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Correlating basis sets for the H atom and the alkali-metal atoms from Li to Rb

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Abstract. Contracted Gaussian-type function sets are developed for correlating p, d, and f functions for a valence electron of the hydrogen atom and alkali-metal atoms from Li to Rb. A segmented contraction scheme is used for its compactness and efficiency. Contraction coefficients and exponents are determined by minimizing the deviation from the *K* orbitals of the atoms. The present basis sets yield an accuracy comparable to the correlation-consistent basis set for the hydrogen atom and also give a similar high accuracy for the alkali-metal atoms. In the calculations of spectroscopic constants of alkali hydrides, the decontraction of the p function plays an important role, especially for LiH. The contributions of d and f functions are nontrivial for KH and RbH.

Keywords: Correlating functions – Polarization functions – Contracted Gaussian-type functions – Hydrogen atom – Alkali-metal atoms

1 Introduction

In molecular calculations, supplementary basis functions that adequately describe the correlation and polarization effects are significant for the accurate determination of molecular properties. We refer to these supplementary basis functions simply as correlating functions in this study. Many correlating sets have been prepared, but only a few sets are available for the hydrogen and alkali-metal atoms. This is because they contain only a single electron in the valence shell and the correlation effect is expected to be fairly small even in molecular systems. However, ad hoc correlating sets are often added to sp sets, since the inclusion of electron correlation effects for these atoms is still inevitable for accurate molecular calculations.

For the hydrogen atom, Dunning [1] reported several correlating sets determined by minimizing the configuration interaction (CI) energies of the ground-state H₂ molecule. These sets show reasonable qualities, but he did not prepare correlating sets for the alkali-metal atoms. Huzinaga et al. [2] constructed small p polarization sets for many atoms including hydrogen and alkali-metals. They determined the orbital exponents to maximize the overlap integral of the radial part with the outermost s function. These sets yield reasonable qualities to describe both polarization and correlation effects, although the d functions are sometimes required for obtaining reliable results. As accurate correlating sets of alkali-metal atoms, Sadlej and Urban [3] reported relatively large sets which give excellent polarizability and electronic moments; however, these sets are not compact enough for molecular applications. Recently, Tatewaki and Koga [4] constructed valence p sets for the alkali-metal atoms, by applying the Root-haan–Hartree–Fock method to the *ns* → *np* excited state. Their sets are adequate for the excited state, but the functions seem to be too diffuse to describe correlation effects. Thus, the aim of the present study is to construct compact, yet efficient, correlating function sets consisting of p, d and f functions for the hydrogen and alkali-metal atoms.

Recently, we proposed a new method for constructing correlating function sets [5, 6, 7, 8, 9]. Our method uses contracted (C) Gaussian-type functions (GTFs) in a segmented form to attain both the efficiency and compactness. Contraction coefficients and exponents of CGTFs are determined so as to minimize the difference between the functions and accurate natural orbitals (NOs) in the correlating space. The method has been successfully applied to the main group elements up to Xe, except for the hydrogen and alkali-metal atoms [5, 6, 8]. These basis sets reproduce more than 99% of atomic correlation energies predicted by accurate NO sets of the same size.

In the present paper, we report correlating basis sets for the hydrogen and alkali-metal atoms from Li to Rb. Our method cannot be applied to these atoms in its original form, since we have no electron pair in the

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valence shell. Thus, we decided to use the K orbitals for ideal correlating orbitals instead of accurate NOs. The K orbital method was proposed by Feller and Davidson [10] to improve the virtual orbitals. They showed that the K orbitals effectively approximate NOs and are adequate for describing correlation effects. In this work, the CGTFs are determined so as to minimize the difference between the functions and the K orbitals. The next section outlines our computational procedures and reports new correlating basis sets. The present basis sets are tested for several diatomic homonuclear and alkali hydride molecules in Sect. 3.

2 Computational method

The K orbitals are obtained by diagonalizing the operator

$$G = \sum_j K_j - \alpha F \quad (1)$$

over the virtual orbital space, where K_j is the exchange integral operator of the j th occupied orbital and F is the Fock operator. The parameter α is recommended to be $\sqrt{n/2}$, where n is a typical virtual orbital occupation number for an important orbital [10]. The resultant K orbitals describe approximately the correlation effects of electron pairs in the occupied orbitals considered in the K_j operator. Although no electron pair exists in the valence shell of the hydrogen and alkali-metal atoms, we apply the K -orbital method to obtain effective correlating orbitals. This can be fairly justified by considering the molecular situation in which extra electrons are supplied from surrounding atoms.

To construct the G operator, we performed self-consistent-field (SCF) calculations on the ground states of the hydrogen atom and the alkali-metal atoms from Li to Rb, by using the ATOMCI program [11]. In these calculations, we used Duijneveldt's (10s) set [12] for hydrogen and the well-tempered sets [13] of (20s), (23s16p), (26s19p), and (28s24p20d) for Li, Na, K, and Rb atoms, respectively. The G operator was constructed from the resultant SCF occupied orbitals, where only the valence s orbital was considered in K_j . For the virtual space to represent G , we prepared six p, six d, and six f primitive GTFs whose exponents are the same as those of the six outermost primitives of the s sets used in the SCF calculations. After orthogonalizing the virtual space against the occupied one, we diagonalized the operator G . Since the recommended value of α is not necessarily appropriate for our case, we determined it for each azimuthal quantum number l , by minimizing CI energies of homonuclear diatomic molecules at the equilibrium internuclear distances, for which we used 1.4 bohr in H_2 and the experimental values in the alkali-metal diatomics [14]. For all the atoms, we obtained only one K orbital which has positive eigenvalue for each l .

Following our previous idea [5], both the contraction coefficients and exponents of CGTFs were determined by minimizing the difference between the CGTFs and the K orbitals. For each l , we define a functional

$$\Delta = \int d\mathbf{r} |\lambda(\mathbf{r}) - \psi(\mathbf{r})|^2 w(\mathbf{r}) , \quad (2)$$

$$\psi(\mathbf{r}) = \sum_{i=1}^M C_i \chi_i(\mathbf{r}) , \quad (3)$$

where $\lambda(\mathbf{r})$ is the K orbital and M is the size of a CGTF basis set $\{\chi_i\}$, and $w(\mathbf{r})$ is a weight function. We employed $1/r^2$ as the weight function $w(\mathbf{r})$, since it was found to give the most appropriate results in a previous work [5]. We added the SCF occupied orbitals to $\{\chi_i\}$ to represent the contribution from the core functions in the construction of the p CGTFs for Na, K, Rb and of the d CGTFs for Rb. The conjugate direction algorithm [15] was used for the nonlinear optimization of contraction coefficients and exponents of the CGTFs, which minimize the functional Δ defined by Eq. (2). This optimization can be performed independently for each l .

In the present study, we constructed p, d, and f correlating CGTFs for all five atoms. For the size of the CGTFs, we used one or three GTFs for p, two for d, and one for f sets. We additionally constructed two GTFs for p sets in H and Li. The exponents and contraction coefficients of the present correlating CGTFs are summarized in Table 1. These results are also available on the internet, <http://setani.sci.hokudai.ac.jp/qc/basis/>.

3 Molecular tests

In order to examine the quality of the present basis set, we performed test calculations on several homonuclear diatomic molecules and alkali hydrides. These molecular calculations were performed with the MOLCAS program [16].

3.1 Homonuclear diatomic molecules

The single and double substitution CI (SDCI) calculations were carried out for H_2 , Li_2 , Na_2 , K_2 , and Rb_2 at their equilibrium internuclear distances, where only the outer two electrons were correlated. For inner and valence sets, we used the atomic SCF orbitals mentioned in the previous section, supplemented by the outermost five s primitives. Hereafter, this set is referred to as set (V). We added the present correlating functions in their single-, double-, and triple-zeta forms, such as (3), (21), and (111). To obtain reference energies, we also used (6p6d6f) primitive GTFs whose exponents are the same as those of the outermost six s primitives. For comparison, Dunning's correlation consistent sets for the hydrogen atom and Huzinaga's p polarization functions for the alkali-metal atoms were also tested in the SDCI calculations. The results of the total energies are summarized in Table 2 for H_2 and Li_2 , and in Table 3 for Na_2 , K_2 , and Rb_2 . The energy lowerings defined as

$$\Delta E^{(c)} = E^{(V+c)} - E^{(V)} , \quad (4)$$

where $E^{(V)}$ is the total CI energy with the set (V) and $E^{(V+c)}$ is that with the set (V) plus the correlating set (c),

Table 1. Exponents and contraction coefficients of correlating contracted Gaussian-type function sets for the H, Li, Na, K, and Rb atoms

Exponents/contraction coefficients									
H									
p	(1)	0.908350	/	1.000000					
	(2)	1.866762		0.503658	/	0.336977	0.759355		
	(3)	2.860673		0.888190		0.303776	/	0.128856	0.619749 0.373113
d	(1)	0.992914	/	1.000000					
	(2)	1.770613		0.593081	/	0.381654	0.721225		
f	(1)	1.451445	/	1.000000					
Li									
p	(1)	0.094257	/	1.000000					
	(2)	0.151249		0.057399	/	0.416260	0.648073		
	(3)	0.529473		0.120808		0.047590	/	0.017257	0.592202 0.461980
d	(1)	0.112687	/	1.000000					
	(2)	0.142216		0.060743	/	0.646765	0.423250		
f	(1)	0.177726	/	1.000000					
Na									
p	(1)	0.069338	/	1.000000					
	(3)	0.555775		0.094473		0.040360	/	-0.036701	0.643703 0.419455
	(1)	0.100892	/	1.000000					
d	(2)	0.128691		0.058334	/	0.616128	0.446370		
	(1)	0.150884	/	1.000000					
f	(1)	0.150884	/	1.000000					
K									
p	(1)	0.041557	/	1.000000					
	(3)	0.253382		0.056121		0.025170	/	-0.072994	0.692577 0.382332
	(1)	0.065105	/	1.000000					
d	(2)	0.273975		0.057199	/	0.080144	0.967129		
	(1)	0.089607	/	1.000000					
f	(1)	0.089607	/	1.000000					
Rb									
p	(1)	0.035922	/	1.000000					
	(3)	0.196301		0.048393		0.022164	/	-0.094962	0.715637 0.369530
	(1)	0.057454	/	1.000000					
d	(2)	0.099919		0.042235	/	0.298511	0.761080		
	(1)	0.075369	/	1.000000					
f	(1)	0.075369	/	1.000000					

and its accuracy $\Delta E^{(c)}/\Delta E^{(6p6d6f)} \times 100$ is also given in these tables.

When the present sets are compared with Dunning's correlation-consistent basis sets for the H_2 molecule, the latter gives a better result for the smallest (1) set, but the difference in the total energies is only 0.0005 hartree. Enlarging the size of contraction to the (2) and (3) sets gives considerable improvements of 0.0018–0.0020 hartrees in the energy lowering. For larger sets such as the (11)(1) and (111)(11)(1) sets, we do not see essential difference between the present and Dunning's correlation-consistent sets.

In the case of the alkali-metal diatomics, we obtained accuracies similar to the H_2 molecule in the energy lowerings relative to the reference (6p6d6f) set. Thus, we expect that the present correlating sets for the alkali-metal atoms from Li to Rb have comparable qualities with the correlation consistent set for the hydrogen atom.

3.2 Alkali hydrides

We performed SCF and CI calculations to obtain the spectroscopic constants of the ground states of the LiH, NaH, KH, and RbH molecules. In these calculations, the electron correlation effect between two valence electrons was only considered, meaning that our CI

calculation corresponds to the full valence CI. The s set of the hydrogen atom was taken from Duijneveldt's (7s) set [12] contracted to (511). For the Li atom, (7211) was prepared by decontracting the (74) set of Tatewaki and Koga [17]. We used the (743/7) set [18] for the Na atom, the (7433/74) set [19] for the K atom, and the (84333/843/8) set for the Rb atom [20], where the outermost s CGTF was split into triple zeta.

The results of the equilibrium internuclear distances, R_e , harmonic vibrational frequencies, ω_e , and dissociation energies, D_e , of LiH, NaH, KH, and RbH are shown in Table 4. The dissociation energy was calculated by subtracting the SCF energies of the separated atoms from the molecular total energy, because both separated atoms have only one s electron in the valence space. We tested several contraction schemes of the correlating basis sets.

On comparing the SCF internuclear distances of LiH obtained from the (3) and (111) p CGTFs, we find the decontraction gives a considerable improvement, about 0.05 bohr, and the resultant R_e value of 3.051 bohr is very close to the 3.046 bohr obtained with the largest (111)(11)(1) set. ω_e also shows a clear difference between the (3) and (111) sets: 1363 cm^{-1} with (3) and 1433 cm^{-1} with (111). The latter value is also close to that obtained with the larger (111)(11)(1) and (111)(11) sets. The (111) set gives a larger dissociation energy than the (3) set,

Table 2. Total energies and energy lowerings (in hartree) for H_2 and Li_2 molecules at the equilibrium internuclear distance. We used 1.4 bohr for H_2 and 5.0510 bohr[14] for Li_2

	Total energy	ΔE^a	Percentage ^b
H_2			
(1)	-1.168837	-0.013985	72.17
(2)	-1.170616	-0.015764	81.36
(3)	-1.170811	-0.015959	82.36
(11)(1)	-1.173023	-0.018171	93.78
(11)(2)	-1.173109	-0.018257	94.22
(21)(1)	-1.173266	-0.018414	95.03
(21)(2)	-1.173372	-0.018520	95.58
(111)(11)(1)	-1.174000	-0.019148	98.82
Dunning			
(1)	-1.169301	-0.014449	74.57
(11)(1)	-1.173215	-0.018363	94.77
(111)(11)(1)	-1.173978	-0.019126	98.71
Li_2			
(1)	-14.895849	-0.019206	71.51
(2)	-14.896996	-0.020353	75.78
(3)	-14.897127	-0.020484	76.27
(11)(1)	-14.901673	-0.025030	93.20
(11)(2)	-14.901748	-0.025105	93.47
(21)(1)	-14.901657	-0.025014	93.14
(21)(2)	-14.901720	-0.025077	93.37
(111)(11)(1)	-14.903336	-0.026693	99.39
Huzinaga (1)	-14.895073	-0.018430	68.62

^a See Eq. (4)

^b The accuracy of ΔE relative to that obtained by the reference (5s6p6d6f) set

implying that the decontraction of the p functions plays an important role for the spectroscopic constants at the SCF level. Comparing the results from the (111), (111)(11), and (111)(11)(1) sets, we see that the d and f functions have little effect on the spectroscopic constants. To confirm the importance of p CGTFs, we calculated the gross atomic orbital populations (GAOP) for LiH at the equilibrium internuclear distance: 2s and 2p GAOPs are 0.43 and 0.29, respectively. Namely, the 2p orbital mixes strongly in the bonding orbitals and we need considerable flexibility for describing the polarization effect. If we use the present sets in a decontracted form, they have enough qualities to account for these effects.

The results of R_e and ω_e obtained by the CI calculations bear a close parallel to those obtained by the SCF calculations. When we include the valence electron correlation, the dissociation energies are in reasonable agreement with the experimental values. The inclusion of f and d functions produces slightly larger dissociation energies.

For heavier systems, NaH, KH, and RbH, decontracting the (3) set to the (21) set introduces a little improvement in R_e and ω_e for the SCF level calculations. However, further splitting of the p CGTF brings no improvement, indicating that the importance of the p functions in the bonding orbital in these systems is much less than the case of the LiH molecule. It is consistent with the magnitude of the valence p GAOPs of Na (0.15), K (0.14), and Rb (0.13). Addition of the d CGTF to the p (21) set yields a little change in the spectroscopic

Table 3. Total energies and energy lowerings (in hartree) for Na_2 , K_2 , and Rb_2 molecules at the equilibrium internuclear distance. We used 5.98, 7.3796, and 7.56 bohr for Na_2 , K_2 , and Rb_2 [14], respectively

	Total energy	ΔE^a	Percentage ^b
Na_2			
(1)	-323.739747	-0.012847	73.70
(3)	-323.739992	-0.013092	75.11
(21)(1)	-323.743608	-0.016708	95.85
(21)(2)	-323.743670	-0.016770	96.21
(111)(11)(1)	-323.744057	-0.017157	98.43
(111)(12)(1)	-323.744061	-0.017161	98.45
Huzinaga (1)	-323.739627	-0.012727	73.01
K_2			
(1)	-1198.343355	-0.010392	67.32
(3)	-1198.343488	-0.010525	68.18
(21)(1)	-1198.347242	-0.014279	92.49
(21)(2)	-1198.347342	-0.014379	93.14
(111)(11)(1)	-1198.348168	-0.015205	98.49
Huzinaga (1)	-1198.343285	-0.010322	66.86
Rb_2			
(1)	-5876.724225	-0.009754	67.20
(3)	-5876.724354	-0.009883	68.08
(21)(1)	-5876.728080	-0.013609	93.75
(21)(2)	-5876.728285	-0.013814	95.17
(111)(11)(1)	-5876.728610	-0.014139	97.40
Huzinaga (1)	-5876.724162	-0.009691	66.76

^a See Eq. (4)

^b The accuracy of ΔE relative to that obtained by the reference (5s6p6d6f) set

constants; however, splitting the d CGTF has a significant effect for the KH and RbH molecules. The importance of the d functions for these molecules is also reflected in the d GAOPs: 0.03 for Li and Na, 0.08 for K, and 0.11 for Rb. Although the effect of the f function is small at the SCF level, a little improvement in the dissociation energies is gained by adding the f function at the CI level.

In the present test calculations, we did not consider the cases in which the np excited or anionic state plays important role. The present correlating sets are insufficient to describe these states. In the Na atom, for example, the (111) set gives 3p excitation energy and electron affinity which deviate by 0.0051 hartrees at SCF level and 0.0016 hartree at CI level from accurate results, respectively. By adding a diffuse p function, we can obtain nearly accurate results.

4 Summary

We developed p, d, and f correlating CGTF sets for the hydrogen and alkali-metal atoms from Li to Rb in a segmented contraction form. The contraction coefficients and exponents of the correlating CGTFs were determined to minimize the difference from the K orbitals.

We performed test calculations for five homonuclear diatomic molecules and four alkali hydrides in their ground states. For H_2 , the present sets show comparable accuracy with the correlation-consistent basis set of

Table 4. The equilibrium internuclear distances, R_e , harmonic vibrational frequencies, ω_e , and dissociation energies, D_e , of LiH, NaH, KH, and RbH molecules obtained by self-consistent field (SCF) and configuration interaction (CI) calculations

Molecule	Set	SCF			CI		
		R_e/bohr	ω_e/cm^{-1}	D_e/eV	R_e/bohr	ω_e/cm^{-1}	D_e/eV
LiH	(1)	3.126	1336	1.262	3.141	1267	1.985
	(3)	3.106	1363	1.311	3.110	1306	2.096
	(21)	3.098	1399	1.350	3.094	1358	2.277
	(111)	3.051	1433	1.449	3.047	1397	2.372
	(21)(2)	3.087	1386	1.368	3.085	1351	2.345
	(21)(11)	3.075	1387	1.376	3.073	1358	2.363
	(111)(11)	3.047	1424	1.458	3.046	1393	2.441
	(111)(11)(1)	3.046	1424	1.459	3.046	1393	2.451
	Exptl. ^a				3.015	1406	2.429
NaH	(3)	3.627	1152	0.866	3.636	1102	1.682
	(21)	3.615	1176	0.895	3.621	1135	1.848
	(111)	3.616	1180	0.899	3.622	1138	1.853
	(21)(2)	3.622	1170	0.906	3.630	1134	1.902
	(21)(11)	3.620	1172	0.911	3.628	1138	1.914
	(111)(11)(1)	3.622	1166	0.915	3.632	1131	1.929
	Exptl. ^a				3.567	1172	1.88
KH	(3)	4.515	911	0.639	4.528	865	1.426
	(21)	4.476	932	0.682	4.484	908	1.619
	(111)	4.475	930	0.686	4.484	903	1.626
	(21)(2)	4.481	926	0.717	4.490	907	1.689
	(21)(11)	4.433	962	0.814	4.448	939	1.781
	(111)(11)(1)	4.435	962	0.820	4.455	936	1.806
	Exptl. ^a				4.238	984	1.86 1.77 ^b
RbH	(3)	4.860	842	0.570	4.878	806	1.348
	(21)	4.807	854	0.612	4.823	835	1.541
	(111)	4.800	845	0.619	4.818	827	1.551
	(21)(2)	4.814	849	0.660	4.831	828	1.621
	(21)(11)	4.790	868	0.714	4.812	851	1.676
	(111)(11)(1)	4.790	868	0.726	4.816	850	1.708
	Exptl.				4.473 ^a	937 ^a	1.75 ^b

^a See Ref. [14]

^b See Ref. [21]

Dunning at the SCF and SDCI levels. For the alkali-metal atoms, the accuracy of the present sets was found to be analogous to that for hydrogen. Thus, we may conclude that the present correlating sets for the alkali-metal atoms have a quality similar to the correlation-consistent basis set reported only for the hydrogen atom. In the calculation of spectroscopic constants of alkali hydrides, the decontraction of the p function is strongly required, especially for LiH. Decontraction of the d CGTF also had a significant effect for the KH and RbH molecules. For reliable molecular calculations both at the SCF and at the CI levels, we recommend the (111), (111)(11), or (111)(11)(1) set for Li and the (21), (21)(11), or (111)(11)(1) set for Na, K, and Rb.

Finally, we note the usage of the present sets. In this work, we did not determine the basis set for inner orbitals; however, our test calculations indicated that the present set can be combined with available basis sets for inner orbitals, which have a sufficient quality for atomic Hartree–Fock orbitals. Furthermore, the present set can also be used with any other polarization/correlating sets having sufficient quality to give satisfactory results in both complete-active-space SCF and CI calculations.

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