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# Contracted Gaussian bases for the first-row atoms applied to neutral and charged diatomic molecules

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## Abstract

A set of contracted Gaussian bases generated with the Generator Coordinate Hartree–Fock method for first-row atoms (H, Li–Ne) is applied to perform molecular ab initio calculations. The primitives 18s 12p Gaussian basis sets were contracted to (5s) for H atom and (7s 5p) for Li–Ne atoms by a standard procedure and enriched with polarization functions in order to perform the calculations. The contracted Gaussian basis sets are then tested for H<sub>2</sub>, BH, B<sub>2</sub>, C<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, F<sub>2</sub>, HF, LiF, BeO, BF, CN<sup>−</sup>, CO and NO<sup>+</sup> molecular species. The molecular properties of interest are Koopmans' ionization potential, bond distances and vibrational frequencies at MP2 level and dipole moments at HF and MP2 levels. The results obtained show that the contracted Gaussian bases used in this work is a useful alternative for ab initio molecular calculations, and that the Generator Coordinate Hartree–Fock method is a legitimate alternative for selection of contracted and polarized Gaussian basis sets. © 2001 Elsevier Science B.V. All rights reserved.

**Keywords:** Generator coordinate Hartree–Fock method; Gaussian basis sets; Neutral diatomic molecules; Charged diatomic molecules

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## 1. Introduction

The Generator Coordinate Hartree–Fock (CGHF) method was introduced in 1986 [1] and has become one of the most powerful technique in the design of basis set for atomic and molecular calculations. One of its first applications was in the generation of Gaussian- and Slater-type orbitals (GTO and STO) universal basis sets [2–4], and afterwards it was applied in the calculation of electronic properties of molecular systems [5]. Also recently, the GCHF method was tested successfully in the generation of

universal Gaussian-type functions (GTF) exponents in relativistic calculations [6–9], and as a tool for choosing polarization functions to be used in GTF basis sets for first- [10] and second-row [11] atoms.

In this work we applied a set of contracted GTF basis sets, previously generated with the Generator Coordinate Hartree–Fock method for first-row atoms (H, Li–Ne) [10], to provide several molecular properties at the HF and MP2 (Second order Moller–Plesset Perturbation Theory) levels, for a group of neutral and charged diatomic molecules, in order to assess their performance in ab initio molecular calculations.

The contracted GTF basis sets used here were obtained from the extended and accurate 18s 12p

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GTF basis sets for the atoms H and Li through Ne [10]. These sets were then contracted to (5s) for H and (7s 5p) for Li–Ne, and augmented with p (H, Li, Be) and d polarization functions chosen with the aid of the integral discretization technique of the GCHF method.

## 2. Computational

In this section we will make a brief presentation of the GCHF method as well as a short description of the contraction of the primitives 18s 12p GTF basis sets and the choice of polarization functions used herein. A deeper and detailed description of these matters can be found elsewhere [1,4,10].

### 2.1. The GCHF method

The GCHF method is a result of choosing the one-electron functions as integral transforms

$$\psi_i(1) = \int \phi_i(1, \alpha) f_i(\alpha) d\alpha, \quad i = 1, \dots, n, \quad (1)$$

where the  $\phi_i$  are the generator functions (GTF in this work), the  $f_i$  the weight functions, and  $\alpha$  the generator coordinate.

The  $\psi_i$  are then employed to build a Slater determinant and the mean value of the total energy,  $\langle E \rangle$ . With the variation of  $\langle E \rangle$  with respect to the  $f_i$ , one can obtain the Griffin–Wheeler–HF (GWHF) equations

$$\int [F(\alpha, \beta) - \epsilon_i S(\alpha, \beta)] f_i(\beta) d\beta = 0, \quad i = 1, 2, \dots, n, \quad (2)$$

where  $\epsilon_i$  are the HF eigenvalues, and  $F(\alpha, \beta)$  and  $S(\alpha, \beta)$  the Fock and overlap kernels, respectively. The Fock and overlap kernels are defined explicitly in Refs. [1,4].

The GWHF Eq. (2) are solved numerically through discretization with a technique that preserves the integral character of the GCHF method, i.e. the integral discretization (ID) technique [12]. The ID technique is implemented through a relabelling of the generator coordinate space  $\alpha$ , viz.

$$\Omega = \frac{\mathcal{L}n\alpha}{A}, \quad A > 1. \quad (3)$$

The new generator coordinate space  $\Omega$  is discretized

for each s and p symmetries in a equally spaced mesh  $\{\Omega_k\}$  so that

$$\Omega_k = \Omega_{\min} + (K - 1)\Delta\Omega, \quad k = 1, \dots, N. \quad (4)$$

In Eq. (4), the set  $\{\Omega_k\}$  is characterized by an initial point  $\Omega_{\min}$ , an increment  $\Delta\Omega$ , and  $N$  (discretization point number), where the discretization point number  $N$  defines the GTF basis set size. The values of  $\Omega_{\min}$  (lowest value) and the highest value  $\Omega_{\max}$  ( $\Omega_{\max} = \Omega_{\min} + (N - 1)\Delta\Omega$ ) are chosen so as to adequately encompass the integration range for the s and p weight functions for several atoms.

The 18s 12p GTF basis sets used in this work were generated by employing Eqs. (3) and (4) and more details on how they were generated can be found in Ref. [10].

### 2.2. The contraction and polarization of the GTF basis sets

From Li through Ne the 18s 12p GTF primitive basis sets were contracted to (7s 5p) through the following contraction scheme: (10,3,1,1,1,1/8,1,1,1,1). For H atom, the 18s GTF primitive basis set was contracted to (5s) through the contraction scheme (8,3,1,1,1) and the four higher exponents of the 18s Gaussian primitive basis set were not taken into account to obtain the contracted (5s) basis set.

The choice of the p and d polarization functions to be used with the contracted GTF bases (5s) for H and (7s 5p) for Li–Ne was made by a combination of Eqs. (3) and (4) and the formula  $\alpha = -2\beta\epsilon$  [13], where  $\alpha$  is the polarization exponent to be used,  $\beta$  a constant that depends on the net charge of the molecule, and  $\epsilon$  the energy of the highest occupied orbital in which the atoms in consideration has an important weight. For a molecule with a positive net charge  $\beta = 0.87$ ; for a neutral net charge  $\beta = 0.75$ ; and for a negative net charge  $\beta = 0.69$  [13]. For the details on the application of the CGHF method as a tool for choosing polarization functions to be used in GTF basis sets see Ref. [10].

## 3. Results and discussion

The set of diatomic molecules chosen for this study is the following: H<sub>2</sub>, B<sub>2</sub>, C<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, F<sub>2</sub>, HF, BH, LiF, BeO, BF, CO, NO<sup>+</sup>, and CN<sup>−</sup>. The molecular

Table 1  
First Koopmans' ionization potential (a.u.)

Molecule <sup>a</sup>	CGTF bases (7s 5p 1d) (this work)	GTF bases 9s 5p 1d (this work) <sup>b</sup>	GTF bases 6-311G* (this work) <sup>c</sup>	GTF bases D95* (this work) <sup>d</sup>	Numerical HF Ref. [17]	Experimental Refs. [20–22]
H <sub>2</sub> <sup>e</sup>	0.595	— <sup>g</sup>	0.596	0.593	— <sup>h</sup>	0.584 [22]
C <sub>2</sub>	0.45829	0.45784	0.45638	0.45803	0.45798	0.44098 [21]
N <sub>2</sub>	0.616	0.612	0.613	0.613	— <sup>h</sup>	0.573 [22]
F <sub>2</sub>	0.66968	0.66621	0.67001	0.66692	0.66693	0.57695 [21]
HF <sup>f</sup>	0.64470	— <sup>g</sup>	0.63798	0.64170	— <sup>h</sup>	0.581 [20]
BH <sup>f</sup>	0.37458	— <sup>g</sup>	0.34620	0.34433	— <sup>h</sup>	0.35646 [21]
LiF	0.473960	— <sup>g</sup>	0.465290	— <sup>g</sup>	0.476127	— <sup>i</sup>
BeO	0.388650	— <sup>g</sup>	0.385330	— <sup>g</sup>	0.388524	0.220491 [21]
BF	0.406470	0.404680	0.403970	0.404200	— <sup>h</sup>	— <sup>i</sup>
CO	0.557	0.554	0.553	0.551	— <sup>h</sup>	0.510 [22]

<sup>a</sup> The interatomic distances are: 1.4, 2.35, 2.068, 2.68, 1.733, 2.329, 2.9553, 2.515, 2.386 and 2.132 a.u., respectively.

<sup>b</sup> Basis from Ref. [14] with one d function added.

<sup>c</sup> Basis from Ref. [15].

<sup>d</sup> Basis from Ref. [16].

<sup>e</sup> The basis for H is (5s 2p).

<sup>f</sup> The GTF basis set is not available for one or both atoms of the molecule.

<sup>g</sup> The basis for H is (5s 2p 1d).

<sup>h</sup> The numerical HF result is not available.

<sup>i</sup> The experimental result is not available.

properties calculated are first Koopmans' ionization potential, MP2 bond lengths, MP2 harmonic vibrational frequencies and HF and MP2 dipole moments.

We compare the results obtained with our contracted GTF basis sets (5s) and (7s 5p) with several standard GTF basis sets from the literature (for which we calculated the above properties), namely: the uncontracted 9s 5p GTF basis sets of Huzinaga [14] (to which we added one d polarization function), the 6-311G\* GTF basis sets of Pople et al. [15], and the D95\* GTF basis sets of Dunning [16]. We also compare our results with the corresponding ones obtained with numerical HF calculations [17,18].

The size of our contracted GTF (CGTF) bases is comparable to the size of the standard GTF bases and all calculations performed in this work were done by using the GAUSSIAN 86 program [19].

### 3.1. First Koopmans' ionization potentials

Table 1 shows the first Koopmans' ionization potential obtained with our CGTF added with one d polarization function, the Huzinaga 9s 5p GTF basis sets with also one d polarization function added (9s 5p 1d), and the 6-311G\* and D95\* GTF basis sets. The

last two columns in Table 1 display, respectively, the first Koopmans' ionization potentials obtained by using numerical approach and experimentally. For some cases, the Huzinaga and D95\* GTF bases are not available for some atoms (see Table 1).

From Table 1 we can see that the first Koopmans' ionization potentials obtained with our (7s 5p 1d) CGTF are similar to the other ones obtained with GTF bases and, in general, all of the GTF bases results overestimate the experimental ones. The performance of our (7s 5p 1d) CGTF is also similar to the other GTF bases when now we compare the results obtained with the CGTF and the GTF bases with those obtained numerically for the first Koopmans' ionization potential.

### 3.2. Bond lengths

In Table 2 we show bond lengths at the MP2 level calculated by using our (7s 5p 1d) CGTF and several GTF bases from the literature. The last column in Table 2 displays the experimental values. For some cases, the Huzinaga and D95\* GTF bases are not available for some atoms (see Table 2).

Here, despite all the GTF bases tested have a very

Table 2  
MP2 bond lengths (a.u.)

Molecule	CGTF bases (7s 5p 1d) (this work)	GTF bases 9s 5p 1d (this work) <sup>a</sup>	GTF bases 6-311G* (this work) <sup>b</sup>	GTF bases D95* (this work) <sup>c</sup>	Experimental [15,24,25]
H <sub>2</sub> <sup>d</sup>	1.386	– <sup>f</sup>	1.394	1.396	1.4 [15]
C <sub>2</sub>	2.381	2.378	2.390	2.409	2.35 [25]
N <sub>2</sub>	2.110	2.112	2.155	2.153	2.068 [25]
F <sub>2</sub>	2.673	2.671	2.668	2.684	2.68 [25]
HF <sup>e</sup>	1.729	– <sup>f</sup>	1.734	1.764	1.733 [15]
BH <sup>e</sup>	2.318	– <sup>f</sup>	2.333	2.342	2.329 [24]
LiF	2.946	– <sup>f</sup>	2.962	– <sup>f</sup>	2.9553 [25]
BF	2.389	2.387	2.397	2.439	2.386 [25]
CO	2.139	2.147	2.151	2.185	2.132 [25]

<sup>a</sup> Basis from Ref. [14] with one d function added.

<sup>b</sup> Basis from Ref. [15].

<sup>c</sup> Basis from Ref. [16].

<sup>d</sup> The basis for H is (5s 2p).

<sup>e</sup> The basis for H is (5s 2p 1d).

<sup>f</sup> The GTF basis set is not available for one or both atoms of the molecule.

close performance when compared to the experimental results, our CGTF present, in general, a better performance in evaluating bond lengths than the other GTF bases.

### 3.3. Harmonic vibrational frequencies

Table 3 shows the harmonic vibrational frequencies at the MP2 level calculated by employing our (7s 5p

1d) CGTF and other GTF bases from the literature. Experimental values for the harmonic vibrational frequencies are also shown. For some cases, the Huzinaga and D95\* GTF bases are not available for some atoms (see Table 3).

When we compare the results obtained with the GTF bases and the experimental values for harmonic vibrational frequencies, we can see that our CGTF, for some cases, present a slightly better

Table 3  
MP2 harmonic vibrational frequencies (a.u.)

Molecule <sup>a</sup>	CGTF bases (7s 5p 1d) (this work)	GTF bases 9s 5p 1d (this work) <sup>b</sup>	GTF bases 6-311G* (this work) <sup>c</sup>	GTF bases D95* (this work) <sup>d</sup>	Experimental [24,26]
H <sub>2</sub> <sup>e</sup>	4458	– <sup>f</sup>	4405	4499	4401 [24]
C <sub>2</sub>	1981	1972	1997	2045	1855 [24]
N <sub>2</sub>	2391	2380	2408	2507	2360 [24]
F <sub>2</sub>	967	917	897	988	923 [26]
HF <sup>g</sup>	4169	– <sup>f</sup>	4099	4300	4139 [24]
BH <sup>g</sup>	2401	– <sup>f</sup>	2428	2467	2366 [24]
LiF	896	– <sup>f</sup>	971	– <sup>f</sup>	914 [26]
BF	1433	1441	1422	1506	1402 [24]
CO	2187	2206	2215	2316	2170 [24]

<sup>a</sup> The interatomic distances are: 1.4, 2.35, 2.068, 2.68, 1.733, 2.329, 2.9553, 2.386 and 2.132 a.u., respectively.

<sup>b</sup> Basis from Ref. [14] with one d function added.

<sup>c</sup> Basis from Ref. [15].

<sup>d</sup> Basis from Ref. [16].

<sup>e</sup> The basis for H is (5s 2p).

<sup>f</sup> The GTF basis set is not available for one or both atoms of the molecule.

<sup>g</sup> The basis for H is (5s 2p 1d).

Table 4  
HF dipole moments (Debye)

Molecule <sup>a</sup>	CGTF bases (7s 5p 1d) (this work)	GTF bases 9s 5p 1d (this work) <sup>b</sup>	GTF bases 6-311G* (this work) <sup>c</sup>	GTF bases D95* (this work) <sup>d</sup>	Numerical HF [17,18]
HF <sup>e</sup>	2.0288	— <sup>f</sup>	2.1919	2.0880	1.9204 [18]
BH <sup>e</sup>	1.7610	— <sup>f</sup>	1.6790	1.9597	— <sup>g</sup>
LiF	6.7815	— <sup>f</sup>	6.3038	— <sup>f</sup>	6.4488 [17]
BeO	7.6691	— <sup>f</sup>	7.1673	— <sup>f</sup>	7.5134 [17]
BF	0.7827	0.8177	0.8656	0.9489	0.8707 [18]
CO	0.3532	0.3364	0.2641	0.2294	0.2647 [18]
NO <sup>+</sup>	0.7266	0.7471	0.7217	0.6543	0.6444 [18]
CN <sup>−</sup>	0.4607	0.3780	0.4469	0.4351	0.4068 [18]

<sup>a</sup> The interatomic distances are: 1.733, 2.329, 2.9553, 2.515, 2.386, 2.132, 2.0088 and 2.214 a.u., respectively.

<sup>b</sup> Basis from Ref. [14] with one d function added.

<sup>c</sup> Basis from Ref. [15].

<sup>d</sup> Basis from Ref. [16].

<sup>e</sup> The basis for H is (5s 2p 1d).

<sup>f</sup> The GTF basis set is not available for one or both atoms of the molecule.

<sup>g</sup> The numerical HF result is not available

performance than the other GTF basis sets. But, in general, there is no clear-cut distinction in the quality of the results, as we already observed for the CISD harmonic vibrational frequencies evaluated previously [10].

### 3.4. HF and MP2 dipole moments

Tables 4 and 5 display various dipole moments calculated at the HF and MP2 levels, respectively,

obtained with our (7s 5p 1d) CGTF and other GTF basis sets. For some cases, the Huzinaga and D95\* GTF bases are not available for some atoms (see Tables 4 and 5).

From Tables 4 and 5 we can see that for both HF and MP2 dipole moment calculations our CGTF as well as the other GTF bases results are not too close to the results obtained numerically. A different behavior happened for the other molecular properties studied and showed in Tables 1–3. Also either HF or

Table 5  
MP2 dipole moments (Debye)

Molecule <sup>a</sup>	CGTF bases (7s 5p 1d) (this work)	GTF bases 9s 5p 1d (this work) <sup>b</sup>	GTF bases 6-311G* (this work) <sup>c</sup>	GTF bases D95* (this work) <sup>d</sup>	Experimental [21,23]
HF <sup>e</sup>	1.9202	— <sup>f</sup>	2.1290	2.0374	1.819 [21]
BH <sup>e</sup>	1.5371	— <sup>f</sup>	1.5787	1.8771	— <sup>g</sup>
LiF	6.6770	— <sup>f</sup>	5.9212	— <sup>f</sup>	6.6 [21]
BeO	6.3427	— <sup>f</sup>	5.7091	— <sup>f</sup>	— <sup>g</sup>
BF	0.8909	0.9438	1.0785	1.0788	1.13 [23]
CO	0.2726	0.2522	0.2693	0.3436	0.112 [21]
NO <sup>+</sup>	0.1775	0.2028	0.2115	0.1711	— <sup>g</sup>
CN <sup>−</sup>	0.7475	0.6693	0.8057	0.7818	— <sup>g</sup>

<sup>a</sup> The interatomic distances are: 1.733, 2.329, 2.9553, 2.515, 2.386, 2.132, 2.0088 and 2.214 a.u., respectively.

<sup>b</sup> Basis from Ref. [14] with one d function added.

<sup>c</sup> Basis from Ref. [15].

<sup>d</sup> Basis from Ref. [16].

<sup>e</sup> The basis for H is (5s 2p 1d).

<sup>f</sup> The GTF basis set is not available for one or both atoms of the molecule.

<sup>g</sup> The experimental result is not available.

MP2 calculations yielded a larger difference between the dipole moments obtained with the CGTF and the other GTF bases, contrary to what happened with the other molecular properties calculated (see Tables 1–3) where most of them showed little differences between the results obtained with the CGTF and other GTF bases.

#### 4. Concluding remarks

Contracted GTF bases for the first-row atoms are employed to perform molecular ab initio calculations in a set of fourteen molecular species. The size of the (5s) and (7s 5p) contracted GTF bases is comparable to the size of GTF standard bases available in the literature and adequate for HF and post-HF calculations for molecules formed with the first-row atoms. The addition of p and d polarization functions to the (5s) and (7s 5p) bases, respectively, leads to good GTF bases as demonstrated with the computation of several molecular electronic properties studied here.

The results presented in this work show that our contracted GTF bases can be used as another and good alternative when one is performing ab initio molecular calculations with first-row atoms. It is interesting to mention that some of the most used GTF basis sets available in ab initio molecular packages are not available for the first-row atoms (for instance the Huzinaga and D95\* GTF basis sets employed in this work).

The outcomes obtained here show that the Generator Coordinate Hartree–Fock method, besides being a powerful method to energy minimization, can be also used as a tool for choosing polarization functions to be used in GTF basis sets.

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