_{\text{mol}}}(MO, 2sp^3)$, the total energy donation to all bonds with which it participates in bonding. The general equation for the radius is given by

$$r_{\text{mol } 2sp^3} = \frac{-e^2}{8\pi\epsilon_0(E_{\text{Coulomb}}(C, 2sp^3) + \sum E_{T_{\text{mol}}}(\text{MO}, 2sp^3))} = \frac{e^2}{8\pi\epsilon_0(e14.825\,751\text{ eV} + \sum |E_{T_{\text{mol}}}(\text{MO}, 2sp^3)|)}. \quad (69)$$

The Coulombic energy $E_{\text{Coulomb}}(\text{mol. atom}, msp^3)$ 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 HO, the energy change for the promotion to the unpaired state is the magnetic energy $E(\text{magnetic})$ [Eq. (52)] at the initial radius r of the AO electron. Then, the energy $E(\text{mol. atom}, msp^3)$ of the outer electron of the atom msp^3 shell is given by the sum of $E_{\text{Coulomb}}(\text{mol. atom}, msp^3)$ and $E(\text{magnetic})$ [Eq. (57)].

For example, the $C2sp^3$ HO of each methyl group of an alkane contributes $-0.929\,18\text{ eV}$ [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 $-0.929\,18\text{ eV}$ 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

$$r_{\text{alkane } C_{\text{methylene}} 2sp^3} = \frac{-e^2}{8\pi\epsilon_0(E_{\text{Coulomb}}(C, 2sp^3) + \sum E_{T_{\text{alkane}}}(\text{methylene } C - C, 2sp^3))} = \frac{e^2}{8\pi\epsilon_0(e14.825\,751\text{ eV} + e0.929\,18\text{ eV} + e0.929\,18\text{ eV})} = 0.815\,49a_0, \quad (70)$$

$$E_{\text{Coulomb}}(C_{\text{methylene}}2sp^3) = \frac{-e^2}{8\pi\epsilon_0(0.815\,49a_0)} = -16.684\,12\text{ eV}, \quad (71)$$

$$E(C_{\text{methylene}}2sp^3) = \frac{-e^2}{8\pi\epsilon_0(0.815\,49a_0)} + \frac{2\pi\mu_0e^2\hbar^2}{m_e^2(0.843\,17a_0)^3} = -16.493\,25\text{ eV}. \quad (72)$$

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, $r_{\text{atom.HO.AO}}$, $E_{\text{Coulomb}}(\text{mol.atom}, msp^3)$, and $E(C_{\text{mol}}2sp^3)$ are calculated using $\Sigma E_{T_{\text{group}}}(\text{MO}, 2sp^3)$, the total energy donation to each bond with which an atom participates in bonding corre-

sponding to the values of $E_T(C-C, C2sp^3)$ of the MO due to charge donation from the AO or HO to the MO given in Tables IV and V.

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 , $-31.635\,368\,31\text{ eV}$, 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 its 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, $E_T(H_2MO)$, is given by the sum of the energy terms [Eqs. (43)–(48)] plus $E_T(\text{AO/HO})$:

$$E_T(H_2MO) = V_e + T + V_m + V_p + E_T(\text{AO/HO}), \quad (73)$$

$$E_T(H_2MO) = -\frac{n_1e^2}{8\pi\epsilon_0\sqrt{a^2-b^2}} \times \left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}-1 \right] + E_T(\text{AO/HO}) = -\frac{n_1e^2}{8\pi\epsilon_0c'} \left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1 \right] + E_T(\text{AO/HO}) \quad (74)$$

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 $E_T(\text{AO/HO})$ is the total energy comprising the difference of the energy $E(\text{AO/HO})$ of at least one atomic or hybrid orbital to which the MO is energy matched and any energy component $\Delta E_{H_2MO}(\text{AO/HO})$ due to the AO or HO's charge donation to the MO.

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

To solve the bond parameters and energies, $c' = a\sqrt{\hbar^24\pi\epsilon_0/m_e e^2 2C_1C_2a} = \sqrt{aa_0/2C_1C_2}$ [Eq. (39)] is substituted into $E_T(H_2MO)$ to give

$$E_T(H_2MO) = -\frac{n_1e^2}{8\pi\epsilon_0\sqrt{a^2-b^2}} \left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}-1 \right] + E_T(\text{AO/HO}) = -\frac{n_1e^2}{8\pi\epsilon_0c'} \left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+c'}{a-c'}-1 \right] + E_T(\text{AO/HO}) = -\frac{n_1e^2}{8\pi\epsilon_0\sqrt{\frac{aa_0}{2C_1C_2}}} \left[c_1c_2\left(2-\frac{a_0}{a}\right)\ln\frac{a+\sqrt{\frac{aa_0}{2C_1C_2}}}{a-\sqrt{\frac{aa_0}{2C_1C_2}}}-1 \right] + E_T(\text{AO/HO}). \quad (76)$$

The total energy is set equal to $E(\text{basis energies})$ 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 $E(\text{AO})$ [e.g., $E(N) = -14.534\ 14\ \text{eV}$] where the first integer can be 1, 2, 3, ..., and each of the second and third integers can be 0, 1, 2, 3, ...

$$E(\text{basis energies}) = n_1(-31.635\ 368\ 31\ \text{eV}) - n_2(-13.605\ 804\ \text{eV}) - n_3 E(\text{AO}). \quad (77)$$

In the case that the MO bonds two atoms other than hydrogen, $E(\text{basis energies})$ 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 , $-31.635\ 368\ 31\ \text{eV}$ [Eq. (11.212)], is the minimum energy possible for a prolate spheroidal MO:

$$E(\text{basis energies}) = n_1(-31.635\ 368\ 31\ \text{eV}). \quad (78)$$

$E_T(\text{H}_2\text{MO})$, is set equal to $E(\text{basis energies})$, and the semimajor axis a is solved. Thus, the semimajor axis a is solved from the equation of the form

$$-\frac{n_1 e^2}{8\pi\epsilon_0 \sqrt{\frac{aa_0}{2C_1 C_2}}} \left[c_1 c_2 \left(2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{\frac{aa_0}{2C_1 C_2}}}{a - \sqrt{\frac{aa_0}{2C_1 C_2}}} - 1 \right] + E_T(\text{AO/HO}) = E(\text{basis energies}). \quad (79)$$

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

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

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

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

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 re-entrant 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

$$f(R) = -\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3} \quad (82)$$

and

$$f'(a) = 2\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3} \quad (83)$$

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

$$\omega = \sqrt{\frac{\frac{-3}{a} f(a) - f'(a)}{m_e}} = \sqrt{\frac{k}{m_e}} = \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3}}, \quad (84)$$

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:

$$\bar{E}_K = \hbar \omega = \hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3}} \quad (85)$$

The Doppler energy of the electrons of the re-entrant orbit is

$$\bar{E}_D \equiv E_{h\nu} \sqrt{\frac{2\bar{E}_K}{m_e c^2}} = E_{h\nu} \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3}}}{m_e c^2}}. \quad (86)$$

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

$$\begin{aligned} \bar{E}_{\text{osc}}(\text{group}) &= n_1(\bar{E}_D + \bar{E}_{\text{Kvib}}) \\ &= n_1 \left(E_{h\nu} \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3}}}{m_e c^2}} + E_{\text{vib}} \right) \end{aligned} \quad (87)$$

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

$$\begin{aligned} \bar{E}_{\text{osc}} &= n_1(\bar{E}_D + \bar{E}_{\text{Kvib}}) \\ &= n_1 \left(E_T(\text{MO})/n_1 \sqrt{\frac{2\bar{E}_K}{m_e c^2}} + \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}} \right). \end{aligned} \quad (88)$$

$E_{T+\text{osc}}(\text{group})$ is given by the sum of $E_T(\text{MO})$ [Eq. (79)] and $\bar{E}_{\text{osc}}$ [Eq. (88)]:

$$\begin{aligned}
E_{T+\text{osc}}(\text{group}) &= E_T(\text{MO}) + \bar{E}_{\text{osc}} \\
&= \left(\left(-\frac{n_1 e^2}{8\pi\epsilon_0 \sqrt{\frac{aa_0}{2C_1 C_2}}} \left[c_1 c_2 \left(2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{\frac{aa_0}{2C_1 C_2}}}{a - \sqrt{\frac{aa_0}{2C_1 C_2}}} - 1 \right] \right. \right. \\
&\quad \left. \left. + E_T(\text{AO/HO}) + E_T(\text{atom-atom}, msp^3 \cdot \text{AO}) \right) \left[1 + \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}}}{m_e c^2}} \right] + n_1 \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}} \right) \\
&= (E(\text{basis energies}) + E_T(\text{atom-atom}, msp^3 \cdot \text{AO})) \left[1 + \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}}}{m_e c^2}} \right] + n_1 \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}}. \quad (89)
\end{aligned}$$

The total energy of the functional group $E_T(\text{group})$ is the sum of the total energy of the components comprising the energy contribution of the MO formed between the participating atoms, $E(\text{basis energies})$, the change in the energy of the AOs or HOs upon forming the bond ($E_T(\text{atom-atom}, msp^3 \cdot \text{AO})$), 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 $E_T(\text{group})$ is

$$E_T(\text{group}) = \left((E(\text{basis energies}) + E_T(\text{atom-atom}, msp^3 \cdot \text{AO})) \left[1 + \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}}}{m_e c^2}} \right] + n_1 \bar{E}_{K\text{vib}} + E_{\text{mag}} \right). \quad (90)$$

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

$$E_{\text{mag}} = c_3 \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 r^3} = c_3 \frac{8\pi\mu_0 \mu_B^2}{r^3}, \quad (91)$$

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

$$E_T(\text{group}) = \left((E(\text{basis energies}) + E_T(\text{atom-atom}, msp^3 \cdot \text{AO})) \left[1 + \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}}}{m_e c^2}} \right] + n_1 \bar{E}_{K\text{vib}} + c_3 \frac{8\pi\mu_0 \mu_B^2}{r^3} \right). \quad (92)$$

The total bond energy of the group $E_D(\text{group})$ is the negative difference of the total energy of the group [Eq. (92)] and the total energy of the two starting orbitals given by the sum of $c_4 E_{\text{initial}}(c_4 \text{AO/HO})$ and $c_5 E_{\text{initial}}(c_5 \text{AO/HO})$:

$$\begin{aligned}
E_D(\text{group}) &= - \left((E(\text{basis energies}) + E_T(\text{atom-atom}, msp^3 \cdot \text{AO})) \left[1 + \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}}}{m_e c^2}} \right] + n_1 \bar{E}_{K\text{vib}} + c_3 \frac{8\pi\mu_0 \mu_B^2}{r^3} \right. \\
&\quad \left. - (c_4 E_{\text{initial}}(c_4 \text{AO/HO}) + c_5 E_{\text{initial}}(c_5 \text{AO/HO})) \right). \quad (93)
\end{aligned}$$

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

$$E(\text{AO/HO}) = -14.634\,89\text{ eV}. \quad (94)$$

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

$$\begin{aligned} E_{\text{mag}}(C2sp^3) &= c_3 \frac{8\pi\mu_o\mu_B^2}{r^3} \\ &= c_3 \frac{8\pi\mu_o\mu_B^2}{(0.91771a_0)^3} \\ &= c_3 0.148\,03\text{ eV}. \end{aligned} \quad (95)$$

Each molecule, independent 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 functional 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 wavefunctions 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 molecules. The results being accurate physical representations rather than pure mathematical curve fits devoid of a connection to reality.

C. Total energy of continuous-chain alkanes

$E_D(C_nH_{2n+2})$, 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

$$\begin{aligned} E_D(C_nH_{2n+2}) &= E_D(\text{C}-\text{C})_{n-1} + 2E_{D_{\text{alkane}}}({}^{12}\text{CH}_3) \\ &\quad + (n-2)E_{D_{\text{alkane}}}({}^{12}\text{CH}_2) \\ &= (n-1)(4.327\,54\text{ eV}) + 2(12.491\,86\text{ eV}) \\ &\quad + (n-2)(7.830\,16\text{ eV}). \end{aligned} \quad (96)$$

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

$$\begin{aligned} E_{D_{\text{exp}}}(C_nH_{2n+2}) &= -\{\Delta H_f(C_nH_{2n+2}(\text{gas})) \\ &\quad - [n\Delta H_f(\text{C}(\text{gas})) \\ &\quad + (2n+2)\Delta H_f(\text{H}(\text{gas}))]\} \\ &= -\{\Delta H_f(C_nH_{2n+2}(\text{gas})) \end{aligned}$$

$$\begin{aligned} &-[n7.427\,74\text{ eV} \\ &\quad + (2n+2)2.259\,353\text{ eV}], \end{aligned} \quad (97)$$

where the heats of formation atomic carbon and hydrogen gas are given by^{31,32}

$$\Delta H_f(\text{C}(\text{gas})) = 716.68\text{ kJ/mole}(7.427\,74\text{ eV/atom}), \quad (98)$$

$$\begin{aligned} \Delta H_f(\text{H}(\text{gas})) \\ = 217.998\text{ kJ/mole}(2.259\,353\text{ eV/atom}). \end{aligned} \quad (99)$$

D. 3-21G and 6-31G* basis-set calculations

The energies of the 3-21G and 6-31G* basis sets were acquired from SPARTAN's precomputed 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 data³ 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 were 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%.

$$E_T = E - \text{TotIP}_{\text{exp}} \quad (100)$$

$$E_T = E - \text{TotIP}_{\text{QM}}. \quad (101)$$

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 $n=2,3,4,\dots,\infty$). Representative functional groups are given in Tables I and II. For example, using Eq. (96), $E_D(C_nH_{2n+2})$ was determined for propane, butane, pentane, hexane, heptane, octane, nonane, decane, undecane, dodecane, and octadecane¹ to compare to the available experimental values. The latter were determined from the corresponding experimental $\Delta H_f(C_nH_{2n+2}(\text{gas}))$ ³² and Eqs. (97)–(99). The results of the determination of the total bond energies are given in Table VI. Similarly, a large array of functional groups and molecules per class for which experimental data were available is given in Tables VI–LXXIV. 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 previously¹ and compared to the experimental values. References for the experimental values are mainly from Refs. 33–36, and they are given for each compound in Ref. 1. For each molecule, the calculated re-

TABLE VI. Summary results of *n*-alkanes.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₃ H ₈	Propane	41.468 96	41.434	−0.000 85
C ₄ H ₁₀	Butane	53.626 66	53.61	−0.000 36
C ₅ H ₁₂	Pentane	65.784 36	65.77	−0.000 17
C ₆ H ₁₄	Hexane	77.942 06	77.93	−0.000 19
C ₇ H ₁₆	Heptane	90.099 76	90.09	−0.000 13
C ₈ H ₁₈	Octane	102.257 46	102.25	−0.000 06
C ₉ H ₂₀	Nonane	114.415 16	114.40	−0.000 12
C ₁₀ H ₂₂	Decane	126.572 86	126.57	−0.000 03
C ₁₁ H ₂₄	Undecane	138.730 56	138.736	0.000 04
C ₁₂ H ₂₆	Dodecane	150.888 26	150.88	−0.000 08
C ₁₈ H ₃₈	Octadecane	223.834 46	223.85	0.000 08

sults 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 Figs. 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 H₂-type-ellipsoidal MO that transitions to the corresponding outer shell of the atom(s) participating in each bond, and the nuclei (not to scale) are shown. In the case of an opaque view of the charge density, the outer orbitals of the atoms at their radii and the ellipsoidal surface of each H- or H₂-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 LXXXV gives the results of MILLSIAN 1.0, the results with 3-21G and 6-31G* basis sets generated from a precomputed 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 were 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 its best performance. SPARTAN 3-21G and 6-31G* typically gave >30% relative error compared to experimental values even for

TABLE VII. Summary results of branched alkanes.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₄ H ₁₀	Isobutane	53.699 22	53.695	−0.000 07
C ₅ H ₁₂	Isopentane	65.856 92	65.843	−0.000 21
C ₅ H ₁₂	Neopentane	65.863 36	65.992	0.001 95
C ₆ H ₁₄	2-methylpentane	78.014 62	78.007	−0.000 10
C ₆ H ₁₄	3-methylpentane	78.014 62	77.979	−0.000 46
C ₆ H ₁₄	2,2-dimethylbutane	78.021 06	78.124	0.001 32
C ₆ H ₁₄	2,3-dimethylbutane	77.995 81	78.043	0.000 61
C ₇ H ₁₆	2-methylhexane	90.172 32	90.160	−0.000 14
C ₇ H ₁₆	3-methylhexane	90.172 32	90.127	−0.000 51
C ₇ H ₁₆	3-ethylpentane	90.172 32	90.108	−0.000 72
C ₇ H ₁₆	2,2-dimethylpentane	90.178 76	90.276	0.001 07
C ₇ H ₁₆	2,2,3-trimethylbutane	90.223 01	90.262	0.000 44
C ₇ H ₁₆	2,4-dimethylpentane	90.244 88	90.233	−0.000 13
C ₇ H ₁₆	3,3-dimethylpentane	90.178 76	90.227	0.000 54
C ₈ H ₁₈	2-methylheptane	102.330 02	102.322	−0.000 08
C ₈ H ₁₈	3-methylheptane	102.330 02	102.293	−0.000 36
C ₈ H ₁₈	4-methylheptane	102.330 02	102.286	−0.000 43
C ₈ H ₁₈	3-ethylhexane	102.330 02	102.274	−0.000 55
C ₈ H ₁₈	2,2-dimethylhexane	102.336 46	102.417	0.000 79
C ₈ H ₁₈	2,3-dimethylhexane	102.311 21	102.306	−0.000 05
C ₈ H ₁₈	2,4-dimethylhexane	102.402 58	102.362	−0.000 40
C ₈ H ₁₈	2,5-dimethylhexane	102.402 58	102.396	−0.000 06
C ₈ H ₁₈	3,3-dimethylhexane	102.336 46	102.369	0.000 32
C ₈ H ₁₈	3,4-dimethylhexane	102.311 21	102.296	−0.000 15
C ₈ H ₁₈	3-ethyl-2-methylpentane	102.311 21	102.277	−0.000 33
C ₈ H ₁₈	3-ethyl-3-methylpentane	102.336 46	102.317	−0.000 19
C ₈ H ₁₈	2,2,3-trimethylpentane	102.380 71	102.370	−0.000 10
C ₈ H ₁₈	2,2,4-trimethylpentane	102.409 02	102.412	0.000 03
C ₈ H ₁₈	2,3,3-trimethylpentane	102.380 71	102.332	−0.000 48
C ₈ H ₁₈	2,3,4-trimethylpentane	102.292 40	102.342	0.000 49
C ₈ H ₁₈	2,2,3,3-tetramethylbutane	102.416 32	102.433	0.000 16
C ₉ H ₂₀	2,3,5-trimethylhexane	114.541 47	114.551	0.000 08
C ₉ H ₂₀	3,3-diethylpentane	114.494 16	114.455	−0.000 34
C ₉ H ₂₀	2,2,3,3-tetramethylpentane	114.574 02	114.494	−0.000 70
C ₉ H ₂₀	2,2,3,4-tetramethylpentane	114.519 60	114.492	−0.000 24
C ₉ H ₂₀	2,2,4,4-tetramethylpentane	114.573 16	114.541	−0.000 28
C ₉ H ₂₀	2,3,3,4-tetramethylpentane	114.582 66	114.484	−0.000 86
C ₁₀ H ₂₂	2-methylnonane	126.645 42	126.680	0.000 27
C ₁₀ H ₂₂	5-methylnonane	126.645 42	126.663	0.000 14

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 three to four significant-figure accuracy compared to one to two significant figures for SPARTAN rendering it practically useless.

In the sets where the SPARTAN results were calculated

TABLE VIII. Summary results of alkenes.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₃ H ₆	Propene	35.560 33	35.632 07	0.002 01
C ₄ H ₈	1-butene	47.718 03	47.784 77	0.001 40
C ₄ H ₈	trans-2-butene	47.931 16	47.903 95	-0.000 57
C ₄ H ₈	Isobutene	47.903 14	47.960 96	0.001 21
C ₅ H ₁₀	1-pentene	59.875 73	59.950 94	0.001 25
C ₅ H ₁₀	trans-2-pentene	60.088 86	60.062 87	-0.000 43
C ₅ H ₁₀	2-methyl-1-butene	60.060 84	60.097 07	0.000 60
C ₅ H ₁₀	2-methyl-2-butene	60.214 33	60.164 44	-0.000 83
C ₅ H ₁₀	3-methyl-1-butene	59.976 62	60.017 27	0.000 68
C ₆ H ₁₂	1-hexene	72.033 43	72.129 54	0.001 33
C ₆ H ₁₂	trans-2-hexene	72.246 56	72.237 33	-0.000 13
C ₆ H ₁₂	trans-3-hexene	72.246 56	72.242 51	-0.000 06
C ₆ H ₁₂	2-methyl-1-pentene	72.218 54	72.294 33	0.001 05
C ₆ H ₁₂	2-methyl-2-pentene	72.372 03	72.372 06	0.000 00
C ₆ H ₁₂	3-methyl-1-pentene	72.134 32	72.191 73	0.000 80
C ₆ H ₁₂	4-methyl-1-pentene	72.105 99	72.210 38	0.001 45
C ₆ H ₁₂	3-methyl-trans-2-pentene	72.372 03	72.332 68	-0.000 54
C ₆ H ₁₂	4-methyl-trans-2-pentene	72.347 45	72.316 10	-0.000 43
C ₆ H ₁₂	2-ethyl-1-butene	72.218 54	72.259 09	0.000 56
C ₆ H ₁₂	2,3-dimethyl-1-butene	72.319 43	72.325 43	0.000 08
C ₆ H ₁₂	3,3-dimethyl-1-butene	72.317 96	72.303 66	-0.000 20
C ₆ H ₁₂	2,3-dimethyl-2-butene	72.497 50	72.384 50	-0.001 56
C ₇ H ₁₄	1-heptene	84.191 13	84.270 84	0.000 95
C ₇ H ₁₄	5-methyl-1-hexene	84.263 69	84.306 08	0.000 50
C ₇ H ₁₄	trans-3-methyl-3-hexene	84.529 73	84.421 12	-0.001 29
C ₇ H ₁₄	2,4-dimethyl-1-pentene	84.448 80	84.493 67	0.000 53
C ₇ H ₁₄	4,4-dimethyl-1-pentene	84.270 12	84.470 87	0.002 38
C ₇ H ₁₄	2,4-dimethyl-2-pentene	84.630 62	84.544 45	-0.001 02
C ₇ H ₁₄	trans-4,4-dimethyl-2-pentene	84.540 76	84.545 49	0.000 06
C ₇ H ₁₄	2-ethyl-3-methyl-1-butene	84.477 13	84.449 10	-0.000 33
C ₇ H ₁₄	2,3,3-trimethyl-1-butene	84.512 74	84.511 29	-0.000 02
C ₈ H ₁₆	1-octene	96.348 83	96.414 21	0.000 68
C ₈ H ₁₆	trans-2,2-dimethyl-3-hexene	96.698 46	96.687 82	-0.000 11
C ₈ H ₁₆	3-ethyl-2-methyl-1-pentene	96.634 83	96.611 13	-0.000 25
C ₈ H ₁₆	2,4,4-trimethyl-1-pentene	96.612 93	96.716 84	0.001 07
C ₈ H ₁₆	2,4,4-trimethyl-2-pentene	96.675 90	96.658 80	-0.000 18
C ₁₀ H ₂₀	1-decene	120.664 23	120.742 40	0.000 65
C ₁₂ H ₂₄	1-dodecene	144.979 63	145.071 63	0.000 63
C ₁₆ H ₃₂	1-hexadecene	193.610 43	193.717 66	0.000 55

TABLE IX. Summary results of alkynes.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₃ H ₄	Propyne	29.429 32	29.404 32	-0.000 85
C ₄ H ₆	1-butyne	41.587 02	41.554 95	-0.000 77
C ₄ H ₆	2-butyne	41.727 65	41.757 05	0.000 70
C ₉ H ₁₆	1-nonyne	102.375 52	102.353 67	-0.000 21

TABLE X. Summary results of alkyl fluorides.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CF ₄	Tetrafluoromethane	21.079 92	21.016	-0.003 03
CHF ₃	Trifluoromethane	19.283 98	19.362	0.004 05
CH ₂ F ₂	Diffuoromethane	18.222 09	18.280	0.003 14
C ₃ H ₇ F	1-fluoropropane	41.867 45	41.885	0.000 41
C ₃ H ₇ F	2-fluoropropane	41.968 34	41.963	-0.000 12

TABLE XI. Summary results of alkyl chlorides.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CCl ₄	Tetrachloromethane	13.431 81	13.448	0.001 23
CHCl ₃	Trichloromethane	14.491 46	14.523	0.002 17
CH ₂ Cl ₂	Dichloromethane	15.372 48	15.450	0.004 99
CH ₃ Cl	Chloromethane	16.263 02	16.312	0.002 99
C ₂ H ₅ Cl	Chloroethane	28.610 64	28.571	−0.001 38
C ₃ H ₇ Cl	1-chloropropane	40.768 34	40.723	−0.001 12
C ₃ H ₇ Cl	2-chloropropane	40.869 23	40.858	−0.000 28
C ₄ H ₉ Cl	1-chlorobutane	52.926 04	52.903	−0.000 44
C ₄ H ₉ Cl	2-chlorobutane	53.026 93	52.972	−0.001 04
C ₄ H ₉ Cl	1-chloro-2-methylpropane	52.998 60	52.953	−0.000 85
C ₄ H ₉ Cl	2-chloro-2-methylpropane	53.210 57	53.191	−0.000 37
C ₅ H ₁₁ Cl	1-chloropentane	65.083 74	65.061	−0.000 34
C ₅ H ₁₁ Cl	1-chloro-3-methylbutane	65.156 30	65.111	−0.000 69
C ₅ H ₁₁ Cl	2-chloro-2-methylbutane	65.368 27	65.344	−0.000 37
C ₅ H ₁₁ Cl	2-chloro-3-methylbutane	65.165 82	65.167	0.000 02
C ₆ H ₁₃ Cl	2-chlorohexane	77.342 33	77.313	−0.000 38
C ₈ H ₁₇ Cl	1-chlorooctane	101.556 84	101.564	0.000 07
C ₁₂ H ₂₅ Cl	1-chlorododecane	150.187 64	150.202	0.000 09
C ₁₈ H ₃₇ Cl	1-chlorooctadecane	223.133 84	223.175	0.000 18

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 suspected. 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 predicted energy. When comparing the rendering of the simple alkane butane (C₄H₁₀) using the two basis sets [Figs. 15(A) and 15(B)] neither shows any resemblance to butane in that they are not even symmetrical, the edge is created artificially and arbitrarily, and the 6-31G* 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 Fig.

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 precomputed 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 3 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

TABLE XII. Summary results of alkyl bromides.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CBr ₄	Tetrabromomethane	11.259 29	11.196	-0.005 66
CHBr ₃	Tribromomethane	12.876 98	12.919	0.003 23
CH ₃ Br	Bromomethane	15.675 51	15.732	0.003 60
C ₂ H ₅ Br	Bromoethane	28.039 39	27.953	-0.003 08
C ₃ H ₇ Br	1-bromopropane	40.197 09	40.160	-0.000 93
C ₃ H ₇ Br	2-bromopropane	40.297 98	40.288	-0.000 24
C ₅ H ₁₀ Br ₂	2,3-dibromo- 2-methylbutane	63.539 58	63.477	-0.000 98
C ₆ H ₁₃ Br	1-bromohexane	76.670 19	76.634	-0.000 47
C ₇ H ₁₅ Br	1-bromoheptane	88.827 89	88.783	-0.000 51
C ₈ H ₁₇ Br	1-bromooctane	100.985 59	100.952	-0.000 33
C ₁₂ H ₂₅ Br	1-bromododecane	149.616 39	149.573	-0.000 29
C ₁₆ H ₃₃ Br	1-bromohexadecane	198.247 19	198.192	-0.000 28

TABLE XIII. Summary results of alkyl iodides.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CHI ₃	Triiodomethane	10.358 88	10.405	0.004 44
CH ₂ I ₂	Diiodomethane	12.946 14	12.921	-0.001 95
CH ₃ I	Iodomethane	15.202 94	15.163	-0.002 63
C ₂ H ₅ I	Iodoethane	27.360 64	27.343	-0.000 66
C ₃ H ₇ I	1-iodopropane	39.518 34	39.516	-0.000 06
C ₃ H ₇ I	2-iodopropane	39.619 23	39.623	0.000 09
C ₄ H ₉ I	2-iodo-2-methylpropane	51.960 57	51.899	-0.001 19

TABLE XIV. Summary results of alkene halides.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₂ H ₃ Cl	Chloroethene	22.467 00	22.505	0.001 70
C ₃ H ₃ Cl	2-chloropropene	35.029 84	35.054 82	0.000 71

TABLE XV. Summary results of alcohols.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CH ₄ O	Methanol	21.110 38	21.131	0.000 97
C ₂ H ₆ O	Ethanol	33.405 63	33.428	0.000 66
C ₃ H ₈ O	1-propanol	45.563 33	45.584	0.000 46
C ₃ H ₈ O	2-propanol	45.720 88	45.766	0.000 98
C ₄ H ₁₀ O	1-butanol	57.721 03	57.736	0.000 26
C ₄ H ₁₀ O	2-butanol	57.878 58	57.922	0.000 74
C ₄ H ₁₀ O	2-methyl-1-propanol	57.793 59	57.828	0.000 60
C ₄ H ₁₀ O	2-methyl-2-propanol	58.153 59	58.126	-0.000 48
C ₅ H ₁₂ O	1-pentanol	69.878 73	69.887	0.000 11
C ₅ H ₁₂ O	2-pentanol	70.036 28	70.057	0.000 29
C ₅ H ₁₂ O	3-pentanol	70.036 28	70.097	0.000 87
C ₅ H ₁₂ O	2-methyl-1-butanol	69.951 29	69.957	0.000 08
C ₅ H ₁₂ O	3-methyl-1-butanol	69.951 29	69.950	-0.000 02
C ₅ H ₁₂ O	2-methyl-2-butanol	70.311 29	70.246	-0.000 92
C ₅ H ₁₂ O	3-methyl-2-butanol	69.960 81	70.083	0.001 74
C ₆ H ₁₄ O	1-hexanol	82.036 43	82.054	0.000 21
C ₆ H ₁₄ O	2-hexanol	82.193 98	82.236	0.000 52
C ₇ H ₁₆ O	1-heptanol	94.194 13	94.214	0.000 21
C ₈ H ₁₈ O	1-octanol	106.351 83	106.358	0.000 06
C ₈ H ₁₈ O	2-ethyl-1-hexanol	106.424 39	106.459	0.000 32
C ₉ H ₂₀ O	1-nonanol	118.509 53	118.521	0.000 10
C ₁₀ H ₂₂ O	1-decanol	130.667 23	130.676	0.000 07
C ₁₂ H ₂₆ O	1-dodecanol	154.982 63	154.984	0.000 01
C ₁₆ H ₃₄ O	1-hexadecanol	203.613 43	203.603	-0.000 05

TABLE XVI. Summary results of ethers.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₂ H ₆ O	Dimethyl ether	32.844 96	32.902	0.001 74
C ₃ H ₈ O	Ethyl methyl ether	45.197 10	45.183	-0.000 30
C ₄ H ₁₀ O	Diethyl ether	57.549 24	57.500	-0.000 86
C ₄ H ₁₀ O	Methyl propyl ether	57.354 80	57.355	0.000 00
C ₄ H ₁₀ O	Isopropyl methyl ether	57.455 69	57.499	0.000 75
C ₆ H ₁₄ O	Dipropyl ether	81.864 64	81.817	-0.000 59
C ₆ H ₁₄ O	Diisopropyl ether	82.066 42	82.088	0.000 26
C ₆ H ₁₄ O	t-butyl ethyl ether	82.102 76	82.033	-0.000 85
C ₇ H ₁₆ O	t-butyl isopropyl ether	94.361 35	94.438	0.000 81
C ₈ H ₁₈ O	Dibutyl ether	106.180 04	106.122	-0.000 55
C ₈ H ₁₈ O	Di-sec-butyl ether	106.381 82	106.410	0.000 27
C ₈ H ₁₈ O	Di-t-butyl ether	106.360 22	106.425	0.000 61
C ₈ H ₁₈ O	t-butyl isobutyl ether	106.656 28	106.497	-0.002 18

TABLE XVII. Summary results of 1° amines.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CH ₅ N	Methylamine	23.882 97	23.857	-0.001 10
C ₂ H ₇ N	Ethylamine	36.040 67	36.062	0.000 60
C ₃ H ₉ N	Propylamine	48.198 37	48.243	0.000 92
C ₄ H ₁₁ N	Butylamine	60.356 07	60.415	0.000 98
C ₄ H ₁₁ N	Sec-butylamine	60.456 96	60.547	0.001 48
C ₄ H ₁₁ N	t-butylamine	60.788 63	60.717	-0.001 18
C ₄ H ₁₁ N	Isobutylamine	60.428 63	60.486	0.000 94

TABLE XVIII. Summary results of 2° amines.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₂ H ₇ N	Dimethylamine	35.768 95	35.765	−0.000 12
C ₄ H ₁₁ N	Diethylamine	60.229 30	60.211	−0.000 30
C ₆ H ₁₅ N	Dipropylamine	84.544 70	84.558	0.000 16
C ₆ H ₁₅ N	Diisopropylamine	84.746 48	84.846	0.001 17
C ₈ H ₁₉ N	Dibutylamine	108.860 10	108.872	0.000 11
C ₈ H ₁₉ N	Diisobutylamine	109.005 22	109.106	0.000 92

TABLE XIX. Summary results of 3° amines.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₃ H ₉ N	Trimethylamine	47.833 38	47.761	−0.001 52
C ₆ H ₁₅ N	Triethylamine	84.306 48	84.316	0.000 12
C ₉ H ₂₁ N	Tripropylamine	120.779 58	120.864	0.000 70

TABLE XX. Summary results of aldehydes.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CH ₂ O	Formaldehyde	15.646 28	15.655	0.000 56
C ₂ H ₄ O	Acetaldehyde	28.187 11	28.198	0.000 39
C ₃ H ₆ O	Propanal	40.344 81	40.345	0.000 00
C ₄ H ₈ O	Butanal	52.502 51	52.491	−0.000 22
C ₄ H ₈ O	Isobutanal	52.603 40	52.604	0.000 01
C ₅ H ₁₀ O	Pentanal	64.660 21	64.682	0.000 34
C ₇ H ₁₄ O	Heptanal	88.975 61	88.942	−0.000 38
C ₈ H ₁₆ O	Octanal	101.133 31	101.179	0.000 45
C ₈ H ₁₆ O	2-ethylhexanal	101.234 20	101.259	0.000 25

TABLE XXI. Summary results of ketones.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₃ H ₆ O	Acetone	40.684 72	40.672	−0.000 31
C ₄ H ₈ O	2-butanone	52.842 42	52.84	−0.000 05
C ₅ H ₁₀ O	2-pentanone	65.000 12	64.997	−0.000 05
C ₅ H ₁₀ O	3-pentanone	65.000 12	64.988	−0.000 05
C ₅ H ₁₀ O	3-methyl-2-butanone	65.101 01	65.036	−0.000 99
C ₆ H ₁₂ O	2-hexanone	77.157 82	77.152	−0.000 08
C ₆ H ₁₂ O	3-hexanone	77.157 82	77.138	−0.000 25
C ₆ H ₁₂ O	2-methyl-3-pentanone	77.258 71	77.225	−0.000 43
C ₆ H ₁₂ O	3,3-dimethyl-2-butanone	77.294 32	77.273	−0.000 28
C ₇ H ₁₄ O	3-heptanone	89.315 52	89.287	−0.000 32
C ₇ H ₁₄ O	4-heptanone	89.315 52	89.299	−0.000 18
C ₇ H ₁₄ O	2,2-dimethyl-3-pentanone	89.452 02	89.458	0.000 07
C ₇ H ₁₄ O	2,4-dimethyl-3-pentanone	89.517 30	89.434	−0.000 93
C ₈ H ₁₆ O	2,2,4-trimethyl-3-pentanone	101.710 61	101.660	−0.000 49
C ₉ H ₁₈ O	2-nonanone	113.630 92	113.632	0.000 01
C ₉ H ₁₈ O	5-nonanone	113.630 92	113.675	0.000 39
C ₉ H ₁₈ O	2,6-dimethyl-4-heptanone	113.776 04	113.807	0.000 27

TABLE XXII. Summary results of carboxylic acids.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CH ₂ O ₂	Formic acid	21.019 45	21.036	0.000 79
C ₂ H ₄ O ₂	Acetic acid	33.559 16	33.537	−0.000 66
C ₃ H ₆ O ₂	Propanoic acid	45.716 86	45.727	0.000 22
C ₄ H ₈ O ₂	Butanoic acid	57.874 56	57.883	0.000 15
C ₅ H ₁₀ O ₂	Pentanoic acid	70.032 26	69.995	−0.000 53
C ₅ H ₁₀ O ₂	3-methylbutanoic acid	70.104 82	70.183	0.001 11
C ₅ H ₁₀ O ₂	2,2-dimethylpropanoic acid	70.316 79	69.989	−0.004 68
C ₆ H ₁₂ O ₂	Hexanoic acid	82.189 96	82.149	−0.000 50
C ₇ H ₁₄ O ₂	Heptanoic acid	94.347 66	94.347	0.000 00
C ₈ H ₁₆ O ₂	Octanoic acid	106.505 36	106.481	−0.000 22
C ₉ H ₁₈ O ₂	Nonanoic acid	118.663 06	118.666	0.000 03
C ₁₀ H ₂₀ O ₂	Decanoic acid	130.820 76	130.795	−0.000 20
C ₁₂ H ₂₄ O ₂	Dodecanoic acid	155.136 16	155.176	0.000 26
C ₁₄ H ₂₈ O ₂	Tetradecanoic acid	179.451 56	179.605	0.000 85
C ₁₅ H ₃₀ O ₂	Pentadecanoic acid	191.609 26	191.606	−0.000 02
C ₁₆ H ₃₂ O ₂	Hexadecanoic acid	203.766 96	203.948	0.000 89
C ₁₈ H ₃₆ O ₂	Stearic acid	228.082 36	228.298	0.000 94
C ₂₀ H ₄₀ O ₂	Eicosanoic acid	252.397 76	252.514	0.000 46

TABLE XXIII. Summary results of carboxylic acid esters.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₂ H ₄ O ₂	Methyl formate	32.710 76	32.762	0.001 56
C ₃ H ₆ O ₂	Methyl acetate	45.248 49	45.288	0.000 87
C ₆ H ₁₂ O ₂	Methyl pentanoate	81.721 59	81.726	0.000 05
C ₇ H ₁₄ O ₂	Methyl hexanoate	93.879 29	93.891	0.000 12
C ₈ H ₁₆ O ₂	Methyl heptanoate	106.036 99	106.079	0.000 40
C ₉ H ₁₈ O ₂	Methyl octanoate	118.194 69	118.217	0.000 18
C ₁₀ H ₂₀ O ₂	Methyl nonanoate	130.352 39	130.373	0.000 16
C ₁₁ H ₂₂ O ₂	Methyl decanoate	142.510 09	142.523	0.000 09
C ₁₂ H ₂₄ O ₂	Methyl undecanoate	154.667 79	154.677	0.000 06
C ₁₃ H ₂₆ O ₂	Methyl dodecanoate	166.825 49	166.842	0.000 10
C ₁₄ H ₂₈ O ₂	Methyl tridecanoate	178.983 19	179.000	0.000 09
C ₁₅ H ₃₀ O ₂	Methyl tetradecanoate	191.140 89	191.170	0.000 15
C ₁₆ H ₃₂ O ₂	Methyl pentadecanoate	203.298 59	203.356	0.000 28
C ₄ H ₈ O ₂	Propyl formate	57.763 66	57.746	−0.000 30
C ₄ H ₈ O ₂	Ethyl acetate	57.638 88	57.548	−0.001 57
C ₅ H ₁₀ O ₂	Isopropyl acetate	69.897 47	69.889	−0.000 13
C ₅ H ₁₀ O ₂	Ethyl propanoate	69.796 58	69.700	−0.001 39
C ₆ H ₁₂ O ₂	Butyl acetate	81.954 28	81.873	−0.000 99
C ₆ H ₁₂ O ₂	t-butyl acetate	82.238 81	82.197	−0.000 51
C ₆ H ₁₂ O ₂	Methyl 2, 2-dimethylpropanoate	82.006 12	81.935	−0.000 87
C ₇ H ₁₄ O ₂	Ethyl pentanoate	94.111 98	94.033	−0.000 84
C ₇ H ₁₄ O ₂	Ethyl 3-methylbutanoate	94.184 54	94.252	0.000 72
C ₇ H ₁₄ O ₂	Ethyl 2, 2-dimethylpropanoate	94.396 51	94.345	−0.000 54
C ₈ H ₁₆ O ₂	Isobutyl isobutanoate	106.443 13	106.363	−0.000 75
C ₈ H ₁₆ O ₂	Propyl pentanoate	106.269 68	106.267	−0.000 03
C ₈ H ₁₆ O ₂	Isopropyl pentanoate	106.370 57	106.384	0.000 13
C ₉ H ₁₈ O ₂	Butyl pentanoate	118.427 38	118.489	0.000 52
C ₉ H ₁₈ O ₂	Sec-butyl pentanoate	118.528 27	118.624	0.000 81
C ₉ H ₁₈ O ₂	Isobutyl pentanoate	118.499 94	118.576	0.000 64

TABLE XXIV. Summary results of amides.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CH ₃ NO	Formamide	23.687 12	23.697	0.000 41
C ₂ H ₅ NO	Acetamide	36.152 22	36.103	−0.001 35
C ₃ H ₇ NO	Propanamide	48.309 92	48.264	−0.000 94
C ₄ H ₉ NO	Butanamide	60.467 62	60.449	−0.000 30
C ₄ H ₉ NO	2-methyl- propanamide	60.515 09	60.455	−0.000 99
C ₅ H ₁₁ NO	Pentanamide	72.625 32	72.481	−0.002 00
C ₅ H ₁₁ NO	2,2-dimethyl- propanamide	72.678 90	72.718	0.000 54
C ₆ H ₁₃ NO	Hexanamide	84.783 02	84.780	−0.000 04
C ₈ H ₁₇ NO	Octanamide	109.098 42	109.071	−0.000 25

TABLE XXV. 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 ₃ H ₇ NO	<i>N,N</i> -dimethylformamide	47.679 454	47.574	0.002 21
C ₄ H ₉ NO	<i>N,N</i> -dimethylacetamide	60.144 55	59.890	−0.004 26
C ₆ H ₁₃ NO	<i>N</i> -butylacetamide	84.636 49	84.590	−0.000 55

TABLE XXVI. Summary results of urea.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CH ₄ N ₂ O	Urea	31.359 19	31.393	0.001 08

TABLE XXVII. Summary results of acid halide.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₂ H ₃ ClO	Acetyl chloride	28.021 74	27.990	−0.001 15

TABLE XXVIII. Summary results of acid anhydrides.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₄ H ₆ O ₃	Acetic anhydride	56.940 96	56.948	0.000 13
C ₆ H ₁₀ O ₃	Propanoic anhydride	81.256 36	81.401	0.001 77

TABLE XXIX. Summary results of nitriles.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₂ H ₃ N	Acetonitrile	25.720 60	25.77	0.001 74
C ₃ H ₅ N	Propanenitrile	37.878 30	37.94	0.001 71
C ₄ H ₇ N	Butanenitrile	50.036 00	50.08	0.000 82
C ₄ H ₇ N	2-methyl- propanenitrile	50.136 89	50.18	0.000 92
C ₅ H ₉ N	Pentanenitrile	62.193 70	62.26	0.001 11
C ₅ H ₉ N	2,2-dimethyl- propanenitrile	62.478 23	62.40	−0.001 32
C ₇ H ₁₃ N	Heptanenitrile	86.509 10	86.59	0.000 89
C ₈ H ₁₅ N	Octanenitrile	98.666 80	98.73	0.000 69
C ₁₀ H ₁₉ N	Decanenitrile	122.982 20	123.05	0.000 57
C ₁₄ H ₂₇ N	Tetradecanenitrile	171.613 00	171.70	0.000 52

TABLE XXX. Summary results of thiols.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
HS	Hydrogen sulfide	3.774 30	3.653	−0.033 20
H ₂ S	Dihydrogen sulfide	7.560 58	7.605	0.005 82
CH ₄ S	Methanethiol	19.602 64	19.575	−0.001 41
C ₂ H ₆ S	Ethanethiol	31.760 34	31.762	0.000 05
C ₃ H ₈ S	1-propanethiol	43.918 04	43.933	0.000 35
C ₃ H ₈ S	2-propanethiol	44.018 93	44.020	0.000 03
C ₄ H ₁₀ S	1-butanethiol	56.075 74	56.089	0.000 24
C ₄ H ₁₀ S	2-butanethiol	56.176 63	56.181	0.000 09
C ₄ H ₁₀ S	2-methyl- 1-propanethiol	56.148 30	56.186	0.000 66
C ₄ H ₁₀ S	2-methyl- 2-propanethiol	56.360 27	56.313	−0.000 84
C ₅ H ₁₂ S	2-methyl- 1-butanethiol	68.306 00	68.314	0.000 12
C ₅ H ₁₂ S	1-pentanethiol	68.233 44	68.264	0.000 44
C ₅ H ₁₂ S	2-methyl- 2-butanethiol	68.517 97	68.441	−0.001 13
C ₅ H ₁₂ S	3-methyl- 2-butanethiol	68.315 52	68.381	0.000 95
C ₅ H ₁₂ S	2,2-dimethyl- 1-propanethiol	68.164 41	68.461	0.004 33
C ₆ H ₁₄ S	1-hexanethiol	80.391 14	80.416	0.000 31
C ₆ H ₁₄ S	2-methyl- 2-pentanethiol	80.675 67	80.607	−0.000 85
C ₇ H ₁₆ S	1-heptanethiol	92.548 84	92.570	0.000 23
C ₁₀ H ₂₂ S	1-decanethiol	129.021 94	129.048	0.000 20

TABLE XXXI. Summary results of sulfides.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₂ H ₆ S	Dimethyl sulfide	31.656 68	31.672	0.000 48
C ₃ H ₈ S	Ethyl methyl sulfide	43.814 38	43.848	0.000 78
C ₄ H ₁₀ S	Diethyl sulfide	55.972 08	56.043	0.001 26
C ₄ H ₁₀ S	Methyl propyl sulfide	55.972 08	56.029	0.001 02
C ₄ H ₁₀ S	Isopropyl methyl sulfide	56.072 97	56.115	0.000 75
C ₅ H ₁₂ S	Butyl methyl sulfide	68.129 78	68.185	0.000 81
C ₅ H ₁₂ S	t-butyl methyl sulfide	68.282 45	68.381	0.001 44
C ₅ H ₁₂ S	Ethyl propyl sulfide	68.129 78	68.210	0.001 17
C ₅ H ₁₂ S	Ethyl isopropyl sulfide	68.230 67	68.350	0.001 74
C ₆ H ₁₄ S	Diisopropyl sulfide	80.489 26	80.542	0.000 65
C ₆ H ₁₄ S	Butyl ethyl sulfide	80.287 48	80.395	0.001 33
C ₆ H ₁₄ S	Methyl pentyl sulfide	80.287 48	80.332	0.000 56
C ₈ H ₁₈ S	Dibutyl sulfide	104.602 88	104.701	0.000 94
C ₈ H ₁₈ S	Di-sec-butyl sulfide	104.804 66	104.701	−0.000 99
C ₈ H ₁₈ S	Di-t-butyl sulfide	104.908 22	104.920	0.000 11
C ₈ H ₁₈ S	Diisobutyl sulfide	104.748 00	104.834	0.000 82
C ₁₀ H ₂₂ S	Dipentyl sulfide	128.918 28	128.979	0.000 47
C ₁₀ H ₂₂ S	Diisopentyl sulfide	129.063 40	129.151	0.000 68

TABLE XXXII. Summary results of disulfides.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₂ H ₆ S ₂	Dimethyl disulfide	34.481 27	34.413	−0.001 99
C ₄ H ₁₀ S ₂	Diethyl disulfide	58.796 67	58.873	0.001 29
C ₆ H ₁₄ S ₂	Dipropyl disulfide	83.112 07	83.169	0.000 68
C ₈ H ₁₈ S ₂	Di-t-butyl disulfide	107.996 53	107.919	−0.000 72

TABLE XXXIII. Summary results of sulfoxides.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₂ H ₆ SO	Dimethyl sulfoxide	35.524 50	35.435	−0.002 53
C ₄ H ₁₀ SO	Diethyl sulfoxide	59.839 90	59.891	0.000 85
C ₆ H ₁₄ SO	Dipropyl sulfoxide	84.155 30	84.294	0.001 65

TABLE XXXIV. Summary results of sulfones.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₂ H ₆ SO ₂	Dimethyl sulfone	40.275 88	40.316	0.001 00

TABLE XXXV. Summary results of sulfites.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₂ H ₆ SO ₃	Dimethyl sulfite	43.950 58	44.042	0.002 07
C ₄ H ₁₀ SO ₃	Diethyl sulfite	68.549 39	68.648	0.001 43
C ₈ H ₁₈ SO ₃	Dibutyl sulfite	117.180 19	117.191	0.000 09

TABLE XXXVI. Summary results of sulfates.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₂ H ₆ SO ₄	Dimethyl sulfate	48.701 96	48.734	0.000 67
C ₄ H ₁₀ SO ₄	Diethyl sulfate	73.300 77	73.346	0.000 61
C ₆ H ₁₄ SO ₄	Dipropyl sulfate	97.616 17	97.609	−0.000 08

TABLE XXXVII. Summary results of nitro alkanes.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CH ₃ NO ₂	Nitromethane	25.149 34	25.107	−0.001 68
C ₂ H ₅ NO ₂	Nitroethane	37.307 04	37.292	−0.000 40
C ₃ H ₇ NO ₂	1-nitropropane	49.464 74	49.451	−0.000 28
C ₃ H ₇ NO ₂	2-nitropropane	49.565 63	49.602	0.000 74
C ₄ H ₉ NO ₂	1-nitrobutane	61.622 44	61.601	−0.000 36
C ₄ H ₉ NO ₂	2-nitroisobutane	61.906 97	61.945	0.000 61
C ₅ H ₁₁ NO ₂	1-nitropentane	73.780 14	73.759	−0.000 28

TABLE XXXVIII. Summary results of nitrite.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CH ₃ NO ₂	Methyl nitrite	24.923 28	24.955	0.001 26

TABLE XXXIX. Summary results of nitrate.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CH ₃ NO ₃	Methyl nitrate	28.185 36	28.117	−0.002 44
C ₂ H ₅ NO ₃	Ethyl nitrate	40.343 06	40.396	0.001 31
C ₃ H ₇ NO ₃	Propyl nitrate	52.500 76	52.550	0.000 93
C ₃ H ₇ NO ₃	Isopropyl nitrate	52.601 65	52.725	0.002 33

TABLE XL. Summary results of conjugated alkenes.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₅ H ₈	Cyclopentene	54.835 65	54.861 17	0.000 47
C ₄ H ₆	1,3 butadiene	42.091 59	42.127 05	0.000 84
C ₅ H ₈	1,3 pentadiene	54.407 76	54.424 84	0.000 31
C ₅ H ₈	1,4 pentadiene	54.037 45	54.118 06	0.001 49
C ₅ H ₆	1,3 cyclopentadiene	49.274 32	49.302 94	0.000 58

TABLE XLI. Summary results of aromatics and heterocyclic aromatics.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₆ H ₆	Benzene	57.260 08	57.263 40	0.000 06
C ₆ H ₅ Cl	Fluorobenzene	57.935 10	57.887	−0.000 83
C ₆ H ₅ Cl	Chlorobenzene	56.552 63	56.581	0.000 51
C ₆ H ₄ Cl ₂	m-dichlorobenzene	55.845 18	55.852	0.000 12
C ₆ H ₃ Cl ₃	1,2,3-trichlorobenzene	55.137 73	55.077	−0.001 11
C ₆ H ₃ Cl ₃	1,3,5-trichlorobenzene	55.295 42	55.255	−0.000 73
C ₆ Cl ₆	Hexachlorobenzene	52.571 30	52.477	−0.001 79
C ₆ H ₅ Br	Bromobenzene	56.179 32	56.391 ^a	0.003 76
C ₆ H ₅ I	Iodobenzene	55.259 93	55.261	0.000 01
C ₆ H ₅ NO ₂	Nitrobenzene	65.187 54	65.217	0.000 46
C ₇ H ₈	Toluene	69.484 25	69.546	0.000 88
C ₇ H ₆ O ₂	Benzoic acid	73.769 38	73.762	−0.000 09
C ₇ H ₅ ClO ₂	2-chlorobenzoic acid	73.061 93	73.082	0.000 27
C ₇ H ₅ ClO ₂	3-chlorobenzoic acid	73.268 20	73.261	−0.000 10
C ₆ H ₇ N	Aniline	64.433 73	64.374	−0.000 93
C ₇ H ₉ N	2-methylaniline	76.623 45	76.643	−0.000 25
C ₇ H ₉ N	3-methylaniline	76.623 45	76.661	0.000 50
C ₇ H ₉ N	4-methylaniline	76.623 45	76.654	0.000 40
C ₆ H ₆ N ₂ O ₂	2-nitroaniline	72.474 76	72.424	−0.000 70
C ₆ H ₆ N ₂ O ₂	3-nitroaniline	72.474 76	72.481	−0.000 09
C ₆ H ₆ N ₂ O ₂	4-nitroaniline	72.474 76	72.476	−0.000 02
C ₇ H ₇ NO ₂	Aniline-2-carboxylic acid	80.908 57	80.941	0.000 41
C ₇ H ₇ NO ₂	Aniline-3-carboxylic acid	80.908 57	80.813	−0.001 18
C ₇ H ₇ NO ₂	Aniline-4-carboxylic acid	80.908 57	80.949	0.000 50
C ₆ H ₆ O	Phenol	61.758 17	61.704	−0.000 87
C ₆ H ₄ N ₂ O ₅	2,4-dinitrophenol	77.613 08	77.642	0.000 37
C ₆ H ₈ O	Anisole	73.390 06	73.355	−0.000 47
C ₁₀ H ₈	Naphthalene	90.746 58	90.791 43	0.000 49
C ₄ H ₅ N	Pyrrole	44.810 90	44.785	−0.000 57
C ₄ H ₄ O	Furan	41.677 82	41.692	0.000 33
C ₄ H ₄ S	Thiophene	40.425 01	40.430	0.000 13
C ₃ H ₄ N ₂	Imidazole	39.763 43	39.741 06	−0.000 56
C ₅ H ₅ N	Pyridine	51.918 02	51.879 27	−0.000 75
C ₄ H ₄ N ₂	Pyrimidine	46.575 97	46.517 94	−0.001 25
C ₄ H ₄ N ₂	Pyrazine	46.575 97	46.513 80	0.000 95
C ₉ H ₇ N	Quinoline	85.404 53	85.486 07	0.001 78
C ₉ H ₇ N	Isoquinoline	85.404 53	85.443 58	0.000 46
C ₈ H ₇ N	Indole	78.522 15	78.514	−0.000 10

^aLiquid.

TABLE XLII. Summary results of DNA bases.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₅ H ₅ N ₅	Adenine	70.854 16	70.798 11	−0.000 79
C ₅ H ₆ N ₂ O ₂	Thymine	69.087 92	69.064 38	−0.000 34
C ₅ H ₅ N ₅ O	Guanine	76.882 12	77.418 49	−0.000 55
C ₄ H ₅ N ₃ O	Cytosine	59.533 78	60.580 56	0.017 28

TABLE XLIII. Summary results of alkyl phosphines.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₃ H ₉ P	Trimethylphosphine	45.809 30	46.873 33	0.022 70
C ₆ H ₁₅ P	Triethylphosphine	82.282 40	82.248 69	−0.000 41
C ₁₈ H ₁₅ P	Triphenylphosphine	168.400 33	167.465 91	−0.005 58

TABLE XLIV. Summary results of alkyl phosphites.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₃ H ₉ O ₃ P	Trimethyl phosphite	61.067 64	60.943 29	−0.002 04
C ₆ H ₁₅ O ₃ P	Triethyl phosphite	98.124 06	97.979 47	−0.001 48
C ₉ H ₂₁ O ₃ P	Tri-isopropyl phosphite	134.899 83	135.006 98	0.000 79

TABLE XLV. Summary results of alkyl phosphine oxides.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₃ H ₉ PO	Trimethylphosphine oxide	53.004 30	52.911 92	−0.001 75

TABLE XLVI. Summary results of alkyl phosphates.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₆ H ₁₅ O ₄ P	Triethyl phosphate	105.319 06	104.404 00	−0.008 76
C ₉ H ₂₁ O ₄ P	Tri- <i>n</i> -propyl phosphate	141.792 16	140.867 78	−0.006 56
C ₉ H ₂₁ O ₄ P	Tri-isopropyl phosphate	142.094 83	141.422 83	−0.004 75
C ₉ H ₂₇ O ₄ P	Tri- <i>n</i> -butyl phosphate	178.265 26	178.077 42	−0.001 05

TABLE XLVII. Summary results of monosaccharides of DNA and RNA.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₅ H ₁₀ O ₄	2-deoxy-D-ribose	77.258 42		
C ₅ H ₁₀ O ₅	D-ribose	81.510 34	83.498 ^a	0.023 81
C ₅ H ₁₀ O ₄	Alpha-2-deoxy-D-ribose	77.466 84		
C ₅ H ₁₀ O ₅	Alpha-D-ribose	82.310 88		

^aCrystal

TABLE XLVIII. Summary results of amino acids.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₄ H ₇ NO ₄	Aspartic acid	68.981 09	70.843 ^a	0.026 28
C ₅ H ₉ NO ₄	Glutamic acid	81.138 79	83.167 ^a	0.024 38
C ₃ H ₇ NO ₄ S	Cysteine	55.024 57	56.571 ^a	0.027 33
C ₆ H ₁₄ N ₂ O ₂	Lysine	95.777 99	98.194 ^a	0.024 61
C ₆ H ₁₄ N ₂ O ₂	Arginine	105.070 07	107.420 ^a	0.021 88
C ₆ H ₉ N ₃ O ₂	Histidine	88.102 32	89.599 ^a	0.016 71
C ₄ H ₈ N ₂ O ₂	Asparagine	71.574 14	73.513 ^a	0.026 37
C ₅ H ₁₀ N ₂ O ₂	Glutamine	83.731 84	85.843 ^a	0.024 59
C ₄ H ₉ NO ₃	Threonine	68.956 78	71.058 ^a	0.029 56
C ₉ H ₁₁ NO ₃	Tyrosine	109.404 27	111.450 ^a	0.018 35
C ₃ H ₇ NO ₃	Serine	56.669 86	58.339 ^a	0.028 61
C ₁₁ H ₁₂ N ₂ O ₂	Tryptophan	126.742 91	128.084 ^a	0.010 47
C ₉ H ₁₁ NO ₂	Phenylalanine	104.906 18	105.009	0.000 98
C ₅ H ₉ NO ₂	Proline	71.768 26	71.332	−0.006 11
C ₅ H ₉ NO ₂	Methionine	79.236 31	79.214	−0.000 28
C ₆ H ₁₃ NO ₂	Leucine	89.121 15	89.047	−0.000 28
C ₆ H ₁₃ NO ₂	Isoleucine	89.029 78	90.612	0.017 46
C ₆ H ₁₃ NO ₂	Valine	76.872 08	76.772	−0.001 30
C ₃ H ₇ NO ₂	Alanine	52.575 49	52.991	0.007 85
C ₂ H ₃ NO ₂	Glycine	40.288 57	40.280	−0.000 21

^aCrystal

TABLE XLIX. Summary results of allotropes of carbon.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C _n	Diamond	3.748 29	3.704	−0.01
C ₆₀	Fullerene	419.755 39	419.733 67	−0.000 05
C _n	Graphite	4.913 59	4.898 66	−0.003 05

TABLE L. Summary results of silanes.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
SiH	Silylidyne	3.075 26	3.020 08	−0.018 27
SiH ₂	Silylene	6.150 52	6.355 23	0.032 21
SiH ₃	Silyl	9.225 78	9.364 94	0.014 86
SiH ₄	Silane	13.572 57	13.345 77	−0.016 99
Si ₂ H ₆	Disilane	21.767 13	22.055 72	0.013 08
Si ₃ H ₈	Trisilane	31.233 22	30.813 34	−0.013 63

TABLE LI. Summary results of alkyl silanes and disilanes.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CH ₃ Si	Methylsilane	25.378 82	25.994 91	0.023 70
C ₂ H ₈ Si	Dimethylsilane	38.456 60	38.648 19	0.004 96
C ₃ H ₁₀ Si	Trimethylsilane	51.534 38	51.335 67	−0.003 87
C ₄ H ₁₂ Si	Tetramethylsilane	64.612 16	64.223 19	−0.006 06
C ₄ H ₁₂ Si	Diethylsilane	62.772 00	63.377 71	0.009 56
C ₆ H ₁₆ Si	Triethylsilane	88.007 48	87.461 41	−0.006 24
C ₈ H ₂₀ Si	Tetraethylsilane	113.242 96	112.065 47	−0.010 51
CH ₃ Si ₂	Methyldisilane	34.567 39	34.739 20	0.004 95
C ₂ H ₁₀ Si ₂	1,1-dimethyldisilane	47.367 64	47.422 83	0.001 16
C ₂ H ₁₀ Si ₂	1,2-dimethyldisilane	47.367 64	47.422 83	0.001 16
C ₃ H ₁₂ Si ₂	1,1,1-trimethyldisilane	60.167 89	60.106 46	−0.001 02
C ₃ H ₁₂ Si ₂	1,1,2-trimethyldisilane	60.167 89	60.106 46	−0.001 02
C ₄ H ₁₄ Si ₂	1,1,1,2-tetramethyldisilane	72.968 15	72.794 42	−0.002 39
C ₄ H ₁₄ Si ₂	1,1,2,2-tetramethyldisilane	72.968 15	72.794 42	−0.002 39
C ₅ H ₁₆ Si ₂	1,1,1,2,2-Pentamethyldisilane	85.768 40	85.478 05	−0.003 40
C ₆ H ₁₈ Si ₂	Hexamethyldisilane	98.568 65	98.326 46	−0.002 46

TABLE LII. 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	8.308 76	8.299 05	−0.001 17
SiO ₂	Silicon dioxide	12.941 90	12.980 73	0.002 99
SiH ₄ O	H ₃ SiOH	18.671 84	19.007 01 ^a	0.017 63
SiH ₄ O ₂	H ₂ Si(OH) ₂	25.042 64	25.042 64 ^a	0.005 63
SiH ₄ O ₃	HSi(OH) ₃	31.413 44	31.470 12 ^a	0.001 80
SiH ₄ O ₄	Si(OH) ₄	37.784 23	38.036 38	0.006 63
C ₃ H ₁₀ SiO	Trimethylsilanol	57.318 95	57.300 73	−0.000 32
C ₂ H ₆ SiO	Vinylsilanol	37.337 84		
CH ₃ SiO ₄	(HO) ₃ SiOCH ₃	47.451 44	49.281 71 ^a	0.037 14
C ₄ H ₁₂ SiO ₄	Tetramethoxysiloxane	83.487 83	84.046 81	0.006 65
C ₆ H ₁₆ SiO ₃	Triethoxysiloxane	102.747 55	102.579 61	−0.001 64
C ₈ H ₂₀ SiO ₄	Tetraethoxysiloxane	132.896 39	133.231 77	0.002 52
C ₆ H ₁₈ Si ₃ O ₃	((CH ₃) ₂ SiO) ₃	123.615 10	123.224 85	−0.003 17
C ₈ H ₂₄ Si ₄ O ₄	((CH ₃) ₂ SiO) ₄	164.820 14	164.790 37	−0.000 18
C ₁₀ H ₃₀ Si ₅ O ₅	((CH ₃) ₂ SiO) ₅	206.025 17	206.355 89	0.001 60
C ₆ H ₁₈ Si ₂ O	Hexamethyldisiloxane	105.246 39	105.201 96	−0.000 42

^aTheory.

TABLE LIII. Summary results of boranes.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
BB	Diboron	3.124 75	3.104 05	−0.006 67
B ₂ H ₆	Diborane	24.942 29	24.890 30	−0.002 09
B ₄ H ₁₀	Tetraborane(10)	44.921 60	45.331 34	0.009 04
B ₅ H ₉	Pentaborane(9)	48.254 62	48.854 11	0.012 27
B ₅ H ₁₁	Pentaborane(11)	54.005 46	53.060 86	−0.017 80
B ₆ H ₁₀	Hexaborane(10)	56.550 63	56.747 39	0.003 47
B ₉ H ₁₅	Nonaborane(15)	85.613 80	84.950 08	−0.007 81
B ₁₀ H ₁₄	Decaborane(14)	89.734 67	89.697 90	−0.000 41

TABLE LIV. Summary results of alkyl boranes.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CH ₃ B	Methylborane	24.609 91	24.493 50	−0.004 75
C ₂ H ₇ B	Dimethylborane	37.088 21	37.177 13	0.002 39
B ₂ CH ₈	Methyldiborane	37.420 60	37.582 59	0.004 31
B ₂ C ₂ H ₁₀	Ethyldiborane	49.578 30	49.507 36	−0.001 43
C ₃ H ₉ B	Trimethylboron	49.566 52	49.761 02	0.003 91
B ₂ C ₂ H ₁₀	1,1-dimethyldiborane	49.898 90	50.201 18	0.006 02
B ₂ C ₂ H ₁₀	1,2-dimethyldiborane	49.898 90	50.201 18	0.006 02
B ₄ CH ₁₂	Methyltetraborane	57.399 90	57.746 04	0.005 99
B ₃ CH ₁₁	Methylpentaborane	60.732 92	61.515 85	0.012 73
B ₂ C ₃ H ₁₂	Trimethyldiborane	62.377 21	62.884 81	0.008 07
B ₄ C ₂ H ₁₄	Ethyltetraborane	69.557 60	69.996 03	0.006 26
B ₅ C ₂ H ₁₃	Ethylpentaborane	72.890 62	73.765 85	0.011 86
B ₂ C ₄ H ₁₄	1,1-diethyldiborane	74.214 30	74.344 20	0.001 75
B ₂ C ₄ H ₁₄	Tetramethyldiborane	74.855 51	75.481 71	0.008 30
B ₃ C ₃ H ₁₅	Propylpentaborane	85.048 32	85.842 39	0.009 25
C ₆ H ₁₅ B	Triethylboron	86.039 62	86.129 41	0.001 04
B ₂ C ₆ H ₁₈	Triethyldiborane	98.850 31	98.594 07	−0.002 60
B ₁₀ CH ₁₆	Methyldecaborane	102.212 98	101.917 75	−0.002 60
C ₈ H ₁₇ B	<i>n</i> -butylboracyclopentane	105.359 16	105.698 74 ^a	0.003 21
B ₁₀ C ₂ H ₁₈	Ethyldecaborane	114.370 68	113.560 66	−0.007 13
C ₉ H ₂₁ B	Tripropylboron	122.512 72	122.597 53	0.000 69
C ₉ H ₂₁ B	Tri-isopropylboron	122.815 39	122.757 98	−0.000 47
B ₂ C ₈ H ₂₂	Tetraethyldiborane	123.486 31	123.740 17	0.002 05
B ₁₀ C ₃ H ₂₀	Propyldecaborane	126.528 38	125.940 75	−0.004 67
C ₁₂ H ₂₇ B	Tri- <i>s</i> -butylboron	159.288 49	158.506 27	−0.004 93
C ₁₂ H ₂₇ B	Tributylboron	158.985 82	159.035 30	0.000 31
C ₁₂ H ₂₇ B	Tri-isobutylboron	159.203 50	159.343 18	0.000 88
C ₁₈ H ₁₅ B	Triphenylboron	172.157 55	172.096 81	−0.000 35
C ₁₅ H ₃₃ B	Tri-3-methylbutylboron	195.676 60	195.780 95	0.000 53
C ₁₈ H ₃₃ B	Tricyclohexylboron	217.247 11	218.237 63	0.004 54
C ₁₈ H ₃₉ B	Tri- <i>n</i> -hexylboron	231.932 02	231.763 40	−0.000 73
C ₂₁ H ₄₅ B	Tri- <i>n</i> -heptylboron	268.405 12	268.222 85	−0.000 68
C ₂₄ H ₅₁ B	Tri- <i>s</i> -octylboron	305.180 89	304.612 92	−0.001 86
C ₂₄ H ₅₁ B	Tri- <i>n</i> -octylboron	304.878 22	304.682 30	−0.000 64

^aCrystal.

TABLE LV. Summary results of alkoxy boranes and borinic acids.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
BH ₃ O	Hydroxyborane	18.293 11	18.225 72	−0.003 70
BH ₃ O ₂	Dihydroxyborane	24.454 60	24.437 77	−0.000 69
BH ₃ O ₃	Boric acid	30.616 10	30.684 31	0.002 22
BC ₂ H ₇ O ₂	Dimethoxyborane	47.753 25	47.723 58	−0.000 62
BC ₃ H ₉ O ₃	Trimethyl borate	65.564 08	65.539 50	−0.000 37
C ₅ H ₁₁ OB	Methoxyboracyclopentane	71.248 58	74.475 66 ^a	0.003 45
C ₆ H ₇ O ₂ B	Phenylborinic acid	77.796 59	78.861 21 ^a	0.013 50
C ₆ H ₁₅ O ₂ B	Di-isopropoxyborane	96.974 71	97.417 37 ^a	0.004 54
BC ₆ H ₁₅ O ₃	Triethyl borate	102.620 50	102.501 97	−0.001 16
C ₈ H ₁₉ OB	Di- <i>n</i> -butylborinic acid	116.195 91	116.451 17	0.002 19
BC ₉ H ₂₁ O ₃	Tri- <i>n</i> -propyl borate	139.093 60	139.113 19	0.000 14
C ₁₂ H ₂₇ OB	<i>n</i> -butyl di- <i>n</i> -butylborinate	164.512 78	165.295 04 ^a	0.004 73
C ₁₂ H ₂₇ O ₂ B	Di- <i>n</i> -butyl <i>n</i> -butylboronate	170.039 74	170.869 64 ^a	0.004 86
BC ₁₂ H ₂₇ O ₃	Tri- <i>n</i> -butyl borate	175.566 70	175.629 01	0.000 35
C ₁₈ H ₁₅ O ₃ B ₃	Phenylborinic anhydride	204.750 82	205.965 48 ^a	0.005 90
C ₁₆ H ₃₆ OB ₂	Di- <i>n</i> -butylborinic anhydride	222.845 51	223.702 32 ^a	0.003 83
C ₂₄ H ₂₀ OB ₂	Diphenylborinic anhydride	240.407 82	241.389 41 ^a	0.004 07

^aCrystal.

TABLE LVI. 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 ₂ H ₇ N	Aminodiborane	32.362 13	31.992 18	−0.011 56
B ₂ C ₂ H ₁₁ N	<i>n</i> -dimethylaminodiborane	57.215 17	57.528 55	0.005 45
C ₆ H ₁₈ N ₃ B	Tris(dimethylamino)borane	108.950 23	108.644 90	−0.002 81
C ₈ H ₂₀ NB	Di- <i>n</i> -butylboronamine	117.454 25	119.491 84 ^a	0.017 05
C ₁₂ H ₂₈ NB	Di- <i>n</i> -butylboron- <i>n</i> -butylamine	166.495 95	167.832 69 ^a	0.007 96
C ₂ H ₁₀ NB	Dimethylaminoborane	49.307 40	49.521 89	0.004 33
BC ₃ H ₁₂ N	Trimethylaminoborane	61.371 83	61.052 05	−0.005 24
BC ₃ H ₁₂ N	Ammoniatrimethylborane	62.918 57	62.522 07	−0.006 34
C ₆ H ₁₈ NB	Triethylaminoborane	97.844 93	97.420 44	−0.004 36
BC ₆ H ₁₈ N	Trimethylaminotrimethylborane	98.806 74	98.270 36	−0.005 46

^aCrystal.

TABLE LVII. Summary results of halidoboranes.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
HB ₂ F ₂	Difluoroboron	17.556 66	17.418 45	−0.007 93
BF ₃	Boron trifluoride	20.269 18	20.097 44	−0.008 55
BF ₂ HO	Difluoroborinic acid	23.718 16	23.647 84	−0.002 97
BFH ₂ O ₂	Fluoroboronic acid	27.167 13	27.181 35	0.000 52
BCH ₃ F ₂	Difluoro-methyl-borane	30.034 96	30.336 24	0.009 93
BC ₂ H ₃ F ₂	Vinyldifluoroborane	36.218 93	36.549 81	0.009 05
BC ₃ H ₉ NF ₃	Trimethylamine-Trifluoroborane	69.509 41	69.113 68	−0.005 73
HBCl ₂	Dichloroboron	13.216 40	13.252 91	0.002 76
BCl ₃	Boron trichloride	13.758 79	13.807 48	0.003 53
BCl ₂ F	Dichlorofluoroborane	15.928 92	15.875 07	−0.003 39
BClF ₂	Chlorodifluoroborane	18.099 05	17.981 69	−0.006 53
C ₂ H ₅ OC ₂ Cl ₂ B	Ethoxydichloroborane	43.379 36	43.557 32	0.004 09
C ₂ H ₄ O ₂ ClB	2-chloro-1,3,2-dioxaborolan	43.688 67	43.993 61 ^a	0.006 93
C ₂ H ₆ NC ₂ Cl ₂ B	Dimethylaminodichloroborane	45.489 27	45.739 40	0.005 47
BC ₂ ClH ₂ O ₂	Dimethoxychloroborane	48.295 65	48.403 90	0.002 24
C ₃ H ₆ O ₂ ClB	4-methyl-2-chloro-1,3,2-dioxaborolan	55.947 26	56.395 37 ^a	0.007 95
BC ₆ H ₅ Cl ₂	Phenylboron dichloride	66.558 38	66.978 20	0.006 27
C ₄ H ₈ O ₂ ClB	4,5-dimethyl-2-chloro-1,3,2-Dioxaborolan	68.234 18	68.723 42 ^a	0.007 12
C ₄ H ₁₀ O ₂ ClB	Diethoxychloroborane	72.999 93	73.077 35	0.001 06
C ₄ H ₁₂ N ₂ ClB	Bis(dimethylamino) Chloroborane	77.219 75	77.380 78	0.002 08
C ₈ H ₁₈ ClB	Di- <i>n</i> -butylchloroborane	110.576 81	110.993 17	0.003 75
C ₁₂ H ₁₀ ClB	Diphenylchloroborane	119.357 96	119.793 35	0.003 63

^aCrystal.

TABLE LVIII. Summary results of organoaluminum.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₂ H ₇ Al	Dimethylaluminum hydride	34.311 71	34.377 97 ^a	0.001 93
C ₃ H ₉ Al	Trimethyl aluminum	47.109 60	46.953 19	−0.003 33
C ₄ H ₁₁ Al	Tiethylaluminum hydride	58.627 11	60.109 48 ^b	0.024 66
C ₆ H ₁₅ Al	Triethylaluminum hydride	83.582 70	83.581 76	−0.000 01
C ₆ H ₁₅ Al	Di- <i>n</i> -propylaluminum hydride	82.942 51	84.405 66 ^b	0.017 33
C ₉ H ₂₁ Al	Tri- <i>n</i> -propyl aluminum	120.055 80	121.064 58 ^b	0.008 33
C ₈ H ₁₉ Al	Di- <i>n</i> -butylaluminum hydride	107.257 91	108.710 51 ^b	0.013 36
C ₈ H ₁₉ Al	Di-isobutylaluminum hydride	107.403 03	108.775 56 ^b	0.012 62
C ₁₂ H ₂₇ Al	Tri- <i>n</i> -butyl aluminum	156.528 90	157.424 29 ^b	0.005 69
C ₁₂ H ₂₇ Al	Tri-isobutyl aluminum	156.746 58	157.589 08 ^b	0.005 35

^aEstimated.^bCrystal.

TABLE LIX. Summary results of scandium coordinate compounds.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
ScF	Scandium fluoride	6.344 74	6.169 25	−0.028 45
ScF ₂	Scandium difluoride	12.119 37	12.195 56	0.006 25
ScF ₃	Scandium trifluoride	19.284 12	19.279 94	−0.000 22
ScCl	Scandium chloride	4.055 15	4.001 92	−0.013 30
ScO	Scandium oxide	7.034 26	7.083 49	0.006 95

TABLE LX. Summary results of titanium coordinate compounds.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
TiF	Titanium fluoride	6.449 97	6.418 71	−0.004 87
TiF ₂	Titanium difluoride	13.775 32	13.663 90	−0.008 15
TiF ₃	Titanium trifluoride	19.639 61	19.646 71	0.000 36
TiF ₄	Titanium tetrafluoride	24.660 85	24.234 70	−0.017 58
TiCl	Titanium chloride	4.562 09	4.561 98	−0.000 03
TiCl ₂	Titanium dichloride	10.020 25	9.874 08	−0.015 17
TiCl ₃	Titanium trichloride	14.286 74	14.229 84	−0.004 00
TiCl ₄	Titanium tetrachloride	17.949 49	17.824 02	−0.007 04
TiBr	Titanium bromide	3.779 36	3.784 66	0.001 40
TiBr ₂	Titanium dibromide	8.916 50	8.930 12	0.001 53
TiBr ₃	Titanium tribromide	12.077 65	12.022 46	−0.004 59
TiBr ₄	Titanium tetrabromide	14.901 22	14.932 39	0.002 09
TiI	Titanium iodide	3.164 46	3.155 04	−0.002 99
TiI ₂	Titanium diiodide	7.355 50	7.292 91	−0.008 58
TiI ₃	Titanium triiodide	9.741 19	9.719 35	−0.002 25
TiI ₄	Titanium tetraiodide	12.100 14	12.145 69	0.003 75
TiO	Titanium oxide	7.027 29	7.003 41	−0.003 41
TiO ₂	Titanium dioxide	13.235 28	13.210 50	−0.001 88
TiOF	Titanium fluoride oxide	12.782 85	12.773 53	−0.000 73
TiOF ₂	Titanium difluoride oxide	18.948 07	18.669 83	−0.014 90
TiOCl	Titanium chloride oxide	11.105 01	11.256 69	0.013 47
TiOCl ₂	Titanium dichloride oxide	15.592 38	15.542 95	−0.003 18

TABLE LXI. Summary results of vanadium coordinate compounds.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
VF ₅	Vanadium pentafluoride	24.060 31	24.241 39	0.007 47
VCl ₄	Vanadium tetrachloride	15.846 35	15.805 70	−0.003 18
VN	Vanadium nitride	4.856 55	4.819 31	−0.007 75
VO	Vanadium oxide	6.378 03	6.602 64	0.034 02
VO ₂	Vanadium dioxide	12.756 06	12.897 29	0.010 95
VOCl ₃	Vanadium trichloride oxide	18.262 79	18.874 69	0.032 42
V(CO) ₆	Vanadium hexacarbonyl	75.267 91	75.633 69	0.004 84
V(C ₆ H ₆) ₂	Dibenzene vanadium	119.806 33	121.201 93 ^a	0.011 51

^aLiquid.

TABLE LXII. Summary results of chromium coordinate compounds.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CrF ₂	Chromium difluoride	10.919 88	10.926 85	0.000 64
CrCl ₂	Chromium dichloride	7.984 49	7.965 13	−0.002 43
CrO	Chromium oxide	4.738 54	4.755 15	0.003 49
CrO ₂	Chromium dioxide	10.025 83	10.049 24	0.002 33
CrO ₃	Chromium trioxide	14.830 00	14.854 04	0.001 62
CrO ₂ Cl ₂	Chromium dichloride Dioxide	17.461 58	17.306 08	−0.008 99
Cr(CO) ₆	Chromium hexacarbonyl	74.225 88	74.618 72	0.005 26
Cr(C ₆ H ₆) ₂	Dibenzene chromium	117.933 45	117.979 71	0.000 39
Cr((CH ₃) ₃ C ₆ H ₃) ₂	Di-(1,2,4-trimethylbenzene) Chromium	191.278 49	192.429 33 ^a	0.005 98

^aLiquid.

TABLE LXIII. Summary results of manganese coordinate compounds.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
MnF	Manganese fluoride	4.038 58	3.975 67	−0.015 82
MnCl	Manganese chloride	3.745 28	3.738 01	−0.001 94
Mn ₂ (CO) ₁₀	Dimanganese decacarbonyl	123.782 99	122.708 95	−0.008 75

TABLE LXIV. Summary results of iron coordinate compounds.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
FeF	Iron fluoride	4.657 26	4.634 64	−0.004 88
FeF ₂	Iron difluoride	10.031 88	9.980 15	−0.005 18
FeF ₃	Iron trifluoride	15.315 08	15.251 94	−0.004 14
FeCl	Iron chloride	2.967 72	2.974 66	0.002 33
FeCl ₂	Iron dichloride	8.078 80	8.286 32	0.025 04
FeCl ₃	Iron trichloride	10.823 48	10.700 65	−0.011 48
FeO	Iron oxide	4.099 83	4.208 95	0.025 93
Fe(CO) ₅	Iron pentacarbonyl	61.756 23	61.918 46	0.002 62
Fe(C ₅ H ₅) ₂	Bis-cyclopentadienyl iron (ferrocene)	98.907 60	98.952 72	0.000 46

TABLE LXV. Summary results of cobalt coordinate compounds.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CoF ₂	Cobalt difluoride	9.451 15	9.755 52	0.031 20
CoCl	Cobalt chloride	3.665 04	3.680 49	0.004 20
CoI ₂	Cobalt dichloride	7.984 67	7.921 06	−0.008 03
CoCl ₃	Cobalt trichloride	9.835 21	9.872 05	0.003 73
CoH(CO) ₄	Cobalt tetracarbonyl hydride	50.332 17	50.360 87	0.000 57

TABLE LXVI. Summary results of nickel coordinate compounds.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
NiCl	Nickel chloride	3.841 84	3.829 34	−0.003 27
NiCl ₂	Nickel dichloride	7.766 28	7.740 66	−0.003 31
Ni(CO) ₄	Nickel tetracarbonyl	50.792 97	50.776 32	−0.000 33
Ni(C ₅ H ₅) ₂	Bis-cyclopentadienyl nickel (nickelocene)	97.730 62	97.846 49	0.001 18

TABLE LXVII. Summary results of copper coordinate compounds.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
CuF	Copper fluoride	4.393 99	4.446 20	0.011 74
CuF ₂	Copper difluoride	7.912 46	7.890 40	−0.002 80
CuCl	Copper chloride	3.912 40	3.808 70	−0.027 23
CuO	Copper oxide	2.932 19	2.909 31	−0.007 87

TABLE LXVIII. Summary results of zinc coordinate compounds.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
ZnCl	Zinc chloride	2.561 75	2.565 29	0.001 38
ZnCl ₂	Zinc dichloride	6.687 49	6.636 75	−0.007 64
Zn(CH ₃) ₂	Dimethylzinc	29.358 15	29.213 67	−0.004 95
(CH ₃ CH ₂) ₂ Zn	Diethylzinc	53.673 55	53.009 87	−0.012 52
(CH ₃ CH ₂ CH ₂) ₂ Zn	Di- <i>n</i> -propylzinc	77.988 95	77.674 64	−0.004 05
(CH ₃ CH ₂ CH ₂ CH ₂) ₂ Zn	Di- <i>n</i> -butylzinc	102.304 35	101.957 82	−0.003 40

TABLE LXIX. Summary results of germanium compounds.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₈ H ₂₀ Ge	Tetraethylgermanium	109.996 86	110.181 66	0.001 68
C ₁₂ H ₂₈ Ge	Tetra- <i>n</i> -propylgermanium	158.627 66	158.630 92	0.000 02
C ₁₂ H ₃₀ Ge ₂	Hexaethyldigermanium	167.889 82	167.898 36	0.000 05

TABLE LXX. Summary results of tin compounds.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
SnCl ₄	Tin tetrachloride	12.957 56	13.037 04	0.006 10
CH ₃ Cl ₃ Sn	Methyltin trichloride	24.695 30	25.691 18 ^a	0.038 76
C ₂ H ₆ Cl ₂ Sn	Dimethyltin dichloride	36.433 04	37.123 69	0.018 60
C ₃ H ₉ ClSn	Trimethyltin chloride	48.170 77	49.006 89	0.017 06
SnBr ₄	Tin tetrabromide	10.986 55	11.019 94	0.003 03
C ₃ H ₉ BrSn	Trimethyltin bromide	47.678 02	48.353 63	0.013 97
C ₁₂ H ₁₀ Br ₂ Sn	Diphenyltin dibromide	117.174 89	117.366 47 ^a	0.001 63
C ₁₂ H ₂₇ BrSn	Tri- <i>n</i> -butyltin bromide	157.097 32	157.265 55 ^a	0.001 07
C ₁₈ H ₁₅ BrSn	Triphenyltin bromide	170.269 05	169.915 11 ^a	−0.002 08
SnI ₄	Tin tetraiodide	9.716 97	9.733 06	0.001 65
C ₃ H ₉ ISn	Trimethyltin iodide	47.360 62	47.698 52	0.007 08
C ₁₈ H ₁₅ SnI	Triphenyltin iodide	169.951 65	167.879 48 ^a	−0.012 34
SnO	Tin oxide	5.618 58	5.547 70	−0.012 78
SnH ₄	Stannane	10.541 37	10.471 81	−0.006 64
C ₂ H ₈ Sn	Dimethylstannane	35.224 94	35.142 01	−0.002 36
C ₃ H ₁₀ Sn	Trimethylstannane	47.566 73	47.773 53	0.004 33
C ₄ H ₁₂ Sn	Diethylstannane	59.540 34	59.503 37	−0.000 62
C ₄ H ₁₂ Sn	Tetramethyltin	59.908 51	60.139 73	0.003 84
C ₅ H ₁₂ Sn	Trimethylvinyltin	66.092 48	66.432 60	0.005 26
C ₅ H ₁₄ Sn	Trimethylethyltin	72.066 21	72.199 22	0.001 84
C ₆ H ₁₆ Sn	Trimethylisopropyltin	84.324 80	84.323 46	−0.000 02
C ₈ H ₁₂ Sn	Tetravinyltin	84.644 38	86.538 03 ^a	0.021 88
C ₆ H ₁₈ Sn ₂	Hexamethyldistannane	91.963 11	91.755 69	−0.002 26
C ₇ H ₁₈ Sn	Trimethyl- <i>t</i> -butyltin	96.814 17	96.478 05	−0.003 48
C ₉ H ₁₄ Sn	Trimethylphenyltin	100.772 19	100.427 16	−0.003 44
C ₈ H ₁₈ Sn	Triethylvinyltin	102.565 58	102.839 06 ^a	−0.002 66
C ₈ H ₂₀ Sn	Tetraethyltin	108.539 31	108.437 51	−0.000 94
C ₁₀ H ₁₆ Sn	Trimethylbenzyltin	112.239 20	112.612 11	0.003 31
C ₁₀ H ₁₄ O ₂ Sn	Trimethyltin benzoate	117.281 49	119.311 99 ^a	0.017 02
C ₁₀ H ₂₀ Sn	Tetra-allyltin	133.535 58	139.206 55 ^a	0.040 74
C ₁₂ H ₂₈ Sn	Tetra- <i>n</i> -propyltin	157.170 11	157.012 53	−0.001 00
C ₁₂ H ₂₈ Sn	Tetraisopropyltin	157.573 67	156.99 52	−0.003 66
C ₁₂ H ₃₀ Sn ₂	Hexaethyldistannane	164.909 31	164.761 31 ^a	−0.000 90
C ₁₉ H ₁₈ Sn	Triphenylmethyltin	182.499 54	180.978 81 ^a	−0.008 40
C ₂₀ H ₂₀ Sn	Triphenylethyltin	194.657 24	192.925 26 ^a	−0.008 98
C ₁₆ H ₃₆ Sn	Tetra- <i>n</i> -butyltin	205.800 91	205.600 55	−0.000 97
C ₁₆ H ₃₆ Sn	Tetraisobutyltin	206.091 15	206.732 34	0.003 10
C ₂₁ H ₂₄ Sn ₂	Triphenyl- trimethyldistannane	214.554 14	212.729 73 ^a	−0.008 58
C ₂₄ H ₂₀ Sn	Tetraphenyltin	223.363 22	221.614 25	−0.007 89
C ₂₄ H ₄₄ Sn	Tetracyclohexyltin	283.709 27	284.576 03	0.003 05
C ₃₆ H ₃₀ Sn ₂	Hexaphenyldistannane	337.145 17	333.270 41	−0.011 63

^aCrystal.

TABLE LXXI. Summary results of lead compounds.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₄ H ₁₂ Pb	Tetramethyl-lead	57.553 66	57.432 64	−0.002 11
C ₈ H ₂₀ Pb	Tetraethyl-lead	106.184 46	105.491 64	−0.006 57

TABLE LXXII. Summary results of alkyl arsines.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₃ H ₉ As	Trimethylarsine	44.739 78	45.631 14	0.019 53
C ₆ H ₁₅ As	Triethylarsine	81.212 88	81.010 84	−0.002 49
C ₁₈ H ₁₅ As	Triphenylarsine	167.330 81	166.492 57	−0.005 03

TABLE LXXIII. Summary results of alkyl stibines.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₃ H ₉ Sb	Trimethylstibine	44.730 78	45.023 78	0.006 51
C ₆ H ₁₅ Sb	Triethylstibine	81.203 88	80.694 02	−0.006 32
C ₁₈ H ₁₅ Sb	Triphenylstibine	167.321 81	165.815 83	−0.009 08

TABLE LXXIV. Summary results of alkyl bismuths.

Formula	Name	Calculated total bond energy (eV)	Experimental total bond energy (eV)	Relative error
C ₃ H ₉ Bi	Trimethylbismuth	42.073 87	42.790 68	0.016 75
C ₆ H ₁₅ Bi	Triethylbismuth	78.546 97	78.391 53	−0.001 98
C ₁₈ H ₁₅ Bi	Triphenylbismuth	164.664 90	163.751 84	−0.005 58

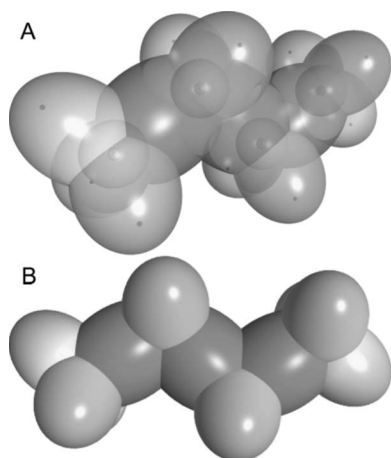


FIG. 5. C₄H₁₀ MO comprising a linear combination of C–H-bond MOs and C–C-bond MOs of the two methyl and two methylene groups. (A) Gray-scale, translucent view of the charge density of the C–C-bond and C–H-bond MOs and the C_{butane}2 sp^3 HOs. Each C–C-bond MO comprises a H₂-type-ellipsoidal MO bridging two C_{butane}2 sp^3 HOs. For each C–H and the C–C bond, the ellipsoidal surfaces of the H₂-type-ellipsoidal MO that transitions to the C_{butane}2 sp^3 HO, the C_{butane}2 sp^3 HO shell, inner most C1s shell, and the nuclei (red, not to scale), are shown. (B) Opaque view highlighting the C–C-bond MOs of the charge density of the C₄H₁₀ MO.

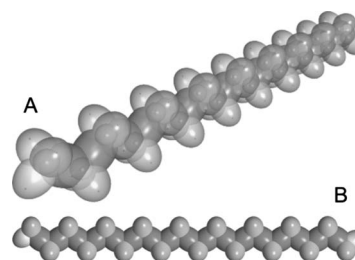


FIG. 6. C₁₈H₃₈ MO comprising a linear combination of C–H-bond MOs and C–C-bond MOs of the 2 methyl and 16 methylene groups. (A) Opaque view of the charge density of the C–C-bond and C–H-bond MOs. Each C–C-bond MO comprises a H₂-type-ellipsoidal MO bridging two C_{octadecane}2 sp^3 HOs. (B) Translucent view highlighting the C–C-bond MOs of the charge-density of the C₁₈H₃₈ MO. For each C–H and the C–C bond, the ellipsoidal surfaces of the H₂-type-ellipsoidal MO that transitions to the C_{octadecane}2 sp^3 HO, the C_{octadecane}2 sp^3 HO shell, innermost C1s shell, and the nuclei (not to scale), are shown.

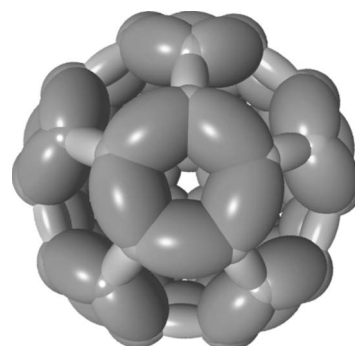


FIG. 7. Opaque pentagonal view of the charge density of the C₆₀ MO highlighting the 20 hexagonal and 12 pentagonal units joined together such that no two pentagons share an edge. The six-six ring edges are C=C bonds and the five-five ring edges are C–C-bonds such that each hexagon is comprised of alternating C=C-bond MOs and C–C-bond MOs and each pentagon is comprised of only C–C-bond MOs.

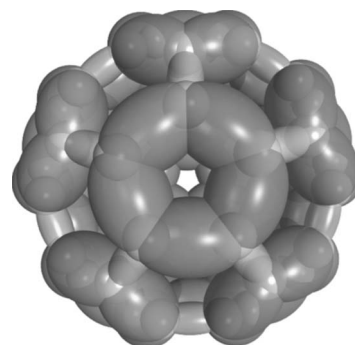


FIG. 8. C₆₀ MO comprising a hollow cage of 60 carbon atoms bound with the linear combination of 60 sets of C–C-bond MOs bridged by 30 sets of C=C-bond MOs. A C=C group is bound to two C–C groups at each vertex carbon atom of C₆₀. Grayscale, translucent pentagonal view of the charge density of the C₆₀-bond MO with each C2 sp^3 HO shown transparently. For each C–C and C=C bond, the ellipsoidal surfaces of the H₂-type-ellipsoidal MO that transitions to the C2 sp^3 HO, the C2 sp^3 HO shell, inner most C1s shell, and the nuclei (not to scale), are shown.

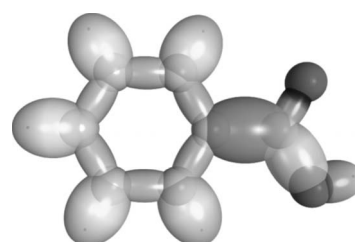


FIG. 9. Grayscale, translucent view of the charge density of benzoic acid.

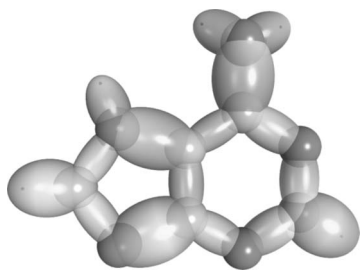


FIG. 10. Grayscale, translucent view of the charge density of adenine.

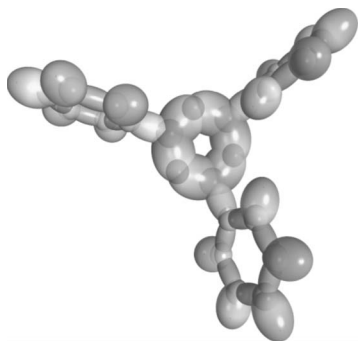


FIG. 11. Grayscale, translucent view of the charge-density of phenylborinic anhydride.

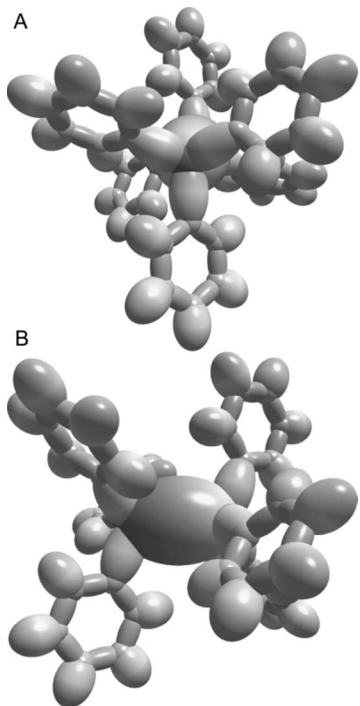
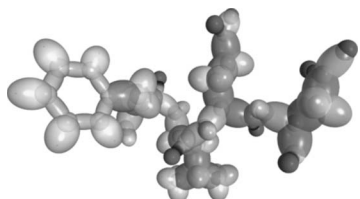
FIG. 12. Grayscale, opaque view of the charge-density of $(\text{C}_6\text{H}_5)_3\text{SnSn}(\text{C}_6\text{H}_5)_3$.

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

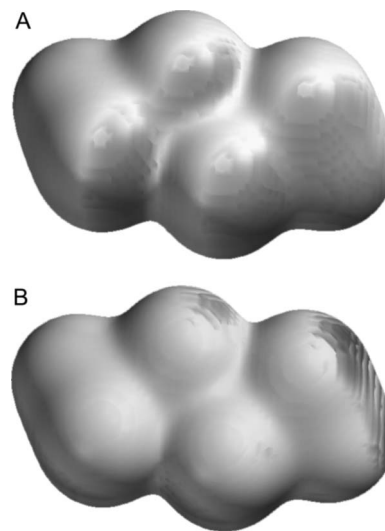
FIG. 14. Grayscale rendering of the charge-density of the representative DNA fragment $\begin{smallmatrix} \text{ACTGACTGACTG} \\ \text{TGACTGACTGAC} \end{smallmatrix}$. Using the nucleotide functional groups, DNA or RNA of any length and complexity may be rendered.FIG. 15. Comparison of the rendering 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 6-31G* 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.

TABLE LXXV. The results (in eV) of MILLSIAN 1.0, the results with 3-21G and 6-31G* basis sets generated from a precomputed 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	−68.6	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
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

TABLE LXXV. (Continued.)

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 (%)
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	−57.6	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
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

TABLE LXXV. (Continued.)

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 (%)
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	-91.2 -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	-0.05 -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
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

TABLE LXXV. (Continued.)

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 (%)
Alkenes (cyclic and 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	−25.1	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- <i>n</i> -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- <i>n</i> -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- <i>n</i> -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- <i>n</i> -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
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
<i>N,N</i> -dimethylacetamide	59.8896	32.6470	−45.5	42.0175	−29.8	N/A	N/A	N/A	N/A	60.1445	0.43
<i>N,N</i> -dimethylformamide	47.5742	31.8634	−33.0	32.4584	−31.8	N/A	N/A	N/A	N/A	47.6795	−0.22
<i>N</i> -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	−75.1	11.3549	−68.2	27.2341	−23.9	35.7689	0.01

TABLE LXXV. (Continued.)

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 (%)
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
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	−98.1	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

TABLE LXXV. (Continued.)

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 (%)
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
<i>m</i> -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
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	30.5620	−0.4	8.1749	−73.5	21.9639	−28.4	30.6161	−0.22
Dihydroxyborane	24.4378	29.5531	20.9	23.6830	−3.1	3.2697	−86.6	18.0813	−26.0	24.4546	0.07
Dimethyloxyborane	47.7236	31.9818	−33.0	46.7967	−1.9	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- <i>n</i> -butyl borate	175.6290	57.5321	−67.2	171.7704	−2.2	49.9574	−71.6	137.4923	−21.7	175.5670	−0.04
Tri- <i>n</i> -propyl borate	139.1132	54.6624	−60.7	136.3390	−2.0	35.2531	−74.7	108.4508	−22.0	139.0940	−0.01
Triethyl borate	102.5020	51.7649	−49.5	100.9489	−1.5	20.8320	−79.6	79.6925	−22.3	102.6200	0.12
Trimethyl borate	65.5395	49.1740	−25.0	65.2338	−0.5	5.5777	−91.5	50.1009	−23.6	65.5640	0.04
Boranes (alkyl)											
Tri-isopropylboron	122.7580	5.0290	−95.9	117.4871	−4.3	51.2874	−58.2	98.1244	−20.1	122.8150	0.05
Triethylboron	86.1294	2.0741	−97.6	82.1202	−4.7	36.7976	−57.3	69.2875	−19.6	86.0396	−0.10
Trimethylborane	49.7610	1.0765	−97.8	46.9473	−5.7	22.3937	−55.2	40.5263	−18.6	49.5665	−0.39
Triphenylboron	172.0968	66.0412	−61.6	169.3322	−1.6	41.9484	−75.6	131.0982	−23.8	172.1580	0.04
Boron chlorides											
Boron trichloride	13.8075	324.7150	2251.7	16.6113	20.3	150.7397	995.2	9.6108	−30.4	13.7588	−0.35
Dichloroboron	13.2529	215.6264	1527.0	14.5239	9.6	98.2622	643.2	10.0616	−24.1	13.2164	−0.28
Phenylborondichloride	66.9782	238.3500	255.9	53.1810	−20.6	86.4038	29.2	50.5704	−24.5	66.5584	−0.63
Boron fluorides											
Boron trifluoride	20.0974	71.0456	253.5	14.5295	−27.7	23.9797	19.2	15.5465	−22.6	20.2692	0.85
Difluoroboron	17.4185	46.4944	166.9	13.0678	−25.0	13.6717	−21.3	13.9433	−20.0	17.5567	0.79
Difluoromethylborane	30.3362	46.5958	53.6	25.7492	−15.1	8.3556	−73.2	24.0609	−20.7	30.0349	−0.99
Vinylidifluoroborane	36.5498	52.6156	44.0	32.3258	−11.6	8.6342	−77.1	28.4969	−22.0	36.2189	−0.91
Bromides											
Bromoform	12.8770	N/A	N/A	6.2342	−51.6	N/A	N/A	N/A	N/A	12.8770	0.00
Bromomethane	15.7321	N/A	N/A	12.9828	−17.5	N/A	N/A	71.2954	353.2	15.6755	−0.36
CH ₃ Br											
Tetrabromomethane	11.2593	N/A	N/A	2.6056	−76.9	N/A	N/A	242.2493	2051.5	11.2593	0.00
Bromides (alkyl)											
1-bromododecane	149.5735	N/A	N/A	143.2627	−4.2	N/A	N/A	178.1153	19.1	149.6160	0.03
1-bromoheptane	88.7830	N/A	N/A	84.1370	−5.2	N/A	N/A	129.4287	45.8	88.8279	0.05

TABLE LXXV. (Continued.)

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-bromohexadecane	198.1915	N/A	N/A	190.5524	−3.9	N/A	N/A	N/A	N/A	198.2470	0.03
1-bromohexane	76.6345	N/A	N/A	72.3145	−5.6	N/A	N/A	119.8000	56.3	76.6702	0.05
1-bromooctane	100.9523	N/A	N/A	95.9666	−4.9	N/A	N/A	139.3294	38.0	100.9860	0.03
1-bromopropane	40.1598	N/A	N/A	36.8634	−8.2	N/A	N/A	90.6387	125.7	40.1971	0.09
2,3-dibromo-2-methylbutane	64.772	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	36.9268	−8.3	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	−26.7	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	−15.4	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-methylbutane	65.3444	110.7170	69.4	52.4563	−19.7	24.8428	−62.0	51.4426	−21.3	65.3682	0.04
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

TABLE LXXV. (Continued.)

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 (%)
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	-22.9	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
Methyl tridecanoate	178.9997	49.2833	-72.5	134.1526	-25.1	55.7073	-68.9	140.2547	-68.9	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											
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

TABLE LXXV. (Continued.)

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 (%)
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											
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)											
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)											
Hexaethyldigermanium	167.8984	N/A	N/A	137.2331	−18.3	N/A	N/A	N/A	N/A	167.8890	−0.01
Tetra- <i>n</i> -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											
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)											
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
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

TABLE LXXV. (Continued.)

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 (%)
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	−52.2	7.7457	−79.7	28.2898	−25.4	37.8783	−0.17
			−29.9								
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
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- <i>n</i> -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

TABLE LXXV. (Continued.)

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 (%)
1,1,2,2-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
Siloxanes											
H ₃ SiOH	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
Tetramethoxysiloxane	84.0468	126.0056	49.9	62.3993	-25.8	20.5035	-76.1	62.5364	-25.6	83.4878	-0.67
Triethoxysiloxane	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 H ₂ O	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

TABLE LXXV. (Continued.)

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 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											
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- <i>n</i> -butyltin	205.6006	N/A	N/A	158.0889	−23.1	N/A	N/A	N/A	N/A	205.8010	0.10
Tetra- <i>n</i> -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
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

TABLE LXXV. (Continued.)

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 (%)
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 SnCl ₄	13.0370	N/A	N/A	17.4750	34.0	N/A	N/A	N/A	N/A	12.9576	-0.61
Tri- <i>n</i> -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- <i>t</i> -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
Triphenyl- trimethyldistannane	212.7297	N/A	N/A	153.0165	-28.1	N/A	N/A	N/A	N/A	214.5540	0.86
Urea											
Urea	31.3930	39.5924	26.1	18.0087	-42.6	N/A	N/A	N/A	N/A	31.3592	-0.11

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 biomolecules such as proteins (Fig. 13) and DNA (Fig. 14) that are enabled by MILLSIAN at a time when the industry is shifting emphasis from small molecules to biotechnology.

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