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A Study on Universal Gaussian Basis Sets for First-Row Atoms

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Analysis of various optimum and non-optimum Gaussian basis sets for first-row elements have indicated that with a minimum increase of the basis set size and without loss of accuracy of the calculated total energy, a single "universal" Gaussian basis set may replace individually optimized Gaussian basis sets for a series of atoms. Such a universal Gaussian basis set may substantially reduce the computational work required for the calculation of molecular integrals in *ab initio* MO calculations.

Key words: Universal Gaussian basis sets for first-row atoms – First-row atoms

1. Introduction

Recent results with rigorously optimized Gaussian basis sets for *ab initio* MO calculations have indicated that optimum exponent sets for first-row atoms are interrelated by a simple "Gaussian Rule" [1]. The orbital exponents α_i in basis sets of the same size (i.e. composed of the same number of *s*, *p*, etc. type functions) are approximately proportional to the square of the nuclear charge, Z^2, and by introducing small correction terms, analogous to Slater's screening constant, the deviations from the exact optima can be minimized. The existence of the "Gaussian Rule" suggests a high degree of "universality" in the optimum Gaussian function representations of different atoms. It is particularly remarkable that the linear coefficients of the best-energy "Uniform Quality" Gaussian expansions of atomic wavefunctions are almost identical [1]. These properties of optimum Gaussian basis sets lead one to consider the extreme case of "universality": the use of *identical* Gaussian basis sets for a series of atoms. The possible advantages of such a "universal Gaussian basis" are considerable: the one-electron and two-electron integrals, once calculated, can be re-used for any set of atoms whenever the internuclear

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separation is the same; by multiplying the nuclear attraction integrals with appropriate constants these integrals can be "corrected" for any nuclear charge Z.

While the "Gaussian Rule" and the near identity of the linear coefficients have indicated an inherent "universality" of optimum Gaussian basis sets [1], in an independent study Silver and Nieuwpoort have explored the applicability of "universal" Slater type basis sets for a series of atoms [2]. Using the "even-tempered" formula of Raffenetti [3] for exponents α_i,

$$\alpha_i = ab^{i-1} \quad (a, b \text{ constants})$$

a universal set of Slater type functions has been proposed [2]. To achieve an accuracy comparable to that of Slater bases individually optimized [4] for atoms B–Ne, the basis set size had to be increased from a total of 18 Slater functions to a total of 27 Slater functions. Consequently, the advantages of this "universal" Slater basis set must be weighed against the 50% increase in the basis set size, that may increase the total number of integrals dramatically. Consequently, the construction of the corresponding Fock matrix may become considerably more tedious, even if many of the integrals are identical.

2. Results and Discussion

Due to the fundamentally different properties of Gaussian type functions, the technique applied for Slater type functions does not appear suitable for the construction of "universal" Gaussian basis sets. The differences are particularly evident in the representation of the core region, near the "cusp" of the wavefunction. Rigorously optimized uniform quality Gaussian basis sets [5–7] fulfill a balance criterion for the generalized "force" components in the coordinate space of the α_i orbital exponents:

$$|g| \leq 5 \times 10^{-5}. \tag{1}$$

Here $|g|$, the measure of balance ("measure of quality") is defined as

$$|g| = \left[\frac{1}{n}\sum_{i=1}^{n}\left(\frac{\partial E}{\partial \ln \alpha_i}\right)^2\right]^{1/2}. \tag{2}$$

Clearly, for an ideally balanced basis set the $\partial E/\partial\alpha_i$ "force" components, consequently the $\alpha_i(\partial E/\partial\alpha_i) = \partial E/\partial \ln \alpha_i$ derivatives are zero and $|g| = 0$. For such "balanced" Gaussian bases the exponents of those functions that are dominant in the core region show considerable deviations from a smooth geometric progression. It is expected that a "universal" Gaussian basis must contain more functions than the basis sets optimized individually for each atom, if comparable accuracy is our goal. On the other hand, the overall economy of *ab initio* calculations requires to keep the dimension of the molecular basis set small. As a compromise, a "universal" Gaussian basis set that may replace small and medium size optimum Gaussian basis sets is likely to offer the most advantages in calculating approximate molecular wavefunctions.

In the present study we have investigated the possibilities of replacing (6^s3^p) and (8^s4^p) Uniform Quality basis sets for first-row atoms with suitable "universal" Gaussian bases. The Gaussian Rule [1] and the relative insensitivity of calculated energies to small re-scaling of exponents [8] have suggested that the optimum basis set for an atom of nuclear charge Z may be used as an approximation to the basis set of the atom of nuclear charge $Z + 1$, since the scaling factor in this case would be $\sim(Z + 1)^2/Z^2$, not very different from unity if Z is large. However, to obtain a similar approximation to the optimum basis set for an atom of nuclear charge Z' much larger or much smaller than Z, the scaling factor $(Z'/Z)^2$ must be rather different from 1.0. In this latter case the deviation from the true optimum basis set would be significant, and the inaccuracy of the approximate basis could well be unacceptable.

To explore the effects of larger scaling factors and the possibilities of utilizing the Gaussian Rule in devising a universal Gaussian basis we have carried out an analysis of (6^s3^p), (8^s4^p) and (10^s5^p) Uniform Quality Gaussian basis sets for the series of first row atoms B–F. Approximate Hartree–Fock wavefunctions have been calculated for these atoms using *all* (6^s3^p) and (8^s4^p) basis sets in *all* possible combinations, i.e. *all* basis sets for *all* five atoms. The results have been analysed in terms of total energies, the virial theorem and the balance parameter $|g|$ ("quality measure" $|g|$) of the resulting approximations to the optimum basis sets. In the following analysis we shall refer to optimum basis sets by the nuclear charge Z of the atom for which the basis was optimized. A $Z_1 \to Z_2$ basis set replacement means that the wavefunction for atom of nuclear charge Z_1 is calculated using the basis optimized for atom of nuclear charge Z_2.

The results for (6^s3^p) and (8^s4^p) type basis sets are summarized in Table 1. Results listed along the diagonals are those obtained with Uniform Quality basis sets optimized directly for the given atom, consequently, the energy values, virial ratios and balance parameters along the diagonals are those closest to the ideal values.

In general, a basis replacement causes a large increase in the calculated total energy. Particularly large increases (for the F → B replacement as large as 1.25 hartree) were obtained for the (6^s3^p) basis sets, as smaller basis sets are more sensitive to variations of the exponents. The energies calculated with (8^s4^p) basis sets show somewhat smaller variations. It is noteworthy that in both series the energies calculated for nitrogen show the smallest variation (0.07 hartree for the (8^s4^p) basis sets). This result is not surprising since the nuclear charge Z of nitrogen is the average value of the nuclear charges of the atoms considered. In general, the larger the difference between the nuclear charges Z_1 and Z_2 of the atoms involved in the basis replacement, the larger the increase of the calculated total energy.

The calculated virial ratios show a similar trend in their deviations from the ideal value of -2. It is noteworthy that replacing basis 1 by basis 2 causes an upward or downward shift in the virial ratio, depending on whether the $(Z_2 - Z_1)$ difference is negative or positive, respectively. This consistent pattern suggests some degree of "universality" of the investigated basis sets and also serves as an indirect evidence

Table 1. Total energies, virial ratios and balance parameters calculated for atoms B–F employing various Uniform Quality (6^s3^p) and (8^s4^p) Gaussian basis sets

(6^s3^p) Basis sets							(8^s4^p) Basis sets					
		Atom						Atom				
Property	Basis	B	C	N	O	F	Basis	B	C	N	O	F
Energy (a.u.)	B	−24.491974	−37.523604	−53.953954	−73.930238	−97.913509	B	−24.524864	−37.666528	−54.325459	−74.630200	−99.050625
	C	−24.439659	−37.622966	−54.243630	−74.424385	−98.589048	C	−24.508093	−37.679939	−54.371268	−74.721823	−99.210404
	N	−24.276578	−37.568081	−54.294611	−74.592010	−98.935927	N	−24.438594	−37.662815	−54.385045	−74.768423	−99.304814
	O	−24.023883	−37.401981	−54.242518	−74.642413	−99.103785	O	−24.301813	−37.600248	−54.369945	−74.781747	−99.350304
	F	−23.685981	−37.116702	−54.069354	−74.584007	−99.161030	F	−24.085353	−37.467546	−54.310305	−74.764939	−99.365407
Virial	B	−1.99999	−2.01793	−2.01896	−2.01641	−2.01573	B	−1.99997	−2.00281	−2.00439	−2.00554	−2.00757
	C	−1.97664	−1.99999	−2.00946	−2.01598	−2.02353	C	−1.99159	−1.99999	−2.00247	−2.00418	−2.00573
	N	−1.94444	−1.98078	−2.00000	−2.00863	−2.01498	N	−1.97288	−1.99349	−2.00000	−2.00225	−2.00395
	O	−1.91275	−1.95517	−1.98491	−1.99999	−2.00843	O	−1.94716	−1.98079	−1.99530	−2.00000	−2.00220
	F	−1.87783	−1.92592	−1.96320	−1.98632	−1.99999	F	−1.91514	−1.96120	−1.98580	−1.99580	−1.99999
Balance $\|g\|$	B	2.195×10^{-7}	9.041×10^{-2}	1.700×10^{-1}	2.645×10^{-1}	3.725×10^{-1}	B	3.219×10^{-5}	1.462×10^{-2}	3.726×10^{-2}	6.786×10^{-2}	9.835×10^{-2}
	C	1.132×10^{-1}	3.272×10^{-6}	6.173×10^{-2}	7.859×10^{-2}	1.365×10^{-1}	C	2.833×10^{-2}	5.146×10^{-6}	1.564×10^{-2}	3.989×10^{-2}	7.372×10^{-2}
	N	2.512×10^{-1}	1.282×10^{-1}	2.697×10^{-6}	7.695×10^{-2}	1.022×10^{-1}	N	7.724×10^{-2}	3.016×10^{-2}	8.218×10^{-6}	1.784×10^{-2}	4.300×10^{-2}
	O	3.686×10^{-1}	2.915×10^{-1}	1.424×10^{-1}	4.619×10^{-6}	9.167×10^{-2}	O	1.357×10^{-1}	8.213×10^{-2}	3.163×10^{-2}	8.643×10^{-6}	2.016×10^{-2}
	F	4.538×10^{-1}	4.484×10^{-1}	3.279×10^{-1}	1.575×10^{-1}	1.188×10^{-5}	F	1.988×10^{-1}	1.485×10^{-1}	8.599×10^{-2}	3.383×10^{-2}	3.647×10^{-5}

for the optimality of the reference basis sets, as it may be deduced from the following argument.

According to the Gaussian Rule, optimum exponents are approximately proportional to the square of the nuclear charge, Z^2. In the $e^{-\alpha r^2}$ radial part of a Gaussian type orbital an $\omega \approx (Z_1/Z_2)^2$ multiplying factor of the orbital exponent is equivalent to a multiplying factor $\omega^{1/2}$ of coordinate r. Considering the electronic Hamiltonian of a many-electron atom,

$$\hat{H} = \hat{T} + \hat{V},$$

where

$$\hat{T} = \left(-\frac{\hbar^2}{2}\sum_{i=1}^{n}\frac{1}{m_e}\nabla_i^2\right)$$

and

$$\hat{V} = -\sum_{i=1}^{n}\frac{Ze^2}{r_{N,i}} + \sum_{i<j}\frac{e^2}{r_{ij}},$$

a direct substitution of $\omega^{1/2}r$ in place of r gives the following relations for the expectation values of kinetic and potential energy operators:

$$\langle\hat{T}_\omega\rangle = \omega^{1/3}\langle T\rangle \tag{3}$$

and

$$\langle\hat{V}_\omega\rangle = \omega^{1/6}\langle\hat{V}\rangle. \tag{4}$$

Here $\langle\hat{T}\rangle$ and $\langle\hat{V}\rangle$ are expectation values obtained for the ideal, perfectly balanced basis, that is well approximated by the Uniform Quality basis set, while $\langle\hat{T}_\omega\rangle$ and $\langle\hat{V}_\omega\rangle$ are expectation values obtained using orbital exponents multiplied by ω.

The virial ratio can then be expressed as

$$\frac{\langle\hat{V}_\omega\rangle}{\langle\hat{T}_\omega\rangle} = \omega^{-1/6}\cdot\frac{\langle\hat{V}\rangle}{\langle\hat{T}\rangle} = -\frac{2}{\omega^{1/6}}. \tag{5}$$

Consequently, whenever ω is larger than 1, i.e. when $Z_1 > Z_2$, the absolute value of the virial ratio is less than 2, while for $Z_1 < Z_2$ it is greater than 2. The fact that the actual virial ratio is better than the one obtained using relation (5) is due to a "resistance" of the electron distribution to "follow" the basis functions, as indicated by major changes in the linear coefficients.

In general the balance parameter $|g|$ is a more reliable measure of the quality of approximate wavefunctions than the virial theorem, particularly, if accurate prediction for properties other than energy is our concern; the improvements in the predicted expectation values of various one-electron properties may be correlated to the improvements in balance parameter $|g|$ [9]. It is apparent from Table 1 that the replacement of (6^s3^p) optimum basis sets results in highly imbalanced basis sets with balance parameters of the order of 10^{-1}, while for (8^s4^p) basis sets the imbalance caused by a replacement is less severe, as indicated by $|g|$ values of the order of 10^{-2}. It is noteworthy that the extent of imbalance is approximately the same for *all* replacements in a given series, although there is a slight increase in the deterioration of the balance as the difference $|Z_1 - Z_2|$ increases.

The above observations may provide some suggestions for the selection of a universal Gaussian basis set. The fact that the energy values calculated for nitrogen show the smallest variations, and the intermediate value of the nuclear charge of nitrogen suggest that the nitrogen (8^s4^p) basis set itself could serve as a universal replacement for the individually optimized (6^s3^p) basis sets for B–F. Indeed, the total energies calculated with this basis set are better than the optimum energies calculated with the (6^s3^p) basis for all five atoms, with the exception of boron, where the (6^s3^p) optimum (−24.491974 a.u.) is much lower than the value (−24.438594 a.u.) obtained with the (8^s4^p) nitrogen basis. However, the (8^s4^p) carbon basis appears as an even better "universal" replacement of individually optimized (6^s3^p) bases, for several reasons. This carbon basis set gives total energies superior to the optimum (6^s3^p) values for *all five* atoms. In addition, the central role of carbon atoms in the overwhelming majority of molecules (i.e. all organic molecules) suggests that our selection of a universal Gaussian basis set should be somewhat biased in favor of the carbon atom.

One may select, however, an alternative more rigorous procedure in searching for a universal basis set. The Gaussian Rule and the results in Table 1 indicate that the true overall optimum of a universal (8^s4^p) basis set for the B–F series lies somewhere between the carbon and nitrogen basis sets. This basis can indeed be determined by optimizing a scaling parameter ω, using a least square criterion for the total energy values of all five atoms, weighing each atom equally. Such least square fit and subsequent application of the Gaussian Rule gives a basis set that corresponds to an optimum basis for a hypothetical "atom" with nuclear charge $Z = 6.75$. In view of the importance of the Carbon atom, however, an equal weighing in this procedure is not necessarily the one that ensures the optimum representation for a large variety of molecules. Considering the applications of a universal basis set for molecular calculations, there is little to gain by using the least square fit basis set instead of using the carbon (8^s4^p) basis directly.

One additional aspect may also suggest the choice of the carbon (8^s4^p) basis set as a universal Gaussian basis. Atoms B–F all have open shell ground states, with some electrons occupying *p*-type orbitals and this has been the reason for selecting them as reference atoms in the search for a universal Gaussian basis. However, a universal basis should be applicable for atoms Li, Be and H as well. Atoms Li and Be do not contain occupied *p* orbitals in their ground states, and the relevant optimum bases are (6^s) and (8^s) type pure *s* basis sets. One may expect that the *p* functions of a universal (8^s4^p) Gaussian basis set, serving as polarization functions in molecular calculations, would ensure that this basis set is superior to or at least an adequate replacement of the optimum (6^s) basis sets, even if the (8^s) subset of the universal basis is not particularly balanced for these atoms. Therefore, the carbon and nitrogen (8^s4^p) bases for Li and Be are expected to give rather similar results in a molecular calculation. Nevertheless, the (8^s) subset of the (8^s4^p) carbon basis set is likely to give a better replacement for these (6^s) bases than the (8^s) subset of the nitrogen basis or that of the basis obtained with the least square fit, since the nuclear charge of carbon deviates the least from that of Be and Li.

It is also apparent from Table 1 that $Z \rightarrow Z + 1$ and $Z \rightarrow Z - 1$ type basis replacements do not result in the same degree of imbalance or loss of accuracy for the corresponding wavefunctions. In general, energies, virial ratios and balance parameters are slightly better for a $Z \rightarrow Z - 1$ type replacement than for a replacement of the $Z \rightarrow Z + 1$ type. This may be explained by recalling relations (3) and (4), and approximating parameter ω by $(Z_2/Z_1)^2$, as implied by the Gaussian Rule. Since the ideal, optimum basis set corresponds to $\omega = 1$, the smaller is the quantity $|\omega - 1|$, the smaller is the deviation of the actual basis from the ideal one. For our two alternatives the two ω parameters, ω_{-1} and ω_{+1} may be approximated as

$$\omega_{-1} = \left(\frac{Z-1}{Z}\right)^2$$

and

$$\omega_{+1} = \left(\frac{Z+1}{Z}\right)^2.$$

Clearly, ω_{-1} is closer to unity than ω_{+1} for any nuclear charge Z larger than 1, consequently a $Z \rightarrow Z - 1$ type basis replacement is more favorable than a $Z \rightarrow Z + 1$ type replacement. This result also suggests that the carbon (8^s4^p) basis set, corresponding to a nuclear charge smaller than that of nitrogen (or that of the hypothetical atom corresponding to the least square fit basis) may offer the best compromise choice for a universal replacement of (6^s3^p) basis sets.

A similar study was carried out on a possible universal replacement of (8^s4^p) optimum basis sets, using (10^s5^p) Gaussian basis sets. Optimum carbon and nitrogen (10^s5^p) basis sets were used to calculate approximate wavefunctions for the B–F series. The calculated total energies, virial ratios and balance parameters are presented in Table 2. The numerical results show the same trends that are characteristic of the (6^s3^p) and (8^s4^p) basis sets. It is remarkable, however, that the balance of all the calculated wavefunctions is much better than for smaller bases, in general the

Table 2. Total energies, virial coefficients and balance parameters calculated for atoms B–F using Universal "C" and "N" (10^s5^p) Gaussian basis sets

	Universal "C" basis			Universal "N" basis		
Atom	Energy (a.u.)	Virial	Balance $\|g\|$	Energy (a.u.)	Virial	Balance $\|g\|$
B	−24.524285	−1.997813	6.606×10^{-3}	−24.503068	−1.990812	2.053×10^{-2}
C	−37.686653	−2.000000	3.534×10^{-5}	−37.682648	−1.998308	7.204×10^{-3}
N	−54.395350	−2.000337	1.859×10^{-3}	−54.397346	−1.999988	4.879×10^{-5}
O	−74.793937	−2.000716	3.236×10^{-3}	−74.801223	−2.000334	2.589×10^{-3}
F	−99.370561	−2.001383	7.526×10^{-3}	−99.389688	−2.000687	4.299×10^{-3}

calculated $|g|$ value is of the order of 10^{-3}. Similarly, the virial coefficients are much closer to the ideal value of -2, than those for smaller bases. Comparing the carbon and nitrogen bases as possible candidates for a universal replacement of all (8^s4^p) basis sets, the most significant difference between these two bases is in the calculated total energies. The nitrogen basis set gives better total energies for atoms C, N, O, F, than the optimum (8^s4^p) bases, however, for boron the energy is considerably higher (by more than 0.02 hartree) than the (8^s4^p) optimum value. On the other hand, the carbon basis set gives approximately the same (only 0.0006 hartree higher) total energy value as the (8^s4^p) optimum value for boron, and for all other atoms the energies are much lower than the (8^s4^p) optima. In agreement with our conclusion above, the carbon (10^s5^p) basis appears to offer the best compromise for a universal replacement of (8^s4^p) optimum Gaussian basis sets.

The orbital exponents of the suggested (8^s4^p) and (10^s5^p) universal Gaussian basis sets (designed as replacements for (6^s3^p) and (8^s4^p) optimum bases, respectively) are listed in Table 3. The calculated total energies, the corresponding energies with individually optimized bases and balance parameters are collected in Table 4. In addition, Table 4 lists the results calculated for atoms H, Li and Be, using the universal bases and the appropriate optimum basis sets. For atoms Li and Be the total energies calculated with the s-subsets of universal bases are considerably higher than the corresponding optimum values and the balance parameters are about an order of magnitude worse than those for the B–F series. These poor results for Li and Be stem from the fact that the pure s-type bases for the ground states of these atoms are of somewhat different character than the s-subsets of bases for the B–F series, as it is evidenced by their larger than average deviations from the Gaussian Rule [1]. In addition, the inferior balance of basis sets generated by a

Table 3. Orbital exponents of recommended (8^s4^p) and (10^s5^p) Universal Gaussian basis sets for first row elements

Function	(8^s4^p) basis	(10^s5^p) basis
s_1	3068.79	8865.83
s_2	460.955	1313.46
s_3	104.933	295.644
s_4	29.5486	82.8185
s_5	9.40810	26.6264
s_6	3.19785	9.34105
s_7	0.52799	3.44459
s_8	0.161943	1.00736
s_9	—	0.390650
s_{10}	—	0.133641
p_1	9.44113	18.3217
p_2	2.00167	4.05072
p_3	0.545707	1.18065
p_4	0.151710	0.377676
p_5	—	0.119460

Table 4. Comparison of Universal and Uniform Quality (U.Q.) Gaussian basis sets for atoms H and Li–F

Atom	Energy (a.u.)		Difference	Balance	Energy (a.u.)		Difference	Balance
	U.Q. (6^s3^p)[a]	Universal (8^s4^p)	ΔE (a.u.)	$\|g\|$	U.Q. (8^s4^p)[a]	Universal (10^s5^p)	ΔE (a.u.)	$\|g\|$
H	−0.4969792	−0.4969675	0.000012	7.9×10^{-3}	−0.4992784	−0.4996427	−0.000364	9.1×10^{-4}
Li	−7.427857	−7.277722	0.150135	1.2×10^{-1}	−7.431749	−7.372570	0.059179	4.1×10^{-2}
Be	−14.556379	−14.484723	0.071656	1.1×10^{-1}	−14.571236	−14.545820	0.025416	3.3×10^{-2}
B	−24.491974	−24.508093	−0.016119	2.8×10^{-2}	−24.524864	−24.524285	0.000579	6.6×10^{-3}
C	−37.622966	−37.679939	−0.056973	5.1×10^{-6}	−37.679939	−37.686653	−0.006714	3.5×10^{-5}
N	−54.294611	−54.371268	−0.076657	1.6×10^{-2}	−54.385045	−54.395350	−0.010305	1.9×10^{-3}
O	−74.642413	−74.721823	−0.079410	4.0×10^{-2}	−74.781747	−74.793937	−0.012190	3.2×10^{-3}
F	−99.161030	−99.210404	−0.049374	7.4×10^{-2}	−99.365407	−99.370561	−0.005154	7.5×10^{-3}

[a] Refs. [5] and [6].

$Z_1 \rightarrow Z_2, Z_1 < Z_2$ basis replacement also contributes to the overall loss of accuracy. Nevertheless, in actual calculations for molecules the presence of p-polarization functions in the universal basis sets may reduce or eliminate the effective energy difference between the universal and optimum basis sets. It is evident that the hydrogen atom is adequately represented by both universal basis sets. Both the energy values and balance parameters are satisfactory.

3. Conclusions

Suitably chosen "universal" (8^s4^p) and (10^s5^p) Gaussian basis sets may replace individually optimized (6^s3^p) and (8^s4^p) basis sets, respectively, for first-row elements without loss of accuracy in the calculated total energies. Both of the proposed universal Gaussian basis sets represent a minimum increase only in the total number of basis functions as compared to those bases they are to replace (the increases are $15 \rightarrow 20$ and $20 \rightarrow 25$, respectively). Consequently, the overall increase in the dimension of a molecular basis and also in the number of integrals may be kept at a minimum; thus the conditions are optimum for utilizing the equivalence of integrals brought about by the use of a universal basis set.

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