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Contracted Gaussian-type basis functions revisited. IV. Atoms Rb to Xe

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Abstract. We report minimal-type contracted Gaussian-type function (GTF) sets, $\#n = (n3333/n33/n3)$ with $n = 5$ and 6, $\#7 =$ (74333/743/74), and $\#8 =$ (84333/843/75), for the fourth-row atoms from Rb to Xe. Test calculations are performed on the Ag_2 molecule. Spectroscopic constants given by split valence sets derived from #5 and #6 are a little contaminated by basis set superposition error. However, we find that the fully valence split #8 set, (8433111/84111/711111), yields essentially the same results as a large GTF set, (22s15p12d), with a general contraction, when p-, d-, and f-type polarization functions are augmented. The present #7 and #8 CGTF sets are recommended for ab initio molecular calculations including fourth-row atoms.

Key words: Contracted Gaussian-type basis sets – Fourth-row atoms – Ag_2 molecule

1 Introduction

Since a pioneering work of O-ohata et al.[1], many contracted Gaussian-type function (CGTF) basis sets have been proposed [2, 3, 4, 5, 6, 7, 8, 9] for molecular calculations, based mainly on the Roothaan–Hartree–Fock (RHF) method [10] applied to the atomic ground state. Among them, the characteristics of minimal-type CGTF sets are the use of independent primitive GTFs (PGTFs) for the major component of individual atomic orbitals (AOs). The CGTF expansion terms for inner AOs are fewer compared to those of ordinary GTF sets [11, 12, 13, 14, 15, 16, 17, 18, 19, 20], where PGTFs are directly used for all AOs with the same angular momentum. In many cases, minimal-type CGTFs have shorter expansions than GTF sets with a segmented or general contracted form of the ordinary GTF sets. As a result, the integral evaluation and storage in the former are much economical than in the latter. Moreover, the minimal-type CGTF sets provide us with a clear physical interpretation for molecular electronic structure than the GTF sets, since the inner and valence CGTFs are well separated and an appropriate decontraction of valence CGTFs explains the effect of molecular environments.

Ditchfield et al. [2] and Hehre and Pople [3] developed minimal-core-double-valence-type CGTFs for the first- and second-row atoms, but they did not extend their sets to heavier atoms. Because they imposed a common use of the PGTFs in the primary CGTFs for AOs in the same shell, a large number of GTFs would be required for shells with different radial functions, such as the $3s$, $3p$, and $3d$ AOs. To our knowledge, only two kinds of minimal-type CGTFs are available after the third-row atoms; one reported by Tatewaki and Huzinaga [4, 5, 6] and the other by Tatewaki and coworkers [7, 8, 9]. The former was developed more than 17 years ago and is insufficiently optimized, yet the basis sizes are small for reliable calculations. On the other hand, the latter authors [7, 8, 9] have reported a systematic development of minimal-type CGTF sets, which improve the problems in the Huzinaga–Tatewaki sets. Typical examples are $(n3/n)$ with $n = 3$–5 and $(n4/n)$ with $n = 6$ and 7 for the first-row atoms [7], $(n33/n3)$ with $n = 3$–6 and (743/74) for the second-row atoms [8], $(n333/n3/n)$ with $n = 3$–6, and $(n433/n4/n)$ with $n = 7$ and 8 for the first-row transition atoms from Sc to Zn [9], where the single-digit figure represents the number of PGTFs for each AO and the oblique symbol separates different symmetries.

The present study extends these works and reports the minimal-type CGTF sets for the fourth-row atoms from Rb (atomic number $Z = 37$) to Xe ($Z = 54$). The next section outlines our computational procedure. The new CGTF sets are presented and discussed in Sect. 3, and a molecular test is given in Sect. 4 for the diatomic Ag_2 molecule.

2 Computational outline

All our CGTF sets were constructed using the RHF method of Roothaan and Bagus [10]. The exponents and expansion

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coefficients of the CGTFs are treated as nonlinear parameters, and are optimized by the Powell method of conjugate directions [21, 22] so as to minimize the total energy. Choosing the Ru atom ($Z = 44$) as a benchmark, we first determined the optimal expansion lengths of respective CGTFs, namely, the structure of our minimal-type CGTF sets. The smallest (33333/333/33) set of Huzinaga et al. [6] was our starting point. We added one or two PGTFs to each symmetry at a time and examined the best pattern of CGTF sets having the same total number of PGTFs. The optimal structures were found to be (n3333/n33/n3) for $n = 4$–6, (74333/743/74), and (84333/843/75). The last pattern was better than (84333/843/84) by 1.8 millihartree in the total energy for the Ru atom. For the sake of simplicity, we hereafter use an abbreviation #n to classify the present CGTF sets, where n (= 3–8) stands for the number of PGTFs for the major component of the 1*s* AO. All the second-row transition atoms Y ($Z = 39$) to Cd ($Z = 48$) have the same CGTF structure as the Ru atom; however, the corresponding #n sets for Rb ($Z = 37$) and Sr ($Z = 38$) exclude a CGTF for the 4*d* AO with an exception that #8 = (84333/843/8), while those for In ($Z = 49$) to Xe ($Z = 54$) include an additional CGTF for the 5*p* AO with three p-type PGTFs. Note also that in the Pd atom ($Z = 46$), the 5*s* AO is vacant and there is no corresponding CGTF.

For the first- and second-row atoms, the CGTF sets with $n \geq 4$ were found [7, 8] to have a sufficient quality to describe the valence AOs; however, it was found [9] that for a third-row atom, a CGTF set with $n \geq 6$ is necessary to obtain an accuracy comparable with the (43/4) set in the first-row atoms. Therefore, the # n sets with $n = 5$–8 are examined and discussed for the fourth-row atoms.

3 CGTF sets for fourth-row atoms

The total energy errors of the present CGTF sets, relative to the numerical Hartree–Fock (NHF) values, are summarized in Table 1. We see that the error increases gradually from Rb to Xe and the ratio of the errors for these two atoms is approximately 2, irrespective of the sizes of the basis set. The largest total energy errors of the #n sets observed at the Xe atom are 1.53, 0.63, 0.13, and 0.06 hartree, respectively, for $n = 5$, 6, 7, and 8. Judging from these values, we expect that the #5 and #6 sets will not be accurate enough in the case of the fourth-row atoms.

The errors, $\Delta\varepsilon_l$, in the orbital energies of the outermost orbitals, relative to the NHF values, are plotted in Fig. 1 as a function of Z, where $l = s$, p, and d specifies the symmetry. In Fig. 1a, $\Delta\varepsilon_s$ has a large peak at Pd, because the 4*s* AO, instead of 5*s*, is outermost in this atom. The #5 and #6 sets give almost the same $\Delta\varepsilon_s$, indicating that the improvements of the innermost 1*s*, 2*p*, and 3*d* AOs bring no refinement of the outermost s orbital. However, a significant improvement is observed for the #7 and #8 sets, which have one or two more PGTFs in the innermost and second-innermost CGTFs compared to the #5 and #6 sets. The result suggests that the improvement in the second-innermost CGTFs, corresponding to the 2*s*, 3*p*, and 4*d* AOs, is effective in improving the quality of the valence *s* AOs. Further improvement in $\Delta\varepsilon_s$ from #7 to #8 is attributed to the increased PGTFs for the 4d CGTF. $\Delta\varepsilon_s$ does not exceed 1.6 millihartree in #7 and 0.5 millihartree in #8, if the Pd atom is not considered.

An analogous Z-dependence is observed for $\Delta\varepsilon_p$ depicted in Fig. 1b. It is interesting that the $\Delta\varepsilon_p$ of #5 and #6 are large for Rb to Cd, whereas those of #7 and #8 are quite small for these atoms. We recall that the #6 and #7 sets use the same number of PGTFs for the 4p CGTF. Then, the improvement in the 4d CGTF is considered to reduce $\Delta\varepsilon_p$, indicating a large electronic interaction between the 4*p* and 4*d* electrons. The small yet almost constant $\Delta\varepsilon_p$ for the 5*p* AOs of In to Xe, irrespective of the CGTF sizes, imply that the 4*d* electrons behave like point charges for the 5*p* electrons. The maximum errors are 7.1 and 1.8 millihartree at the Pd atom in the case of the #7 and #8 sets, respectively.

$\Delta\varepsilon_d$ is plotted against Z in Fig. 1c. Its Z dependence is not very different from that of $\Delta\varepsilon_s$ and $\Delta\varepsilon_p$, as already discussed. An essential difference is that $\Delta\varepsilon_d$ of #5 and #6 is large for Rb and Sr, which do not have 4*d* electrons and the corresponding CGTFs. A drastic reduction in the error is again observed for the #7 and #8 sets, in which the maximal $\Delta\varepsilon_d$ are 6.4 and 1.3 millihartree, respectively.

Table 1. Contracted Gaussian-type basis function total energy errors relative to the numerical Hartree–Fock (*NHF*) values in hartrees

Z	Atom	Electronic configuration	Term	NHF	#5	#7	#8	37
37	Rb	$[\mathrm{Kr}]5s$	^{2}S	−2,938.357454	0.759876	0.310267	0.064474	0.029038
38	Sr	$[\mathrm{Kr}]5s^2$	^{1}S	−3,131.545686	0.793186	0.322453	0.067623	0.030558
39	Y	$[\mathrm{Kr}]5s^2 4d$	^{2}D	−3,331.684170	0.825266	0.337330	0.070985	0.034085
40	Zr	$[\mathrm{Kr}]5s^2 4d^2$	^{3}F	−3,538.995065	0.864021	0.354317	0.074690	0.035685
41	Nb	$[\mathrm{Kr}]5s4d^4$	^{6}D	−3,753.597728	0.912712	0.379355	0.079592	0.037540
42	Mo	$[\mathrm{Kr}]5s4d^5$	^{7}S	−3,975.549500	0.956479	0.399649	0.083698	0.039300
43	Tc	$[\mathrm{Kr}]5s^2 4d^5$	^{6}S	−4,204.788737	0.992880	0.412380	0.086681	0.040966
44	Ru	$[\mathrm{Kr}]5s4d^7$	^{5}F	−4,441.539488	1.052432	0.446195	0.092843	0.043134
45	Rh	$[\mathrm{Kr}]5s4d^8$	^{4}F	−4,685.881704	1.102913	0.470917	0.097563	0.045128
46	Pd	$[\mathrm{Kr}]4d^{10}$	^{1}S	−4,937.921024	1.174604	0.515953	0.105836	0.047807
47	Ag	$[\mathrm{Kr}]5s4d^{10}$	^{2}S	−5,197.698473	1.208834	0.523252	0.107314	0.049271
48	Cd	$[\mathrm{Kr}]5s^2 4d^{10}$	^{1}S	−5,465.133143	1.248871	0.535546	0.110162	0.051167
49	In	$[\mathrm{Cd}]5p$	^{2}P	−5,740.169156	1.288706	0.547175	0.113301	0.053032
50	Sn	$[\mathrm{Cd}]5p^2$	^{3}P	−6,022.931695	1.332696	0.562272	0.117044	0.055119
51	Sb	$[\mathrm{Cd}]5p^3$	^{4}S	−6,313.485321	1.378764	0.578898	0.121114	0.057329
52	Te	$[\mathrm{Cd}]5p^4$	^{3}P	−6,611.784059	1.426390	0.596528	0.125401	0.059639
53	I	$[\mathrm{Cd}]5p^5$	^{2}P	−6,917.980896	1.475513	0.615131	0.129897	0.062047
54	Xe	$[\mathrm{Cd}]5p^6$	^{1}S	−7,232.138364	1.526001	0.634568	0.134573	0.064552

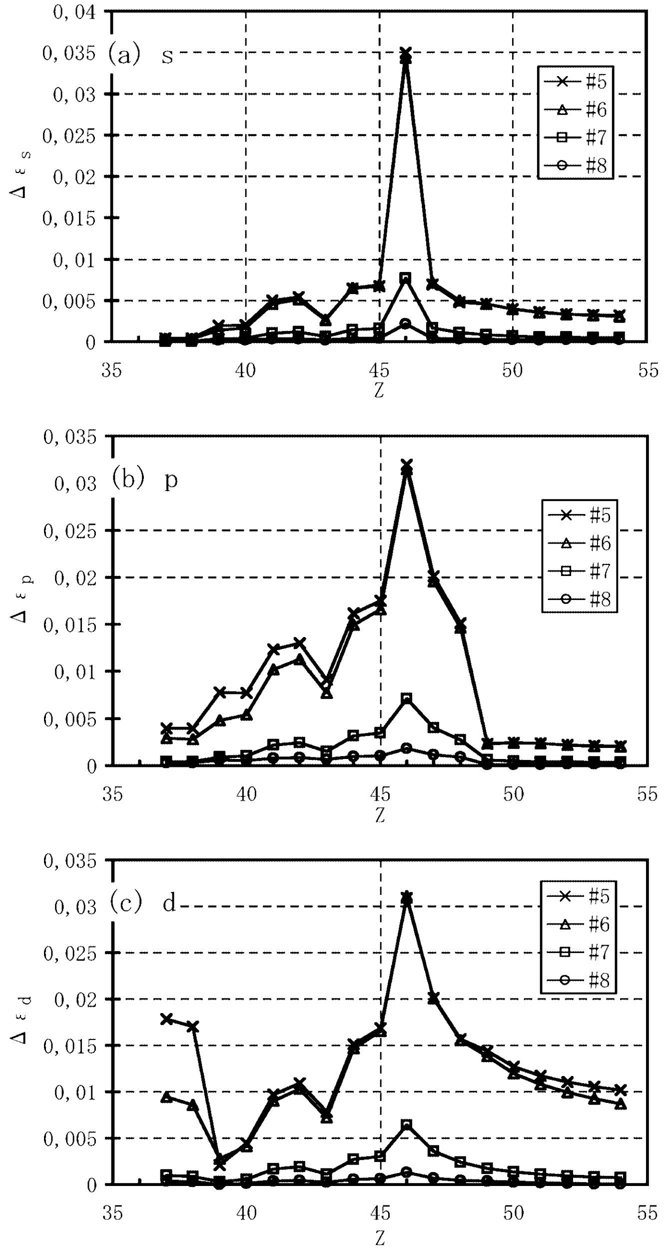

Fig. 1a–c. The orbital energy errors of the outermost orbitals relative to the numerical Hartree–Fock values in hartrees. **a** *s* orbital; **b** *p* orbital; **c** *d* orbital

When we move from #5 to #6, the accuracy of the valence AOs is much improved for the first-row transition atoms [9], but the present study shows that it is not improved for the second-row transition atoms. The corresponding improvement for these atoms is observed at the step from #6 to #7. The result means that for the fourth-row and heavier atoms, the number of PGTFs in the second-innermost CGTFs is important as well as that in the first. We cannot therefore use the same type of CGTF sets such as (*n*333.../*n*33.../*n*3...), if a molecule is composed of atoms belonging to different rows. If we balance $\Delta\varepsilon_l$ for the 2*p*, 3*p*, 3*d*, and 4*d* AOs of the first-, second-, third-, and fourth-row atoms, the (43/4), (433/43), (6333/63/6), and (74333/743/74) sets will be appropriate, for example.

4 Molecular tests

Our test calculations were performed on the Ag_2 molecule. A large number of the 4*d* electrons in this molecule provide a severe test of basis sets. For molecular calculations, the valence parts of the present four CGTF sets, #5, #6, #7, and #8, are split as (533321/53111/5111), (633321/63111/6111), (743321/74111/71111), and (843321/84111/72111), respectively. These are hereafter designated as S#5P0, S#6P0, S#7P0, and S#8P0, where the initial S stands for split-valence CGTF set and P0 means no polarization functions are added. We next prepared three sets of the polarization functions P*m*:

- P1: two 2p-type polarization functions [6] with the exponents 0.095 and 0.039 for 5*s* electrons.
- P2: P1 and one 3d-type polarization function with the exponent 0.115 for 5s electrons. The exponent value was determined to give the same average radius as the 5s AO.
- P3: P2 and three 4f-type polarization functions [6] with the exponents 3.785, 1.229, and 0.359 for 4*p* and 4*d* electrons.

The CGTF sets S#*n* combined with these polarization function sets P*m* are christened as S#*n*P*m*, where $n = 5$–8 and $m = 0$–3. We also prepared a reference primitive GTF set of (22s15p12d) [20] contracted to [18*5,1*4/11*3,1*4/7*2,1*5] = [9s,7p,7d] by a kind [14] of general contraction [13]. The total energy of the reference set is only 1.1 millihartree above the atomic Hartree–Fock limit. The reference basis set combined with the polarization functions is referred to as RefP*m*.

The calculated spectroscopic constants are listed in Table 2 and are compared them the experimental values [28, 29]. We estimated the dissociation energies, D_e, by the difference in the molecular total energies at $R = R_e$ and at $R = 50$ bohr except that in self-consistent-field (SCF) calculations, the latter energy was taken from the complete-active-space (CAS) SCF result, which gives the correct SCF dissociation limit. At the SCF level of calculation, D_e from the S#5P*m* and S#6P*m* are larger (at most 0.2 eV) than those from S#7P*m*, S#8P*m*, and RefP*m* for any *m*, owing to the basis set superposition error (BSSE) [23, 24, 25, 26]. The S#7P*m* D_e also shows a small BSSE, but the S#8P*m* D_e ($m \neq 0$) gives almost perfect agreement with the reference values. The S#*n*P*m* ($m \neq 0$) approaches RefP*m* as *n* increases. A similar discussion holds for D_e resulting from CAS SCF calculations, where the electron correlation of the outermost shell is taken into account by the two configurations $5s\sigma_g{}^2$ and $5s\sigma_u{}^2$.

The situation largely changes when single- and double-excitation configuration interaction calculations from $5s\sigma_g^2$ and $5s\sigma_u^2$ (referred to as 2SDCI) and 2SDCI calculations with Davidson correction [27] (referred to as CIQ) are performed, where the 4*p*, 4*d*, and 5*s* electrons are correlated. D_e from S#*n*P*m* generally decreases from $n = 6$ to 8 and the differences between S#8P*m* and RefP*m* are large. The smallest D_e value given by S#8P*m* ($m \geq 2$) indicates the insufficiency of basis functions for the 4*p*, 4*d*, and 5*s* regions. We are reminded that RefP*m* uses four s, four p, and five d PGTFs for these regions. When the valence parts of S#7 and S#8 are further modified as (7433111/74111/71111), (8433111/84111/

Table 2. Spectroscopic constants of Ag_2 obtained by self-consistent-field (*SCF*), complete-active-space (*CAS*) SCF, single- and double-excitation configuration interaction (*2SDCI*), and 2SDCI with Davidson correction (*CIQ*) calculations. The dimensions of the CI matrixes are 358,316, 358,316, 434,080, 434,080, 450,618, 450,618, 535,136, and 768,994 for S#*n*P3 (n = 5–8), S#7*m*P3, S#8*m*P3, S#8*m*,P3, and RefP3, respectively. The (SCF and 2SDCI) total energies of these basis sets at R = 5.0 bohr are (−10,393.069330, −10,393.960659), (−10,394.416991, −10,395.308385), (−10,395.197277, −10,396.097315), (−10,395.311070, −10,396.208150), (−10,395.199608, −10,396.115203), (−10,395.312580, −10,396.225380), (−10,395.312703, −10,396.233678), and (−10,395.405911, −10396.337603) hartree

	D_e (eV)				R_e (bohr)				ω_e (cm^{-1})			
Basis	SCF	CAS	2SDCI	CIQ	SCF	CAS	2SDCI	CIQ	SCF	CAS	2SDCI	CIQ
S#5P0	0.224	0.586	0.812	0.851	5.256	5.397	5.220	5.201	141	113	142	145
S#6P0	0.224	0.586	0.810	0.849	5.256	5.397	5.221	5.202	141	113	141	144
S#7P0	0.184	0.553	0.816	0.861	5.297	5.461	5.257	5.235	138	103	140	144
S#8P0	0.177	0.547	0.833	0.885	5.296	5.467	5.251	5.227	137	101	139	142
RefP0	0.201	0.558	0.900	0.966	5.282	5.446	5.204	5.174	139	105	145	149
S#5P1	0.491	0.771	1.233	1.371	5.220	5.318	5.114	5.087	146	126	157	161
S#6P1	0.497	0.777	1.239	1.377	5.218	5.315	5.112	5.084	146	127	157	161
S#7P1	0.350	0.637	1.112	1.250	5.296	5.418	5.184	5.157	141	114	155	159
S#8P1	0.324	0.611	1.115	1.260	5.307	5.438	5.192	5.164	138	110	153	157
RefP1	0.325	0.610	1.099	1.243	5.282	5.446	5.204	5.174	139	105	145	149
S#5P2	0.369	0.653	1.170	1.316	5.259	5.375	5.155	5.130	144	119	157	161
S#6P2	0.362	0.646	1.162	1.308	5.260	5.378	5.156	5.131	143	118	156	160
S#7P2	0.344	0.630	1.071	1.220	5.300	5.424	5.206	5.166	141	113	151	157
S#8P2	0.325	0.612	1.058	1.208	5.307	5.437	5.214	5.175	138	110	149	155
RefP2	0.326	0.611	1.118	1.266	5.304	5.433	5.171	5.140	138	110	151	155
S#5P3	0.420	0.685	1.134	1.296	5.277	5.380	5.116	5.062	142	119	158	166
S#6P3	0.412	0.677	1.124	1.286	5.279	5.384	5.118	5.064	141	118	157	165
S#7P3	0.386	0.654	1.104	1.269	5.316	5.430	5.143	5.087	137	112	155	164
S#8P3	0.370	0.638	1.088	1.252	5.316	5.432	5.143	5.088	136	110	153	162
RefP3	0.369	0.636	1.185	1.365	5.315	5.430	5.097	5.046	136	111	158	164
S#7*m*P3	0.385	0.654	1.212	1.393	5.317	5.431	5.103	5.052	137	112	159	165
S#8*m*P3	0.369	0.637	1.195	1.376	5.316	5.432	5.100	5.049	136	110	158	164
S#8*m*,P3	0.369	0.637	1.193	1.374	5.316	5.432	5.100	5.049	136	110	158	164
RefP3	0.369	0.636	1.185	1.365	5.315	5.430	5.097	5.046	136	111	158	164
Experimental[a]	1.67				4.78				192			

[a] See Refs. [28, 29]. Half the zero-point vibration energy is added to D_0^0

72111), and (8433111/84111/711111) (referred to as S#7*m*, S#8*m*, and S#8*m′*) and are augmented by P3, the resultant S#7*m*P3, S#8*m*P3, and S#8*m′*P3 sets give favorable results. Especially the larger two sets give complete agreement with RefP3 at all levels of calculation, which also reveals the improvements are brought mainly by the decontraction of the valence *s* part.

In most cases, the equilibrium internuclear distances, R_e, from the S#5P*m* and S#6P*m* sets are predicted to be shorter than RefP*m* reflecting BSSE, though its amount is smaller than 0.1 bohr. On the other hand, the S#7P*m* and S#8P*m* with $m \geq 2$ give larger R_e in 2SDCI and CIQ than the reference set, indicating again the insufficiency of the valence GTFs in the 4*p*, 4*d*, and 5*s* regions. The error is about 0.05 bohr. Similar trends are observed for the vibrational constant, ω_e. Finally, we note that the spectroscopic constants given by S#8*m*P3, S#8*m′*P3 and RefP3 are essentially the same as those reported by Tsuchiya et al. [30]: $D_e = 0.37$ eV, $R_e = 5.33$ bohr, and $\omega_e = 127$ cm^{-1} from SCF calculations and $D_e = 1.41$ eV, $R_e = 4.98$ bohr, and $\omega_e = 167$ cm^{-1} by singles and doubles coupled-cluster methods with perturbative triples.

5 Summary

We have developed minimal-type CGTF sets, #*n* = (*n*3333/*n*33/*n*3) with $n = 5$ and 6, #7 = (74333/743/74), and #8 = (84333/843/75), for the second-row transition atoms from Y to Cd. Analogous CGTF sets for the remaining fourth-row atoms Rb, Sr, and In to Xe have also been constructed. Error analysis in the total and orbital energies of the atoms has shown that the #*n* sets with $n \geq 7$ are recommended for reliable calculations for the fourth row. Molecular test calculations were performed on Ag_2. Examination of the calculated spectroscopic constants D_e, R_e, and ω_e has again shown that the valence decontracted #*n* sets with $n \geq 7$ are best suited for so-called ab initio molecular calculations. The basis sets discussed in the present work are given in http://www.nsc.nagoya-cu.ac.jp/˜htatewak.

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