Contribution to the “Klaus Ruedenberg-Volume”

Molecular calculations with $B$ functions

E.O. Steinborn$^a$, H.H.H. Homeier$^a$, I. Ema$^b$, R. Lopez$^b$ and G. Ramírez$^b$

$^a$Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-93040 Regensburg, Germany.

$^b$Departamento de Química Física Aplicada, Facultad de Ciencias C-XIV, Universidad Autónoma de Madrid, 28049 Madrid, Spain.

ABSTRACT
A program for molecular calculations with $B$ functions is reported and its performance is analyzed. All the one- and two-center integrals, and the three-center nuclear attraction integrals are computed by direct procedures, using previously developed algorithms. The three- and four-center electron repulsion integrals are computed by means of Gaussian expansions of the $B$ functions. A new procedure for obtaining these expansions is also reported. Some results on full molecular calculations are included to show the capabilities of the program and the quality of the $B$ functions to represent the electronic functions in molecules.

1 Introduction

Although there is a general agreement in the best quality of exponential type orbitals (ETO) for describing the electronic function in atoms and molecules, the difficulties in solving some molecular integrals (in particular the three- and four-center two-electron repulsion integrals) have strongly restricted their use in molecular calculations, in benefit of the more easy to handle Gaussian type orbitals (GTO).

In a previous article, a program for molecular calculations with Slater type orbitals (STO) has been reported. In that program, some of the molecular integrals (all the one- and two-center and the three-center nuclear attraction) were computed by direct algorithms, and the remaining ones by means of Gaussian expansions of the STO. The aim of that program was to provide a bridge and a reference for further works in this field, mainly to those dealing with the direct calculation of all the integrals. The present work has been developed in the same spirit, using in this case a different type of ETO, the reduced Bessel functions ($B$ functions) that have been already proposed by Steinborn et al. for molecular calculations.

In the real case, the $B$ functions are defined as:

$$B_{n,l}^m(\alpha, r) = [2^{n+l} (n + l)!]^{-1/2} k_{n-1/2}(\alpha r) (\alpha r)^l z_l^m(\theta, \phi)$$

(1)
where

\[ \hat{k}_\gamma(z) = \sqrt{\frac{2}{\pi}} z^{\gamma} K_\gamma(z) \]  \hspace{1cm} (2)

are the corresponding reduced Bessel functions, with \( K_\gamma \) being the Macdonald function, \( z^m_l \) are real spherical harmonics:

\[ z^m_l(\theta, \phi) = \left[ \frac{(2l + 1) (l - |m|)!}{(1 + \delta_{m,0}) \pi (l + |m|)!} \right] (-1)^m P^{|m|}_l (\cos \theta) \Phi_m(\phi) \]  \hspace{1cm} (3)

\( P^{|m|}_l \) being the corresponding Legendre functions, and the functions \( \Phi \) are defined as:

\[ \Phi_m(\phi) = \begin{cases} 
  \cos m\phi & \text{for } m \geq 0 \\
  \sin |m|\phi & \text{for } m < 0
\end{cases} \]  \hspace{1cm} (4)

The simplicity of the Fourier transform of the \( B \) functions has been proposed as an advantage to be exploited in the development of algorithms for molecular integrals calculations with this kind of ETO.

In the next sections, the algorithms used in the program will be summarized and some results will be reported to show the quality of the \( B \) functions for molecular calculations and to compare with both the commonly used Gaussian functions and with the STO.

2 Algorithms

The present program for molecular integrals with \( B \) functions closely follows the scheme of that previously reported for the STO. The one- and two-center and the three-center nuclear attraction integrals are computed by direct procedures previously developed and the remaining ones are computed by means of Gaussian expansions of the \( B \) functions.

The integrals computed with direct procedures are obtained with an average cost about 0.1 milliseconds per integral actually computed measured on a Digital AlphaServer 8400, for an accuracy of at least twelve decimal places.

The remaining integrals have been computed by using Gaussian expansions, as mentioned above. The expansions have been obtained by a procedure different than the usual least-squares method. This procedure, that is summarized in the appendix, is much easier to apply than the least-squares, and yields expansions that tend to better approximate the tails of the functions.

The integrals between the Gaussian primitives are evaluated with the algorithm proposed by Saunders slightly modified, and a test for avoiding calculation of negligible Gaussian contributions to a given set of integrals is also included.

The program for the calculation of the integrals has been implemented in a modular way, so that the subroutines corresponding to each type of integrals can be easily replaced by others when required. The main structure can therefore be kept unaltered when trying new algorithms for a given type of integrals.

The package includes routines for the direct minimization of the energy in RHF and ORHF calculations but, since the integrals are stored in external files in a very easy-to-handle way, the interface with other standard programs for minimizing the energy (both in Hartree-Fock and post-Hartree-Fock calculations) is straightforward.
3 Results

We have first analyzed the quality of the Gaussian expansions for representing the \( B \) functions. In Table 1 we collect the least-squares error of the expansions for different principal quantum numbers in the functions. We want to recall here that the least-squares error has not been used as criterion for attaining the present expansions. As it can be seen in the table, the quality of the expansions improves as the \( n \) quantum number increases. This is so because the Gaussian expansions obtained with the current procedure tend to better reproduce the tail of the functions, but present some problems to reproduce the peak in the origin for the functions with \( n = 1 \). This causes a loss of accuracy in the integrals involving these latter functions. In consequence, the program uses expansions optimized by minimizing the least-squares error for \( \hat{k}_{1/2} \) (which are the same as those of the STO 1s [14]), and expansions obtained with the current procedure for the rest.

Then, we have carried out full RHF calculations on several systems to test the performance of the program and to analyze the qualities of the \( B \) functions for molecular calculations. The corresponding exponents of the single-zeta and double-zeta basis sets used in the calculations are collected in Tables 2 and 3. These basis sets are optimized for atoms and have been taken from references [15, 16]. The geometries are summarized in Table 4.

In Tables 5 and 6, the energy values and the computational cost are analyzed for expansions of different length with both types of basis sets. The computational cost of the integrals calculated by direct procedures is included in the second column of each table, and columns 3 to 8 collect both the value of the electronic energy and the time required for the integrals computed with the Gaussian expansions for the B-10G, B-15G and B-20G expansions. As it can be seen in these tables, the direct procedures enable us to obtain highly accurate integrals in a very fast way. This should spur for a further search on direct procedures for all the integrals.

Nevertheless, an accuracy sufficient for testing purposes can be attained with a moderate cost by using not very long expansions (such as the B-10G) of the \( B \) functions. In fact, the results obtained with these expansions are also sufficiently accurate to give an idea about the quality of the \( B \) functions in molecular calculations. In Table 7 a comparison between the results obtained with \( B \) and STO basis sets of same length is made. The table clearly illustrates that, despite that the energy values with STO are slightly lower in the single zeta basis sets, the double zeta of both types yield results of similar quality, thus confirming the capabilities of the \( B \) functions for high-quality molecular calculations.

4 Conclusions

A program for computing molecular integrals with \( B \) functions has been implemented and tested. The program combines techniques of direct computation for the one- and two-center integrals and the three-center nuclear attraction integrals with others based on Gaussian expansions for the remaining ones. Direct procedures yield highly accurate results at low computational cost. The Gaussian expansions lead to a lower ratio accuracy/cost, but still acceptable for calculations in medium size systems. The expansions obtained by the moments procedure reported herein are good enough for all cases except the \( \hat{k}_{1/2} \) function because of the peak in the origin in this latter. An expansion based in
the least-squares procedure is preferable in this case, and has been used in the program. Finally, basis sets of $B$ functions have a good quality for reproducing the electronic wave function in molecules, comparable with that of STO.

5 Appendix: Gaussian expansions of $B$ functions

The procedure used to obtain Gaussian expansions of the B functions is based on the fitting of the value of the functions at the origin and the moments of the unnormalized spherical part of the $B$-function, i.e., an expansion:

$$\hat{k}_{n-1/2}(r) \approx \sum_{i=1}^{N} c_i e^{-\alpha_i r^2}$$

is chosen with the requirement that a given number of the moments of the reduced Bessel functions are reproduced:

$$\int_0^\infty dr \ r^{k-1} \hat{k}_{n-1/2}(r) = \sum_i c_i \int_0^\infty dr \ r^{k-1} e^{-\alpha_i r^2} \quad k = 1, 2, ...$$

Replacing the integrals by their final values [19, 20], the following equalities are obtained:

$$2^{k+n-3/2} \Gamma \left( \frac{k}{2} + n \right) \Gamma \left( \frac{k+1}{2} \right) = \frac{1}{2} \sum_i c_i \frac{\Gamma \left( \frac{k+1}{2} \right)}{\alpha_i^{k+1}}$$

Introducing the definitions:

$$Q_0 = \hat{k}_{n-1/2}(0)$$

$$Q_k \equiv 2^{k+n-1/2} \Gamma \left( \frac{k}{2} + n \right)$$

and

$$r_i \equiv \frac{1}{\sqrt{\alpha_i}}$$

Eq. (7) can be rewritten as:

$$Q_k = \sum_{i=1}^{N} c_i r_i^k \quad k = 0, 1, 2N - 1$$

Since an expansion of length $N$ implies $2N$ unknowns, $c_i$, $r_i$, a total of $2N$ moments ($k = 0, 1, ... 2N - 1$) can be exactly reproduced. This can be accomplished by solving a system with $2N$ equations that can be written in matrix form:

$$\begin{pmatrix}
Q_0 \\
Q_1 \\
\vdots \\
Q_{N-1} \\
Q_N \\
\vdots \\
Q_{2N-1}
\end{pmatrix} =
\begin{pmatrix}
r_1^0 & r_2^0 & \cdots & r_N^0 \\
r_1^1 & r_2^1 & \cdots & r_N^1 \\
\vdots & \vdots & \ddots & \vdots \\
r_1^{N-1} & r_2^{N-1} & \cdots & r_N^{N-1} \\
r_1^N & r_2^N & \cdots & r_N^N \\
\vdots & \vdots & \ddots & \vdots \\
r_1^{2N-1} & r_2^{2N-1} & \cdots & r_N^{2N-1}
\end{pmatrix}
\begin{pmatrix}
c_1 \\
c_2 \\
\vdots \\
c_N
\end{pmatrix}$$
It should be noted that in this system, both the \( c_i \) and the \( r_i \) are unknown. To solve it, the system must be partitioned in two, one corresponding to the upper half equalities and the other to the lower half ones. By defining:

\[
Q \equiv \begin{pmatrix}
Q_0 \\
Q_1 \\
\vdots \\
Q_{N-1}
\end{pmatrix} \quad \quad \quad \quad Q' \equiv \begin{pmatrix}
Q_N \\
Q_{N+1} \\
\vdots \\
Q_{2N-1}
\end{pmatrix} \quad \quad \quad \quad c \equiv \begin{pmatrix}
c_1 \\
c_2 \\
\vdots \\
c_N
\end{pmatrix}
\tag{13}
\]

\[
T \equiv \begin{pmatrix}
1 & 1 & \ldots & 1 \\
r_1 & r_2 & \ldots & r_N \\
\vdots & \vdots & \ddots & \vdots \\
r_1^{N-1} & r_2^{N-1} & \ldots & r_N^{N-1}
\end{pmatrix} \quad \quad \quad \quad T' \equiv \begin{pmatrix}
r_1^N & r_2^N & \ldots & r_N^N \\
r_1^{N+1} & r_2^{N+1} & \ldots & r_N^{N+1} \\
\vdots & \vdots & \ddots & \vdots \\
r_1^{N-1} & r_2^{N-1} & \ldots & r_N^{N-1}
\end{pmatrix}
\tag{14}
\]

it is clear that Eq. (12) is equivalent to:

\[
Q = T \ c \quad \quad \quad \quad Q' = T' \ c
\tag{15}
\]

Solving for the first one:

\[
c = T^{-1} \ Q
\tag{16}
\]

and replacing in the second one, it follows:

\[
Q' = T' \ T^{-1} \ Q
\tag{17}
\]

To attain directly the general solution of this latter equation can be rather difficult. However, one can start by the first cases \((N = 1, 2, \ldots)\) and proceed by induction. In this way, it can be found that the set \( \{r_i\}_{i=1}^{N} \) that fulfills the equation coincides with the roots of the \( N \)-th degree polynomial:

\[
\sum_{i=0}^{N} a_i^{(n)} \ r^i = 0 \quad a_i^{(N)} = 1
\tag{18}
\]

where the coefficients, \( a_i^{(N)} \) are the solutions of the linear system:

\[
\begin{pmatrix}
Q_N \\
Q_{N+1} \\
\vdots \\
Q_{2N-1}
\end{pmatrix} = - \begin{pmatrix}
Q_0 & Q_1 & \ldots & Q_{N-1} \\
Q_1 & Q_2 & \ldots & Q_N \\
\vdots & \vdots & \ddots & \vdots \\
Q_{N-1} & Q_N & \ldots & Q_{2N-2}
\end{pmatrix} \begin{pmatrix}
a_0^{(N)} \\
a_1^{(N)} \\
\vdots \\
a_{N-1}^{(N)}
\end{pmatrix}
\tag{19}
\]

Finally, once the \( r_i \) are obtained by solving Eq. (18), the \( c_i \) can be readily attained by Eq. (13) and the values of \( \alpha_i \) follow from (14). Gaussian expansions of the sigma part of the \( B \) functions ranging from a single Gaussian to 20 Gaussians have been obtained. The standard limits for the three- and four-center integrals are \( N - L < 9 \).

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Dedication
We dedicate this article to Professor Klaus Ruedenberg with thankful appreciation of his pioneering work on molecular integrals with exponential-type basis functions in molecular calculations.

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Table 1: Least-squares errors$^a$, $\Delta^2$, in the Gaussian expansions of $\hat{k}_{n-1/2}(r)$ obtained with the method of moments.

| Number of Gaussians | $n$ index of the $\hat{k}_{n-1/2}$ function |
|---------------------|---------------------------------------------|
|                     | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   |
| 1                   | 2.7(-1) | 5.9(-2) | 2.5(-2) | 1.4(-2) | 8.9(-3) | 6.1(-3) | 4.5(-3) | 3.4(-3) |
| 2                   | 3.2(-2) | 3.6(-3) | 8.7(-4) | 3.1(-4) | 1.3(-4) | 7.0(-5) | 3.9(-5) | 2.4(-5) |
| 3                   | 7.1(-3) | 4.6(-4) | 7.2(-5) | 1.8(-5) | 5.6(-6) | 2.2(-6) | 9.5(-7) | 4.6(-7) |
| 4                   | 2.0(-3) | 8.4(-5) | 8.8(-6) | 1.5(-6) | 3.7(-7) | 1.1(-7) | 3.9(-8) | 1.5(-8) |
| 5                   | 7.0(-4) | 1.9(-5) | 1.4(-6) | 1.8(-7) | 3.4(-8) | 8.0(-9) | 2.3(-9) | 7.4(-10) |
| 6                   | 2.8(-4) | 5.0(-6) | 2.7(-7) | 2.7(-8) | 3.9(-9) | 7.3(-10) | 1.7(-10) | 4.7(-11) |
| 7                   | 1.2(-4) | 1.5(-6) | 6.0(-8) | 4.6(-9) | 5.3(-10) | 8.2(-11) | 1.6(-11) | 3.7(-12) |
| 8                   | 5.7(-5) | 4.9(-7) | 1.5(-8) | 9.0(-10) | 8.4(-11) | 1.1(-11) | 1.8(-12) | 3.5(-13) |
| 9                   | 2.8(-5) | 1.8(-7) | 4.1(-9) | 2.0(-10) | 1.5(-11) | 1.6(-12) | 2.2(-13) | 3.8(-14) |
| 10                  | 1.5(-5) | 6.8(-8) | 1.2(-9) | 4.8(-11) | 3.0(-12) | 2.7(-13) | 3.2(-14) | 4.6(-15) |
| 11                  | 8.3(-6) | 2.8(-8) | 4.0(-10) | 1.2(-11) | 6.5(-13) | 5.0(-14) | 5.0(-15) | 6.4(-16) |
| 12                  | 4.8(-6) | 1.2(-8) | 1.4(-10) | 3.5(-12) | 1.5(-13) | 9.9(-15) | 8.7(-16) | 9.6(-17) |
| 13                  | 2.9(-6) | 5.4(-9) | 4.9(-11) | 1.0(-12) | 3.8(-14) | 2.1(-15) | 1.6(-16) | 1.6(-17) |
| 14                  | 1.8(-6) | 2.6(-9) | 1.9(-11) | 3.3(-13) | 1.0(-14) | 4.9(-16) | 3.3(-17) | 2.8(-18) |
| 15                  | 1.1(-6) | 1.3(-9) | 7.4(-12) | 1.1(-13) | 2.9(-15) | 1.2(-16) | 7.0(-18) | 5.3(-19) |
| 16                  | 7.3(-7) | 6.3(-10) | 3.0(-12) | 3.7(-14) | 8.6(-16) | 3.1(-17) | 1.6(-18) | 1.1(-19) |
| 17                  | 4.9(-7) | 3.3(-10) | 1.3(-12) | 1.4(-14) | 2.7(-16) | 8.5(-18) | 3.8(-19) | 2.3(-20) |
| 18                  | 3.3(-7) | 1.8(-10) | 5.8(-13) | 5.1(-15) | 8.7(-17) | 2.4(-18) | 9.6(-20) | 5.1(-21) |
| 19                  | 2.3(-7) | 9.8(-11) | 2.6(-13) | 2.0(-15) | 2.9(-17) | 7.1(-19) | 2.5(-20) | 1.2(-21) |
| 20                  | 1.6(-7) | 5.5(-11) | 1.2(-13) | 7.9(-16) | 1.0(-17) | 2.2(-19) | 6.9(-21) | 3.0(-22) |
### Table 2: Single-Zeta BTO exponents.

| Orbital | Zn   | S                | B                | C                | N                | O                | F                | H                |
|---------|------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|
| 1s      | 28.979194 | 15.396775       | 4.649767       | 5.636105       | 6.621925       | 7.607778       | 8.593356       | 1.000000       |
| 2s      | 9.212368   | 4.468108        | 1.076139       | 1.346562       | 1.612481       | 1.885508       | 2.154463       |
| 3s      | 4.615722   | 1.723750        | 1.226030       | 1.581274       | 1.929475       | 2.238550       | 2.561510       |
| 4s      | 0.966290   | 5.987867        |                 |                 |                 |                 |                 |
| 2p      | 13.015418  |                 | 1.684294       |                 |                 |                 |                 |
| 3p      | 4.754359   |                 |                 |                 |                 |                 |                 |
| 3d      | 4.660219   |                 |                 |                 |                 |                 |                 |

### Table 3: Double-Zeta BTO exponents.

| Orbital | Zn   | S                | B                | C                | N                | O                | F                | H                |
|---------|------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|
| 1s      | 41.443334 | 16.517740       | 7.809120       | 9.121695       | 7.308276       | 8.306577       | 9.356483       | 1.200000       |
| 1s      | 29.336793 | 11.035952       | 3.907381       | 5.156559       | 4.211759       | 5.330563       | 6.202314       | 1.000000       |
| 2s      | 23.592780 | 5.492259        | 4.173803       | 5.447762       | 3.434959       | 2.910067       | 3.089333       |
| 2s      | 12.264347 | 4.467502        | 1.204488       | 1.495602       | 1.724930       | 1.873454       | 2.040237       |
| 3s      | 11.550144 | 2.255074        | 2.213227       | 2.726540       | 3.240492       | 3.686133       | 4.174972       |
| 3s      | 5.617435  | 1.566569        | 1.004047       | 1.255198       | 1.496401       | 1.655654       | 1.847191       |
| 4s      | 4.425408  | 9.438960        |                 |                 |                 |                 |                 |
| 4s      | 1.140164  | 5.089873        |                 |                 |                 |                 |                 |
| 2p      | 19.000918 | 2.008415        |                 |                 |                 |                 |                 |
| 2p      | 11.734571 | 1.206954        |                 |                 |                 |                 |                 |
| 3p      | 5.624098  |                 |                 |                 |                 |                 |                 |
| 3p      | 3.506195  |                 |                 |                 |                 |                 |                 |
| 3d      | 7.339257  |                 |                 |                 |                 |                 |                 |
| 3d      | 3.134250  |                 |                 |                 |                 |                 |                 |
Table 4: Geometries used for molecular calculations

| Molecule | Geometry         | Bond distances and angles<sup>a</sup> |
|----------|------------------|----------------------------------------|
| BH<sub>3</sub> | Planar           | \( R_{BH} = 2.25 \)                    |
| B<sub>2</sub>H<sub>6</sub> | See fig. 1       | \( R_{BH} = 2.26013 \) \( R'_{BH} = 2.53037 \) \( R_{BB} = 3.35430 \) \( \angle_{HBB} = 119^\circ \) |
| CH<sub>4</sub> | Regular tetrahedron | \( R_{CH} = 2.0665 \) |
| C<sub>2</sub>H<sub>2</sub> | Linear           | \( R_{HC} = 2.002 \) \( R_{CC} = 2.281 \) |
| C<sub>2</sub>H<sub>4</sub> | Planar           | \( R_{HC} = 2.02203 \) \( R_{CC} = 2.55116 \) \( \angle_{HCH} = 120^\circ \) |
| C<sub>2</sub>H<sub>6</sub> | Alternate        | \( R_{HC} = 2.08250 \) \( R_{CC} = 2.91588 \) \( \angle_{HCH} = 109.32^\circ \) \( \angle_{HCC} = 109.62^\circ \) |
| HCN      | Linear           | \( R_{HC} = 2.0 \) \( R_{CN} = 2.187 \) |
| SF<sub>6</sub> | Regular octahedron | \( R_{SF} = 2.88769 \) |
| Zn<sub>3</sub> | Equilateral triangle | \( R_{ZnZn} = 5.03593 \) |

<sup>a</sup> Distances in a.u. and angles in degrees.

Table 5: Electronic Energy RHF with Single-Zeta basis set of BTO.<sup>a</sup>

| Molecule | time(direct.alg.) | 10G time | 15G time | 20G time | 20G time |
|----------|-------------------|----------|----------|----------|----------|
| BH<sub>3</sub> | 0.04              | -26.2978760 | 1.6       | -26.2978758 | 6.1       | -26.2978762597 | 16.4       |
| B<sub>2</sub>H<sub>6</sub> | 0.6               | -52.591815 | 41.3      | -52.591817 | 156.9     | -52.5918199842 | 410.4      |
| H<sub>2</sub>O | 0.1               | -75.6136703 | 0.5       | -75.61366972 | 1.9       | -75.6136697787 | 5.0        |
| HCN      | 0.2               | -92.4898386 | 2.6       | -92.48983974 | 9.7       | -92.4898398408 | 25.0       |
| CH<sub>4</sub> | 0.04              | -40.0629604 | 3.5       | -40.0629605 | 13.7      | -40.0629611447 | 36.3       |
| C<sub>2</sub>H<sub>2</sub> | 0.3               | -76.5372092 | 6.3       | -76.5372103 | 24.4      | -76.5372106538 | 61.6       |
| C<sub>2</sub>H<sub>4</sub> | 0.4               | -77.7418899 | 19.8      | -77.7418903 | 74.8      | -77.7418909888 | 192.4      |
| C<sub>2</sub>H<sub>6</sub> | 0.6               | -78.970476 | 40.4      | -78.9704946 | 155.8     | -78.9704966047 | 404.1      |
| SF<sub>6</sub> | 9.9               | -988.79773 | 598.7     | -988.79379 | 2277.8    | -988.7938448335 | 5836.4     |
| Zn<sub>3</sub> | 82.4              | -5306.54329 | 275.4     | -5306.54320060 | 614.4     | -5306.5432005659 | 1679.2     |

<sup>a</sup> Energy in Hartrees.
Table 6: Electronic Energy RHF with Double-Zeta basis set of BTO.\(^a\)

| Molecule | time(directalg.) | 10G          | time | 15G          | time | 20G          | time |
|----------|------------------|--------------|------|--------------|------|--------------|------|
| BH3      | 0.5              | -26.373450   | 23.1 | -26.3734463  | 90.0 | -26.373446526 | 234.7 |
| B2H6     | 5.3              | -52.757514   | 595.0| -52.757528   | 229.0| -52.757530595 | 5967.9|
| H2O      | 0.3              | -75.998708   | 7.3  | -75.99870643 | 28.0 | -75.9987064604| 73.0 |
| HCN      | 2.5              | -92.801141   | 36.4 | -92.8011484  | 135.6| -92.8011486868| 350.0|
| CH4      | 0.9              | -40.182804   | 51.6 | -40.1828002  | 202.8| -40.1828008395| 532.5|
| C2H2     | 3.0              | -76.773130   | 89.1 | -76.7731380  | 336.4| -76.7731382182| 872.2|
| C2H4     | 4.2              | -77.99422    | 281.3| -77.9942558  | 1070.7| -77.9942574766| 2791.2|
| C2H6     | 5.1              | -79.197399   | 589.0| -79.1974595  | 2255.7| -79.1974630394| 5853.2|
| SF6      | 141.5            | -993.7002    | 8683.5| -993.70374   | 33498.9| -993.7038527430| 87495.1|
| Zn3      | 744.6            | -5332.8974   | 2007.0| -5332.89797  | 6802.8| -5332.8979948489| 16198.3|

\(^a\) Energy in Hartrees.

Table 7: RHF electronic energy with both Slater and B basis sets.\(^a\)

|         | Bessel(SZ) [16] | Slater(SZ) [17] | Bessel(DZ) [16] | Slater(DZ) [18] |
|---------|----------------|-----------------|-----------------|-----------------|
| BH3     | -26.297876     | -26.319008      | -26.373450      | -26.375009      |
| B2H6    | -52.591815     | -52.630434      | -52.757514      | -52.758232      |
| H2O     | -75.613670     | -75.687535      | -75.998708      | -76.000535      |
| HCN     | -92.489839     | -92.572795      | -92.801148      | -92.833977      |
| CH4     | -40.062960     | -40.101608      | -40.182800      | -40.183596      |
| C2H2    | -76.537209     | -76.596599      | -76.773130      | -76.803955      |
| C2H4    | -77.741890     | -77.810378      | -77.99422       | -78.004891      |
| C2H6    | -78.970476     | -79.041644      | -79.197399      | -79.199828      |
| SF6     | -988.79773     | -989.887733     | -993.7002       | -993.705704     |
| Zn3     | -5306.54329    | -5313.330879    | -5332.8974      | -5332.907860    |

\(^a\) Energy in Hartrees.
