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Density matrix averaged atomic natural orbital (ANO) basis sets for correlated molecular wave functions

III. First row transition metal atoms

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Abstract. Generally contracted basis sets for the first row transition metal atoms Sc–Zn have been constructed using the atomic natural orbital (ANO) approach, with modifications for allowing symmetry breaking and state averaging. The ANOs are constructed by averaging over the three electronic configurations d^n, $d^{n-1}s$, and $d^{n-2}s^2$ for the neutral atom as well as the ground state for the cation and the ground state atom in an external electric field. The primitive sets are $21s15p10d6f4g$. Contraction to $6s5p4d3f2g$ yields results that are virtually identical to those obtained with the corresponding uncontracted basis sets for the atomic properties, which they have been designed to reproduce. Slightly larger deviations are obtained with the $5s4p3d2f1g$ for the polarizability, while energetic properties still have only small errors. The design objective has been to describe the ionization potential, the polarizability and the valence spectrum as accurately as possible. The result is a set of well-balanced basis sets for molecular calculations, which can be used together with basis sets of the same quality for the first and second row atoms.

Key words: Basis sets – Atomic natural orbitals – General contraction

1 Introduction

The general contraction scheme based on atomic natural orbitals (ANOs) [1] has proved to be an excellent way of constructing compact basis sets for correlated molecular wave functions [2–4]. The possibility of handling large primitive basis sets, the minimization of contraction errors, the computational efficiency and the explicit treatment of electron correlation in the basis set construction process are some of its well-known advantages.

Nevertheless, the original approach has two important limitations: First of all, the natural orbitals are obtained from a calculation on the atomic ground state. A bias towards this state therefore occurs. This unbalanced treatment may have negative consequences in molecular calculations since other electronic states are also important in chemical bond formation. Secondly, the contraction, which is based on the correlation energy, does not allow full flexibility in the outermost regions of the wave function, which is required for an accurate description of properties, like the polarizability.

A procedure, which treats different electronic states and the atomic polarization in a balanced way has recently been proposed [5]. The contraction coefficients in the basis sets are obtained by computing the natural orbitals from an averaged density matrix. Singles and doubles configuration interaction calculations (SDCI) are performed for the atom in the electronic ground state, the cation, anion, and the neutral atom in the electronic ground state placed in a weak homogeneous electric field. The final density matrix used to construct the ANOs is obtained as the spherical average of the density matrices of the individual wave functions.

Density matrix averaged ANO basis sets for the first and second row atoms H–Ar have recently been published [5, 6]. They have been shown to yield simultaneously accurate values for the ionization potential, electron affinity and polarizability of the atoms. The truncation errors for these properties were found to be small. A number of calculations on small- and medium-sized molecules have been performed, which show that these basis sets give results of high quality (see e.g. [7]).

We present here corresponding basis sets for the first row transition metal atoms Sc–Zn. For these elements, the use of an averaging technique to construct the ANO basis sets is not only an interesting modification but an essential procedure. The reason is the occurrence of several low-lying atomic states arising from different atomic configurations with very different basis set requirements. A balanced treatment of these states is of fundamental importance for the description of molecular systems, since the chemical bond may drastically change the electronic structure of the involved atom and/or may yield significant mixtures of the atomic states. This aim can be easily achieved by including the states in the averaging procedure described above. Such basis sets have recently been discussed for Ti and Ni [4]. After completing this work we became aware of a very similar ANO basis set for first row transition metal atoms, which had been compiled by Bauschlicher. It is published back-to-back with this work [3]. Tests performed by Bauschlicher show that the performance of the two basis sets is very similar.

The basis sets compiled here have been devised in a similar fashion as was done for the first and second row atoms [5, 6]. The size of the primitive set has been chosen to yield a similar accuracy as for the lighter elements. Thus, a set of balanced basis sets is obtained. This line of development will continue to fill in the gaps of K–Ca and heavier elements, primarily Ga–Kr. The same type of basis sets for the atoms H–Kr, but based on a smaller set of primitive functions, have recently been published [8]. All these basis sets are part of the basis set library of the quantum chemistry software MOLCAS-3 [9].

2 The primitive basis set

The basis sets reported in this work are aimed to be of comparable quality as the basis sets in [5, 6]. As starting primitives we have chosen the basis sets of Partridge [10], with the size $20s12p9d$, since they have low truncation errors at the SCF level, ranging from 0.302 mH for Sc to 0.882 mH for Zn. These primitive sets were augmented with 5 f-type and 3 g-type polarization functions optimized with respect to the energy of a correlated wave function where the $3d$ and $4s$ electrons were correlated. These sets yield good energies for the atoms, but lack in the description of the outer regions, affecting in particular the computed polarizabilities. Additional functions were therefore added in the following way: One extra diffuse function was added to each shell in an even-tempered fashion, except for the p-shell where three functions were added. This was done in order to obtain an accurate description of the $4p$ shell, which is nearly degenerate with the $4s$ shell. It has usually considerable population in molecular systems and contains the most important correlation functions for the $4s$ electron pair. Hence, the final primitive sets are of the size $21s15p10d6f4g$. It should be noted that the use of such primitive sets for the whole row leads to a slight unbalance in the treatment of the atoms, Sc being slightly better described than Zn, but this should be of little consequence in molecular calculations.

3 Contraction procedure

The contraction of these basis sets follows closely the procedure of the previous work for the first and second row atoms [5, 6] with slight differences because of the particular features of transition metal systems. One of them is the number of electrons that have to be correlated, which is often larger than in the lighter atoms. It is therefore more important here to use a size-consistent correlation procedure instead of the SDCI procedure, which was used in the previous work. For the calculations reported in this paper the modified coupled pair functional (MCPF) method has been used [11]. It is known to yield satisfactory results for those transition metal systems in which a single configurational wave function is a good zeroth-order approximation. It is, however, not a method, which gives highly accurate results. This should be born in mind when comparing the computed properties with experiment.

Another difference between the transition metals and the first- and second-row atoms is the character of the states which are relevant, when the atom is chemically bound. First- and second-row atoms can have different charges in different molecular surroundings, but it is rare to find transition metal atoms with a negative charge. Instead, configurations with a different number of d electrons become important for chemical bonding involving transition metals. The averaging procedure has consequently been performed over a different set of atomic states.

Zerovalent transition metal chemistry is an important field, which is often computationally demanding. Emphasis has therefore been put on the description of the three most important electronic configurations in the valence spectra, namely $d^{n-2}s^2$, $d^{n-1}s$, and d^n. The energetically lowest terms for each of these configurations have been included in the averaging procedure.

Transition metal atoms form compounds with different oxidation states. The aim of this work has been to try to construct basis sets that can properly describe the electronic structure in a balanced way in all such compounds. Fortunately, the actual positive charge on the transition metal atoms rarely exceeds $+1.0$–$+1.5$ in systems that are not excessively charged. In addition, when electrons are removed from an atom, the demands on the basis set normally decreases. Thus, we have chosen to include only monovalent cations into the contraction procedure.

Some properties of an atom depends on the quality of the basis set far from the nucleus. The polarizability has been used here as a measure of these properties. In order to obtain accurate polarizabilities for the atoms, calculations were performed with the atom placed in a weak electric field. The resulting density matrix was included in the averaging. The field strength was chosen in such a way that the first virtual orbital of each shell obtained in the averaging primarily describes correlation and state differences, while the second contains mainly the polarizability effects.

In summary, the following states are included: The lowest term for $d^{n-2}s^2$, $d^{n-1}s^1$ and $d^n s^0$; the cationic ground state, $d^{n-2}s^1$ or $d^{n-1}s^0$; and the atomic ground state in a weak electric field. See Table 1 for the weights used and Table 2 for the strengths of the field employed. Figures 1–3 show the ^{10}log of the eigenvalues of the averaged density matrices for the atoms Sc, Cr, and Zn. The corresponding figures for the other atoms show a similar behavior and need therefore not be presented. These eigenvalues are averaged occupation numbers and are good measures of the importance of an individual functions in the basis set. With a cutoff at 10^{-6} almost all of the correlation energy in the primitive set is retained in the contracted set, with a systematic reduction for tighter thresholds. This is illustrated for Zn in Table 3.

A general rule is to include all functions with an average occupation number above a certain threshold, say 10^{-4}, which would lead to a basis set of size $6s5p4d3f2g$ for copper, where the $6g$ function has an occupation slightly less than 10^{-4}. The resulting contracted basis sets exhibit an approximate shell structure where the average occupation numbers for a given shell, e.g. $5s$–$5g$, are approximately the same. This is not completely correct, especially for the lighter elements (cf. Fig. 1), but can serve as a guideline of selecting the size of the basis set.

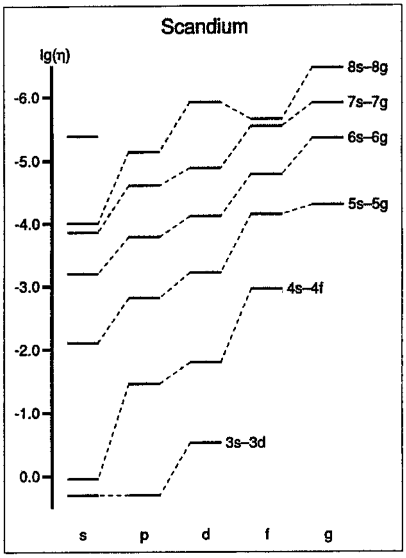
Table 1. Weight of states included in averaging

State	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
M ($d^{n-2}s^2$)	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.25	0.33
M ($d^{n-1}s$)	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.25	
M (d^n)	0.20	0.20	0.20	0.20	0.20	0.20	0.20	0.20		
M$^+$ ($d^{n-2}s$)	0.20	0.20			0.20	0.20				0.33
M$^+$ (d^{n-1})			0.20	0.20			0.20	0.20	0.25	
M ($d^{n-2}s^2$)[a]	0.20	0.20	0.20		0.20	0.20	0.20	0.20		0.33
M ($d^{n-1}s$)[a]				0.20					0.25	

[a] With external electric field applied

Table 2. Strength of external electric field applied (a.u.)

Atom	Field
Sc	0.0100
Ti	0.0100
V	0.0100
Cr	0.0025
Mn	0.0100
Fe	0.0150
Co	0.0150
Ni	0.0100
Cu	0.0050
Zn	0.0200



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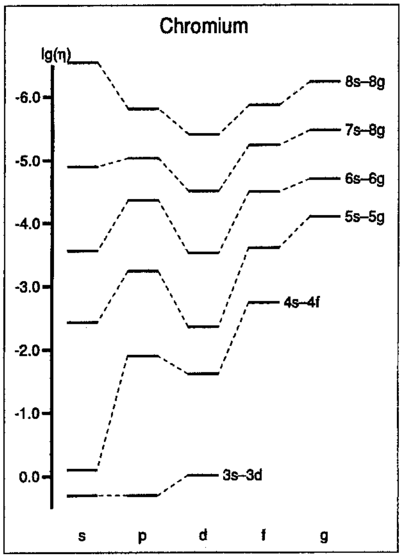

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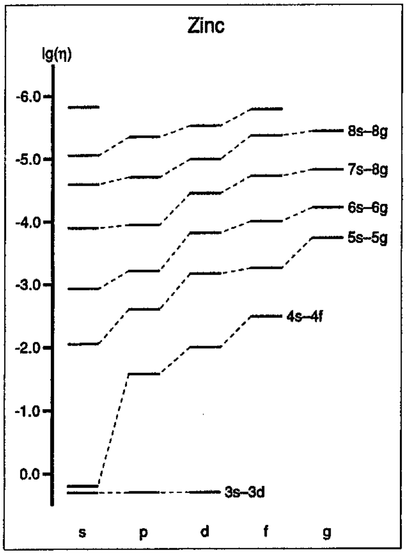

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Fig. 1. Logarithm of the average ANO occupation numbers of Sc (1), Cr (2), and Zn (3)

4 Test calculations

In order to assess the quality of the basis sets, a number of test calculations have been performed, both for the atoms under consideration and for the corresponding hydrides. The present basis sets were also used in a recent study of copper and nickel hydrides and dimers and were found to give accurate results for the spectroscopic properties and the electric dipole moments [12]. Firstly, the atomic properties which are most important for a correct description of the molecular systems have been calculated. Truncation errors have been computed for the

Table 3. Truncation error of the correlation energy for Zn

Basis	E_{SCF}	E_{MCPF}	ΔE_{corr}	% ΔE_{corr}
Primitive	− 1777.84728435	− 1778.35764837	− 0.51036402	100.0
8*s*7*p*6*d*5*f*4*g*	− 1777.84728068	− 1778.35585613	− 0.50857545	99.6
7*s*6*p*5*d*4*f*3*g*	− 1777.84727401	− 1778.35206009	− 0.50478608	98.9
6*s*5*p*4*d*3*f*2*g*	− 1777.84725241	− 1778.34112825	− 0.49387583	96.8
5*s*4*p*3*d*2*f*1*g*	− 1777.84693051	− 1778.30650096	− 0.45957045	90.0
4*s*3*p*2*d*1*f*0*g*	− 1777.83947981	− 1778.21615682	− 0.37667702	73.8

Table 4. States employed in the calculation of the hydrides

Atom	State
Sc	$^1\Sigma^+$
Ti	$^4\Phi$
V	$^5\Delta$
Cr	$^6\Sigma^+$
Mn	$^7\Sigma^+$
Fe	$^4\Delta$
Co	$^3\Phi$
Ni	$^2\Delta$
Cu	$^1\Sigma^+$
Zn	$^2\Sigma^+$

valence spectra as well as for the ionization potential and the polarizability. Secondly, the behavior of the molecular properties has been studied. The effect of the contraction on the spectroscopic constants, dipole moments, and dipole derivatives for the first-row transition metal hydrides has been analyzed. The calculations have been performed for the ground states (cf. Table 4). All these calculations have been carried out with the MCPF method. Only the 3*d* and 4*s* electrons have been correlated, leaving the core uncorrelated. It is well-known that correlation of the 3*p* electrons will influence the atomic and molecular properties for transition metal atoms and molecules (see e.g. [12]), which must be remembered when comparing the computed properties with experiment. The influence of the relativistic corrections has been evaluated using first-order perturbation theory and including the mass–velocity and the one-electron Darwin terms.

4.1 Atoms

Tables 5, 6 show the computed energy differences between the low-lying atomic states corresponding to the occupations $d^{n-2}s^2$, $d^{n-1}s$, and d^n. They have been calculated both for the primitive basis sets (labeled by P in the tables) and for four different contractions. The number of basis functions used was chosen according to the principle of adding complete shells with respect to the principal quantum number of the atom. For example if we use the functions 1*s*–6*s* for a transition metal atom, we use for the other shells: 2*p*–6*p*, 3*d*–6*d*, 4*f*–6*f*, and 5*g*–6*g*, resulting in

Table 5. $d^{n-2}s^2 \rightarrow d^{n-1}s$ excitation energy (eV)

Basis	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu
P[a]	1.74	1.21	0.44	− 1.29	2.41	1.08	0.75	0.12	− 1.75
A[a]	1.74	1.21	0.44	− 1.29	2.42	1.08	0.75	0.11	− 1.76
B[a]	1.74	1.20	0.44	− 1.29	2.42	1.08	0.75	0.11	− 1.76
C[a]	1.74	1.20	0.43	− 1.30	2.43	1.08	0.74	0.10	− 1.78
D[a]	1.73	1.18	0.41	− 1.39	2.46	1.08	0.72	0.08	− 1.83
Exp[b]	1.43	0.81	0.25	− 1.00	2.14	0.87	0.42	− 0.03	− 1.49

[a] P = $21s15p10d6f4g$, A = $8s7p6d5f4g$, B = $7s6p5d4f3g$, C = $6s5p4d3f2g$, D = $5s4p3d2f1g$

[b] Values (j-averaged) from Ref. [13]

Table 6. $d^{n-2}s^2 \rightarrow d^n$ excitation energy (eV)

Basis	Sc	Ti	V	Cr	Mn	Fe	Co	Ni
P[a]	4.68	4.07	2.88	3.20	6.19	4.79	4.00	2.31
A[a]	4.68	4.07	2.87	3.19	6.20	4.79	3.99	2.31
B[a]	4.68	4.07	2.87	3.19	6.20	4.79	3.98	2.30
C[a]	4.67	4.06	2.86	3.18	6.20	4.78	3.92	2.27
D[a]	4.65	4.02	2.81	3.10	6.22	4.76	3.92	2.22
Exp[b]	4.19	3.35	2.47	3.40	5.59	4.07	3.36	1.71

[a] P = $21s15p10d6f4g$, A = $8s7p6d5f4g$, B = $7s6p5d4f3g$, C = $6s5p4d3f2g$, D = $5s4p3d2f1g$

[b] Values (j-averaged) from Ref. [13]

a basis set of the size $6s5p4d3f2g$. The procedure is justified by the occupation numbers that are obtained in the averaging procedure. They usually form an approximate shell structure. The major factor that determines these occupation numbers is the principal quantum number, whereas the angular quantum number gives only finer details, see Figs 1–3. The occupation number of a basis function is a good measure of its importance in the correlated wave function. The four contracted basis sets for the metal atoms which have been used range from $8s7p6d5f4g$ (labeled A) to $5s4p3d2f1g$ (labeled D). The largest one comprises 130 basis functions and is estimated to be saturated with respect to the primitive basis set. The smallest one comprises 55 functions and shows small but nonnegligible truncation errors.

As can be seen in Tables 5 and 6, the truncation errors for the excitation energies are very small. The largest contracted basis sets give virtually the same results for both the excitation energies as the uncontracted sets. The intermediate sets (B and C) give errors within the range 0–0.04 eV, except for one of the differences of the cobalt atom. Even for the smallest basis sets are the contraction errors (absolute values) not larger than 0.1 eV. The results for the computed ionization potentials, which have been compiled in Table 7, are similar. The effect of truncation is negligibly small for the basis sets $8s7p6d5f4g$ and $7s6p5d4f3g$. The $6s5p4d3f2g$ yields absolute errors smaller than 0.4 eV. More significant deviations occur, however, for the $5s4p3d2f1g$ basis sets.

Experimental data have also been included in the tables. When comparing the calculated values to experiment one must, however, take into account that the calculations have been performed at the MCPF level of approximation correlating only the valence electrons. The MCPF method is known to be inadequate for computing these excitation energies.

The polarizability was computed by using the finite field approach with an external field of 0.01 a.u. The obtained values are given in Table 8.

The accurate computation of polarizabilities with ANO basis sets is known to be particularly difficult. Indeed, the results show that it is more affected by truncation. Nevertheless, the two largest contracted basis sets yield small errors. Deviations with respect to the values obtained with the primitive sets are larger for the 6*s*5*p*4*d*3*f*2*g* basis set although they do not exceed 12%. The smallest basis sets give, however, errors between 6% and 43%.

Even though the contraction errors for the atomic properties have been shown to be small, it has been reported that significant errors can be obtained when calculating the relativistic energy contributions [4]. We have therefore evaluated the relativistic effect on the separation between the low-lying states of the nickel atom. The results are given in Table 9. As is well known, the relativistic

Table 7. Ionization potential (eV)

Basis	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
P[a]	5.76	6.62	6.69	6.44	7.23	7.67	7.90	7.30	7.35	9.08
A[a]	5.76	6.62	6.68	6.44	7.23	7.67	7.90	7.30	7.35	9.08
B[a]	5.76	6.62	6.68	6.44	7.22	7.66	7.89	7.30	7.34	9.08
C[a]	5.81	6.61	6.67	6.44	7.21	7.65	7.87	7.28	7.33	9.05
D[a]	5.91	6.61	6.63	6.42	7.20	7.63	7.84	7.26	7.27	9.02
Exp[b]	6.56	6.83	6.74	6.76	7.43	7.90	7.86	7.63	7.72	9.39

[a] P = 21*s*15*p*10*d*6*f*4*g*, A = 8*s*7*p*6*d*5*f*4*g*, B = 7*s*6*p*5*d*4*f*3*g*, C = 6*s*5*p*4*d*3*f*2*g*, D = 5*s*4*p*3*d*2*f*1*g*
[b] Values from Ref. [13]

Table 8. Polarizability (a.u.)

Basis	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
P[a]	142.28	114.34	97.34	94.72	75.52	63.93	57.71	51.10	53.44	42.85
A[a]	142.30	114.36	97.34	94.40	75.54	66.27	57.64	51.02	52.96	42.65
B[a]	142.30	114.38	97.24	93.44	75.44	64.56	57.42	50.26	50.00	42.16
C[a]	142.18	114.14	96.84	83.52	73.64	63.45	55.95	45.44	40.72	40.23
D[a]	126.18	107.46	87.06	67.84	60.58	53.26	45.36	36.36	30.48	31.24

[a] P = 21*s*15*p*10*d*6*f*4*g*, A = 8*s*7*p*6*d*5*f*4*g*, B = 7*s*6*p*5*d*4*f*3*g*, C = 6*s*5*p*4*d*3*f*2*g*, D = 5*s*4*p*3*d*2*f*1*g*

Table 9. Relativistic contributions to the excitation energies for the nickel atom (eV)

Basis set	$^3F \rightarrow {}^3D$	$^3F \rightarrow {}^1S$
21*s*15*p*10*d*6*f*4*g*	0.36	0.59
8*s*7*p*6*d*5*f*4*g*	0.38	0.62
7*s*6*p*5*d*4*f*3*g*	0.40	0.64
6*s*5*p*4*d*3*f*2*g*	0.40	0.66
5*s*4*p*3*d*2*f*1*g*	0.38	0.62

contributions are important for an accurate description of the valence spectra. The effect of truncation does not seem to behave in a systematic way, but the absolute errors are smaller than 0.1 eV, which contradicts the results of Bauschlicher and Taylor [4].

4.2 Hydrides

Although a good performance of the constructed basis sets for calculations on atoms has been shown, this does not guarantee a corresponding good performance for molecules. Hence, additional test calculations have been carried out for the transition metal hydrides. The MCPF method was again used. Two of the basis sets have already been employed in a previous study [12] yielding satisfactory results.

When performing calculations on molecules it is important to have basis sets that have a balanced quality for all the atoms in the molecule. For the hydrogen atom, we have used the ANO basis set of [5], which we believe to be of the same quality as the Sc–Zn basis sets of this work. According to the procedure described above, the size of the hydrogen atom basis set was selected with the criterion that the same number of virtual functions are included. For example, *1s*–*3s* for hydrogen yield a TZ description of the valence just as *4s*–*6s* does for transition metal atoms. Thus, the *6s5p4d3f2g* basis set of the transition metal atoms are used together with a *3s2p1d* basis set for hydrogen. The largest basis sets used have the size *8s7p6d5f4g*/*5s4p3d* and are expected to be saturated. They will be therefore taken as references for the analysis of the truncation errors, since calculations with totally uncontracted sets become impracticably large. The following properties were computed: equilibrium distance (r_e), bond energy (D_e), vibrational frequency (ω_e), dipole moment (μ), and dipole moment derivative ($d\mu/dR$). The three first molecular constants were computed with the relativistic effects included, while the electric properties were evaluated only at the nonrelativistic level. The spectroscopic constants were obtained from a parabolic fit in r^{-1} with a 0.1 a.u. grid around the minimum of the potential curve.

Table 10 shows the optimized bond distance for the hydrides computed with the four contracted basis sets. The contraction errors (absolute values) with respect to the largest basis sets do not exceed from 0.003 a.u. (*7s6p5d4f3g*/*4s3p2d* contraction), 0.012 a.u. (*6s5p4d3f2g*/*3s2p1d* contraction), and 0.021 a.u. (*5s4p3d2f1g*/*2s1p* contraction). The discrepancy between the results for the most flexible basis sets and experiment ranges from 0.104 a.u. for iron hydride to − 0.020 a.u. for titanium hydride. As has already been pointed out, this error is largely due to the correlation treatment and not to the basis set. The contribution of the relativistic effects to the results is far from negligible. The shortening of the bonds computed with MCPF and the largest basis sets, ranges from 0.045 a.u. for copper hydride to − 0.004 a.u. for scandium hydride.

The computed dissociation energies of the hydrides are compiled in Table 11. The behavior of the different basis sets is similar to that obtained for the optimized bond lengths. The two intermediate basis sets yield results which do not differ very much from the values obtained with the largest basis sets. The most important deviations is obtained for the *6s5p4d3f2g*/*3s2p1d* basis set of copper, where it is 0.05 eV. In contrast, the contraction *5s4p3d2f1g*/*2s1p* gives larger errors in some cases. For instance, the dissociation energies for the chromium and copper hydrides are 0.09 eV smaller than the values obtained with the *8s7p6d5f4g*/*5s4p3d*

Table 10. Equilibrium distance [r_e (a.u.)] for the hydrides including relativistic corrections

Basis	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
A[a]	3.392	3.420	3.230	3.060	3.287	2.936	2.860	2.759	2.761	2.997
B[a]	3.393	3.420	3.231	3.061	3.287	2.934	2.857	2.758	2.763	2.996
C[a]	3.389	3.419	3.230	3.063	3.286	2.936	2.857	2.755	2.773	2.995
D[a]	3.382	3.416	3.227	3.061	3.294	2.942	2.862	2.764	2.782	3.009
Exp[b]		3.4		3.14	3.29	3.04	2.861[c]	2.747[d]	2.764[e]	3.014[f]

[a] A = *8s7p6d5f4g/5s4p3d*, B = *7s6p5d4f3g/4s3p2d*, C = *6s5p4d3f2g/3s2p1d*, D = *5s4p3d2f1g/2s1p*
[b] Values from Ref. [14] except as noted
[c] Ref. [15]
[d] Ref. [16]
[e] Ref. [17]
[f] Ref. [18]

Table 11. Dissociation energies [D_e (eV)] for the hydrides including relativistic corrections

Basis	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
A[a]	2.39	2.10	2.36	2.21	1.70	1.67	1.90	2.97	2.80	0.97
B[a]	2.37	2.10	2.35	2.20	1.69	1.66	1.89	2.97	2.79	0.96
C[a]	2.36	2.07	2.33	2.17	1.67	1.64	1.88	2.96	2.75	0.95
D[a]	2.32	2.06	2.31	2.12	1.62	1.66	1.89	2.92	2.71	0.91
Exp[b]	2.09[c]	2.09[c]	2.13[d]	2.03[e]	1.36	1.70	2.09	2.70	2.75	0.95[f]

[a] A = *8s7p6d5f4g/5s4p3d*, B = *7s6p5d4f3g/4s3p2d*, C = *6s5p4d3f2g/3s2p1d*, D = *5s4p3d2f1g/2s1p*
[b] Values obtained as $D_e = D_0 + 1/2h\omega_e$. D_0 values taken from Ref. [14] except as noted
[c] D_0 value
[d] D_0 value taken from Ref. [19]
[e] Value obtained from the D_0 value reported in Ref. [19]
[f] Value from Ref. [18]

basis sets. The experimental data reported in Table 11 have been calculated by adding the term $h\omega_e/2$ to the experimental D_0 values, except for the hydrides in which no vibration frequency has been found in the literature. The most important deviation between these results and the theoretical ones (largest basis sets) occurs for manganese hydride, where it is 0.34 eV (absolute value). Nevertheless, it is smaller than 0.1 eV for diatoms like FeH or CuH. The relativistic effect on the bond strength is significant. It ranges from − 0.23 eV for cobalt hydride to + 0.16 eV for chromium molecule.

Table 12 collects the vibration frequency for the hydrides obtained with the different basis sets. Truncation errors are small for all the contractions and the absolute deviation does not exceed 40 cm^{-1}, even for the *5s4p3d2f1g/2s1p* basis set. The difference between the experimental and the calculated values lies within the expected range for the largest basis sets, except for chromium hydride where it is larger than 200 cm^{-1} (which only proves that the MCPF method is inadequate for this molecule, as expected). The relativistic contributions are very small for the atoms on the left half of the row and for Zn, where it ranges from 3 to 7 cm^{-1}, but they are important for the atoms Fe–Cu, ranging from 52 to 84 cm^{-1}

Table 12. Vibrational constant [ω_e (cm^{-1})] for the hydrides including relativistic corrections

Basis	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
A[a]	1591	1516	1624	1800	1547	1908	1889	1979	1959	1651
B[a]	1553	1514	1622	1789	1547	1907	1889	1974	1924	1649
C[a]	1567	1524	1625	1792	1551	1907	1889	1977	1919	1651
D[a]	1574	1525	1631	1828	1548	1904	1887	1962	1999	1641
Exp[b]				1581	1548	1827	1925	2001[c]	1941	1608[d]

[a] A = $8s7p6d5f4g/5s4p3d$, B = $7s6p5d4f3g/4s3p2d$, C = $6s5p4d3f2g/3s2p1d$, D = $5s4p3d2f1g/2s1p$

[b] Values from Ref. [14] except as noted

[c] Value from Ref. [16]

[d] Value from Ref. [18]

The computation of accurate dipole moments for transition metal compounds is known to be a difficult problem. This property is very sensitive to the quality of the wave function. Indeed, an unbalanced treatment of the low-lying atomic states may yield significant errors in μ. The MCPF method has been used to compute the dipole moments for the hydrides, yielding results, which are in reasonable agreement with experiment for the two cases (TiH and NiH), where the experimental value is known [20]. In Table 13 we present the MCPF results obtained with the different contracted basis sets, and compare them with the earlier calculations and experiment. Dipole moments have been computed as expectation values of the MCPF wave function at the nonrelativistic level.

The truncation errors are very different from one basis set to another. Whereas the $7s6p5d4f3g/4s3p2d$ contraction yields negligible deviations with respect to the results given by the largest basis sets and the $6s5p4d3f2g/3s2p1d$ basis set yield values which do not differ more than 0.03 D, the smallest contractions yield important absolute errors. For the chromium and zinc molecules they are actually larger than 0.2 D. Comparison with the earlier theoretical results reported in Ref. [20] shows that the two sets of results are very similar, except for chromium hydride where the difference is larger than 1.5 D. We have no explanation for this discrepancy. We can also compare the present results for NiH and CuH with those obtained in an earlier study, where the CASSCF method was used in combination with multiconfigurational second-order perturbation theory [12]. This method gives the dipole moments 2.43 and 2.73 D for NiH and CuH, respectively. The values decrease to 2.32 and 2.66 D when $3s$, $3p$ correlation effects are added. These results are accurate and show that the MCPF method has a tendency to overestimate the ionic character of the wave function, which is typical for single configuration based correlation methods.

The trends observed for the dipole derivatives are very similar as can be seen from the values in Table 14. The values obtained with the intermediate contracted basis sets show almost negligible truncation errors while, in some cases, they increase for the least flexible basis set. Again, the results for CrH deviates most from the values reported by Chong et al. [20].

It is well known that ANO basis sets give small errors due to basis set superposition (BSSE). In order to analyze the BSSE for the basis sets presented here, we have performed calculations on the copper atom with a set of copper ghost orbitals located at a distance of 4.194 a.u. from the atom (corresponding to the equilibrium distance in Cu_2 [23]). At the SCF level, superposition errors for the two smallest basis sets were computed to be negligible: 0.0006 eV ($6s5p4d3f2g$) and

Table 13. Dipole moments [μ(D)] for the hydrides

Basis	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
A[a]	1.38	2.11	1.97	2.21	1.12	2.88	2.89	2.53	2.82	0.52
B[a]	1.38	2.11	1.97	2.21	1.12	2.88	2.89	2.53	2.82	0.51
C[a]	1.35	2.11	1.97	2.24	1.11	2.86	2.88	2.51	2.80	0.51
D[a]	1.34	2.14	2.05	2.46	1.29	2.88	2.85	2.48	2.74	0.74
MCPF[b]	1.37	2.19	2.02	3.81	1.24	2.90	2.74	2.56	2.95	0.59
Exp		2.455[c]						2.4 ± 0.1[d]		

[a] A = *8s7p6d5f4g/5s4p3d*, B = *7s6p5d4f3g/4s3p2d*, C = *6s5p4d3f2g/3s2p1d*, D = *5s4p3d2f1g/2s1p*

[b] Theoretical data from Ref. [20]

[c] Value from Ref. [21]

[d] Value from Ref. [22]

Table 14. Dipole moments derivative [$d\mu/dR$ (D/a.u.)] for the hydrides

Basis	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
A[a]	1.29	1.22	1.08	0.49	1.71	1.48	1.20	1.11	0.75	1.08
B[a]	1.29	1.22	1.08	0.48	1.71	1.48	1.20	1.11	0.75	1.07
C[a]	1.28	1.29	1.07	0.49	1.69	1.47	1.19	1.08	0.74	1.04
D[a]	1.26	1.31	1.08	0.44	1.69	1.51	1.20	1.04	0.82	1.03
MCPF[b]	1.41	1.28	1.16	1.48	1.73	1.61	1.18	1.00	0.78	1.08

[a] A = *8s7p6d5f4g/5s4p3d*, B = *7s6p5d4f3g/4s3p2d*, C = *6s5p4d3f2g/3s2p1d*, D = *5s4p3d2f1g/2s1p*

[b] Theoretical data from Ref. [20]

0.005 eV (*5s4p3d2f1g*). At the MCPF level, the corresponding values were 0.024 eV (*6s5p4d3f2g*) and 0.050 eV (*5s4p3d2f1g*).

5 Conclusions

We have presented a series of ANO basis sets for the first row transition metal atoms, that have been obtained by averaging over the three electronic configurations d^n, $d^{n-1}s$, and $d^{n-2}s^2$ for the neutral atom as well as the ground state for the cation and the ground state atom in an external electric field. They differ in this respect from parallel work by Bauschlicher Jr., who did not include the d^n configuaration (only for Ni) or the polarizing field in the averaging procedure. Instead the outermost *s* and *p* primitives were uncontracted. Comparisons between the two basis sets made for Cu_2 and NiH show that they are of very similar accuracy. The d^n configuration is important mainly in zero-valent compounds like ferrocene. Further testing is needed in order to judge the importance of this configuration in the averaging procedure.

Contraction of the present basis set to *6s5p4d3f2g* yields results that are virtually identical to those obtained with the corresponding uncontracted basis sets for the atomic properties that they have been designed to reproduce. Slightly larger deviations are obtained with the *5s4p3d2f1g* for the polarizability, while energetic properties still have only small errors.

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Appendix

The basis sets are included in this article for completeness, but it is rather awkward to type all 4350 numbers, and you are encouraged to send an e-mail to one of the authors to receive the basis sets electronically: teobor@garm.teokem.lu.se (BOR) or ibmpow@garm.teokem.lu.se (POW).

Under normal circumstances we recommend a contraction "shell-wise" i.e. using the principal quantum number as the cutoff criteria. A *8s7p6d5f4g* basis set is virtually saturated with respect to the primitive basis set and using larger basis sets is meaningless. A *6s5p4d3f2g* basis set shows very small contraction errors and is of sufficient quality for many applications while the next smaller basis set, *5s4p3d2f1g*, shows a significant degradation of quality, and is not recommended except if computational economy prevents the usage of a larger set. As a compromise it is usually better to truncate the *dfg* space while using a larger sp space, thus a *6s5p3d2f1g* (or *7s6p4d3f2g*) can be recommended when computational effort is an issue. Under such circumstances it might be wise to use also a smaller primitive basis [8].

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Sc atom

Exponents for s-functions

2715278.	406598.4	92530.04	26207.92	8549.429	3085.975	1203.172	498.4869
216.7360	97.87476	45.20433	20.21187	9.574751	4.540346	1.995687	0.942215
0.417845	0.095761	0.051351	0.023878	0.009551			

Contraction matrix for s-function

1s	2s	3s	4s	5s	6s	7s	8s
0.00000904	-0.00000260	0.00000093	-0.00000020	0.00000033	-0.00000050	0.00000060	-0.00000010
0.00007025	-0.00002060	0.00000725	-0.00000180	0.00000259	-0.00000380	0.00000508	-0.00000060
0.00036936	-0.00010830	0.00003813	-0.00000940	0.00001336	-0.00001890	0.00002328	-0.00000320
0.00155734	-0.00045720	0.00016110	-0.00003970	0.00005779	-0.00008580	0.00011736	-0.00001470
0.00563817	-0.00166130	0.00058525	-0.00014420	0.00020373	-0.00028470	0.00033930	-0.00004710
0.01806446	-0.00537480	0.00189710	-0.00046690	0.00068535	-0.00103110	0.00144768	-0.00017810
0.05144548	-0.01567320	0.00554026	-0.00136660	0.00191409	-0.00262930	0.00299552	-0.00042980
0.12707079	-0.04083870	0.01453926	-0.00358060	0.00531269	-0.00814650	0.01185638	-0.00142260
0.25490555	-0.09186680	0.03306537	-0.00818040	0.01128466	-0.01500180	0.01553214	-0.00240110
0.36017448	-0.16483380	0.06115124	-0.01512000	0.02309854	-0.03719520	0.05878879	-0.00667270
0.26994142	-0.18091270	0.07020757	-0.01759940	0.02223441	-0.02357950	0.00528309	-0.00314330
0.06163753	0.05165397	-0.02111350	0.00550800	0.00012429	-0.02279820	0.09434564	-0.00609790
-0.00137010	0.50474999	-0.27065280	0.07005315	-0.12218900	0.23648629	-0.46579960	0.04625288
0.00205343	0.50458120	-0.44054920	0.12312721	-0.14779690	0.13085046	0.10415482	0.01739344
-0.00095410	0.09393705	0.06285392	-0.02804590	-0.03470180	0.23841114	-0.88418510	0.04824636
0.00043552	-0.00297080	0.71691262	-0.24417280	0.64622191	-1.77116600	4.00662690	-0.40686840
-0.00018700	0.00248254	0.44287952	-0.32519970	0.15556924	1.29776820	-4.97894900	0.46797935
0.00009671	-0.00080170	0.02330734	0.35832951	-2.27616700	3.27082980	7.87419890	0.69915480
-0.00009370	0.00076538	-0.01372210	0.60752195	1.15412310	-6.65044700	-9.85628200	-3.30406900
0.00004126	-0.00033710	0.00463010	0.20971754	0.73089925	4.26392470	5.32791980	4.81968330
-0.00000960	0.00007798	-0.00096690	0.00735932	0.10275994	-0.71246510	-1.36913800	-2.85896200

Exponents for p-functions

4609.885	1092.156	354.3368	134.8076	56.60258	25.33410	11.74033	5.569259
2.594958	1.196351	0.535059	0.220776	0.088310	0.035324	0.014130	

Contraction matrix for p-function

2p	3p	4p	5p	6p	7p	8p
0.00019182	-0.00006450	0.00001892	-0.00002410	0.00003139	-0.00000370	0.00006720
0.00168006	-0.00056470	0.00016799	-0.00021600	0.00028193	-0.00009380	0.00033047
0.00927532	-0.00314160	0.00092264	-0.00117490	0.00153073	-0.00018100	0.00327359
0.03752902	-0.01284830	0.00382999	-0.00492860	0.00643366	-0.00216920	0.00731896
0.11490240	-0.04053780	0.01193472	-0.01520350	0.01981904	-0.00187070	0.04399471
0.25439248	-0.09287680	0.02796506	-0.03616710	0.04726485	-0.01843640	0.04132905
0.37991661	-0.14765040	0.04354371	-0.05550180	0.07284368	0.00517068	0.21606005
0.30955557	-0.11280680	0.03528510	-0.04666140	0.06440105	-0.07381960	-0.04754280
0.08713977	0.15761618	-0.06168620	0.08722143	-0.11917420	0.14285677	0.23806451
0.00256096	0.47136955	-0.15801900	0.22269449	-0.38254400	-0.09680990	-2.55856900
0.00122683	0.43009952	-0.22299720	0.36197365	-0.39389800	0.45403423	4.31709930
-0.00047590	0.10180833	0.15843483	-0.88835790	2.19800400	-1.45299000	-3.68183000
0.00022635	-0.00184220	0.70244749	-0.40959980	-2.39692000	2.62863880	2.28377620
-0.00011100	0.00290251	0.28120425	0.91905928	0.89636097	-3.13249300	-1.07370600
0.00003471	-0.00078270	0.01348198	0.21314873	0.35148686	1.96084820	0.28495095

Exponents for d-functions

110.2197 32.80041 12.31300 5.063819 2.225547 0.992343 0.436361 0.185705
0.073441 0.029376

Contraction matrix for d-function

3d	4d	5d	6d	7d	8d
0.00082585	-0.00072360	0.00088824	-0.00079750	0.00131877	-0.00369500
0.00668105	-0.00582090	0.00727289	-0.00574830	0.01552580	-0.02134390
0.02815944	-0.02479120	0.03053473	-0.02734940	0.04659408	-0.13480300
0.08372592	-0.07372960	0.09263052	-0.07108940	0.20849078	-0.28299330
0.17840105	-0.15786200	0.19890523	-0.19284550	0.28675455	-1.07102300
0.26729481	-0.22085100	0.26567709	-0.17873910	0.58272511	2.60623010
0.30373222	-0.20962350	0.09014133	-0.03909720	-2.16466900	-2.43683400
0.29501849	0.05386544	-0.65848460	1.37404170	2.18450990	1.45019450
0.19903618	0.43826457	-0.39701430	-1.98588300	-1.25616900	-0.66794290
0.09880504	0.51004476	0.89538505	1.16147000	0.44271166	0.22240725

Exponents for f-functions

2.841500 1.126300 0.446400 0.176900 0.070100 0.027800

Contraction matrix for f-function

4f	5f	6f	7f	8f
0.03457755	-0.09573200	0.13599954	-0.18947700	0.31414809
0.09785268	-0.21698380	0.33213274	-0.51944710	0.70431127
0.34953556	-0.57644500	0.49380454	0.66751872	-1.35290100
0.54494830	0.14682811	-1.24770000	0.04262355	1.41191830
0.23054038	0.57506501	0.81525437	-0.93623980	-1.28621700
0.03096216	0.20992137	0.20469111	1.06981160	0.85106694

Exponents for g-functions

1.607100 0.631700 0.248300 0.097600

Contraction matrix for g-function

5g	6g	7g	8g
-0.03124780	-0.17126050	-0.45988690	-0.87389880
-0.19912470	-0.40228810	-0.18438610	1.12606360
-0.43510610	0.05517028	0.75066198	-0.85961910
-0.16454480	0.44274085	-0.69961420	0.42599543

Ti atom

Exponents for s-functions

3014643.	451432.9	102733.8	29098.17	9492.330	3426.346	1335.896	553.5026
240.6925	108.7293	50.26457	22.58004	10.71432	5.093546	2.244183	1.059570
0.468849	0.106143	0.055262	0.025465	0.010186			

Contraction matrix for s-function

1s	2s	3s	4s	5s	6s	7s	8s
0.00000891	-0.00000260	0.00000094	-0.00000020	0.00000033	-0.00000070	0.00000070	-0.00000080
0.00006931	-0.00002050	0.00000732	-0.00000180	0.00000263	-0.00000530	0.00000531	-0.00000530
0.00036438	-0.00010770	0.00003850	-0.00000950	0.00001351	-0.00002630	0.00002922	-0.00003280
0.00153639	-0.00045480	0.00016265	-0.00004010	0.00005873	-0.00012000	0.00011605	-0.00011140
0.00556285	-0.00165290	0.00059092	-0.00014580	0.00020574	-0.00039620	0.00045565	-0.00053040
0.01782861	-0.00534850	0.00191602	-0.00047270	0.00069769	-0.00144350	0.00134216	-0.00122050
0.05081175	-0.01560890	0.00559924	-0.00138220	0.00193149	-0.00365790	0.00441363	-0.00535560
0.12571796	-0.04072220	0.01471713	-0.00363470	0.00543140	-0.01144970	0.01006047	-0.00838210
0.25299347	-0.09187640	0.03356771	-0.00830710	0.01140247	-0.02093470	0.02766255	-0.03603000
0.35959434	-0.16550280	0.06237534	-0.01548490	0.02391928	-0.05291360	0.04026955	-0.02489570
0.27246952	-0.18360090	0.07240544	-0.01810670	0.02240972	-0.03314180	0.07324128	-0.12295430
0.06359557	0.04772324	-0.01969540	0.00495788	0.00244168	-0.03572990	-0.05679990	0.17036170
-0.00122450	0.50578507	-0.27814850	0.07274548	-0.12994700	0.34737593	-0.16965990	-0.02547000
0.00201172	0.50661982	-0.44779230	0.12462260	-0.14412390	0.19621750	-0.76563180	1.42375220
-0.00093570	0.09464746	0.07571834	-0.03012510	-0.04266210	0.21600547	1.37733270	-3.69996800
0.00042046	-0.00280280	0.72182448	-0.25472070	0.68771072	-2.54289500	0.71862212	3.42508630
-0.00017760	0.00244130	0.43305367	-0.31128130	0.08970366	2.53447060	-2.56707700	-1.00954000
0.00008641	-0.00072980	0.02190391	0.39641780	-2.20071600	0.65481184	5.20872300	-2.39533300
-0.00008290	0.00069792	-0.01256510	0.58239439	1.16817660	-3.07838800	-5.98295700	5.66622560
0.00003762	-0.00031470	0.00450143	0.19898058	0.68247571	2.18525880	1.89911920	-5.71171100
-0.00000900	0.00007494	-0.00096630	0.00465101	0.09670204	-0.12137220	0.47574667	2.69579320

Exponents for p-functions

5181.157	1227.461	398.2712	151.5867	63.69633	28.54733	13.26129	6.310352
2.951875	1.365370	0.611415	0.252548	0.101019	0.040408	0.016163	

Contraction matrix for p-function

2p	3p	4p	5p	6p	7p	8p
0.00018724	-0.00006430	0.00001778	-0.00002460	0.00003719	-0.00005500	0.00003441
0.00164139	-0.00056350	0.00015781	-0.00021600	0.00030354	-0.00044230	0.00074567
0.00908304	-0.00314250	0.00086992	-0.00120360	0.00181821	-0.00268410	0.00167516
0.03689507	-0.01290430	0.00362099	-0.00495220	0.00694324	-0.01009190	0.01739889
0.11355987	-0.04095070	0.01136286	-0.01573360	0.02391533	-0.03527760	0.01936750
0.25317899	-0.09460300	0.02679911	-0.03658610	0.05029716	-0.07263650	0.14811200
0.38016762	-0.15139560	0.04214155	-0.05944900	0.09593973	-0.14494120	-0.00414360
0.31019996	-0.11414090	0.03368180	-0.04678460	0.05786017	-0.14247940	0.63592456
0.08777409	0.16320565	-0.05898500	0.07944795	-0.08846610	0.31125939	-1.91295700
0.00294909	0.47321733	-0.15122720	0.27628381	-0.65664460	1.43894680	1.31107870
0.00131937	0.42451323	-0.20347950	0.27142188	0.11031284	-2.78088700	0.71779745
-0.00042150	0.10183772	0.11806167	-0.79246970	1.61485710	1.85240650	-2.24014800
0.00021981	-0.00167870	0.69383947	-0.46317480	-1.74849600	-0.07210230	2.90907530
-0.00010630	0.00283921	0.31458515	0.84321160	0.31630342	-1.14942500	-2.70645000
0.00003319	-0.00076640	0.01638688	0.29045090	0.63388041	0.97774753	1.42394160

Exponents for d-functions

134.3565 40.04189 15.12976 6.276990 2.781410 1.253602 0.557405 0.239759
0.095287 0.038115

Contraction matrix for d-function

3d	4d	5d	6d	7d	8d
0.00082946	-0.00066820	0.00107015	-0.00145030	0.00228582	-0.00312940
0.00686716	-0.00549600	0.00903555	-0.01239650	0.01652191	-0.02947250
0.02978288	-0.02413250	0.03925759	-0.05422370	0.08713506	-0.13216440
0.08973599	-0.07293950	0.12440155	-0.17800620	0.25177544	-0.53635380
0.19339831	-0.15795350	0.25010252	-0.33545420	0.54086998	-0.22595440
0.28934684	-0.21643350	0.28000335	-0.18766830	-0.64286510	1.99762740
0.31794406	-0.18224060	-0.08899850	0.78380039	-0.80912680	-2.72669200
0.27588611	0.12624548	-0.62602520	0.22363428	1.85337250	2.16382570
0.15938332	0.44805135	-0.24875410	-1.28760100	-1.65105200	-1.24025100
0.07054351	0.48413331	0.81573964	0.96413095	0.76643894	0.47141590

Exponents for f-functions

4.246400 1.683100 0.667100 0.264400 0.104800 0.041500

Contraction matrix for f-function

4f	5f	6f	7f	8f
0.03908396	-0.12201770	0.23859369	-0.46302000	0.67086609
0.13383140	-0.36711890	0.55423570	-0.38522010	-0.49903890
0.36510792	-0.49912310	-0.19514490	1.12623010	-0.23268570
0.49496780	0.25518397	-0.73517000	-0.89607750	0.95139916
0.25144472	0.52213820	0.65679222	0.01836808	-1.38173800
0.03832938	0.11207232	0.26902177	0.58238478	1.10757900

Exponents for g-functions

2.401700 0.944000 0.371000 0.145800

Contraction matrix for g-function

5g	6g	7g	8g
0.10521998	-0.38795830	-0.54015460	-0.97127230
0.33971686	-0.55192540	0.06154673	1.42790710
0.56411761	0.18037356	0.63268065	-1.20652500
0.28531137	0.60415486	-0.67377870	0.63051175

V atom

Exponents for s-functions

3321857. 497435.6 113202.7 32063.33 10459.62 3775.506 1472.040 609.9331
265.2634 119.8607 55.44891 24.98372 11.88056 5.660311 2.495703 1.177866
0.520044 0.115965 0.058938 0.026946 0.010778

Contraction matrix for s-function

1s	2s	3s	4s	5s	6s	7s	8s
0.00000883	-0.00000260	0.00000095	-0.00000020	0.00000041	-0.00000070	0.00000070	-0.00000100
0.00006866	-0.00002040	0.00000739	-0.00000170	0.00000326	-0.00000540	0.00000520	-0.00000680
0.00036099	-0.00010750	0.00003887	-0.00000920	0.00001661	-0.00002720	0.00002906	-0.00004150
0.00152213	-0.00045390	0.00016423	-0.00003870	0.00007314	-0.00012220	0.00011320	-0.00014450
0.00551165	-0.00165010	0.00059669	-0.00014080	0.00025215	-0.00041000	0.00045534	-0.00066690
0.01766850	-0.00534000	0.00193533	-0.00045670	0.00087231	-0.00146550	0.00130153	-0.00160130
0.05038288	-0.01559340	0.00565819	-0.00133560	0.00235836	-0.00380660	0.00443916	-0.00669230
0.12480875	-0.04072340	0.01489218	-0.00351830	0.00683812	-0.01159340	0.00968596	-0.01124660
0.25172615	-0.09208410	0.03404071	-0.00805470	0.01385685	-0.02209190	0.02820132	-0.04474820
0.35922653	-0.16636470	0.06349336	-0.01508270	0.03069543	-0.05334350	0.03801966	-0.03654160
0.27416445	-0.18580410	0.07421806	-0.01773950	0.02615091	-0.03823630	0.07857070	-0.14943220
0.06486325	0.04585458	-0.01908000	0.00455364	0.00874491	-0.02907220	-0.06832350	0.19110584
-0.00116620	0.50807061	-0.28571740	0.07165822	-0.17680100	0.34559817	-0.14736410	0.06905681
0.00198280	0.50692043	-0.45245900	0.12029781	-0.15916140	0.25792818	-0.82902110	1.69200910
-0.00092240	0.09430995	0.09007795	-0.03297310	-0.08362760	0.02175315	1.63122450	-4.96967400
0.00040988	-0.00270220	0.72508737	-0.24733060	1.01147820	-2.40280600	0.23192924	5.29396380
-0.00017020	0.00240065	0.42300422	-0.28548310	-0.22802420	2.70767500	-2.15214700	-2.39720300
0.00007885	-0.00067900	0.02042977	0.35331149	-2.26950100	-0.25108400	4.89520660	-0.66756870
-0.00007520	0.00064630	-0.01164770	0.59079651	1.60659870	-2.02543500	-5.96357100	3.38722670
0.00003493	-0.00029880	0.00432259	0.22227516	0.30163731	1.79308710	2.17030290	-4.30186600
-0.00000850	0.00007268	-0.00095410	0.00404189	0.13033433	-0.03372380	0.37871365	2.24684740

Exponents for p-functions

5777.377 1368.674 444.1233 169.0991 71.10191 31.90311 14.85109 7.085227
3.324422 1.541164 0.690520 0.285424 0.114170 0.045668 0.018267

Contraction matrix for p-function

2p	3p	4p	5p	6p	7p	8p
0.00018364	-0.00006410	0.00001786	-0.00002930	0.00003757	-0.00005740	0.00004717
0.00161110	-0.00056260	0.00015831	-0.00025550	0.00031060	-0.00047960	0.00079787
0.00893306	-0.00314410	0.00087602	-0.00143690	0.00184297	-0.00281000	0.00232320
0.03640766	-0.01295560	0.00365295	-0.00589370	0.00715633	-0.01104480	0.01874096
0.11255928	-0.04131800	0.01154370	-0.01897940	0.02447013	-0.03724580	0.02910045
0.25238886	-0.09610600	0.02735364	-0.04405560	0.05280936	-0.08169560	0.15830173
0.38048748	-0.15458390	0.04343197	-0.07318490	0.09891909	-0.15309860	0.05462061
0.31047820	-0.11487580	0.03382935	-0.05429490	0.06201692	-0.15863690	0.54869931
0.08808031	0.16825757	-0.06114900	0.10392677	-0.12794370	0.44880841	-2.07482200
0.00320003	0.47522201	-0.15596350	0.35080196	-0.64800290	1.23670600	1.80041500
0.00136798	0.41995647	-0.19423340	0.21455923	0.26641426	-2.69004000	0.18305779
-0.00038780	0.10071516	0.12128512	-0.91179100	1.37800780	1.90754510	-1.88871400
0.00021436	-0.00165100	0.68002867	-0.29944180	-1.66822500	-0.15905240	2.71073900
-0.00010280	0.00277481	0.32526772	0.79383862	0.32032507	-1.09269000	-2.58362000
0.00003206	-0.00074620	0.01640418	0.24053483	0.68719137	0.95690944	1.36049790

Exponents for d-functions

155.8527 46.49771 17.62999 7.354672 3.274051 1.482482 0.661351 0.284826
0.112899 0.045160

Contraction matrix for d-function

3d	4d	5d	6d	7d	8d
0.00082402	-0.00073700	0.00111483	-0.00160610	0.00235870	-0.00279830
0.00690787	-0.00615680	0.00949818	-0.01385620	0.01838356	-0.03231840
0.03046120	-0.02746690	0.04217370	-0.06229780	0.09402233	-0.12735110
0.09234492	-0.08414480	0.13485535	-0.20931580	0.30787651	-0.62960570
0.19856961	-0.18070830	0.27482529	-0.38597190	0.49646648	0.12458911
0.29427802	-0.23594040	0.27099699	-0.04116230	-0.93727640	1.60105310
0.31782364	-0.15454830	-0.17801220	0.90020360	-0.26353080	-2.59638700
0.27361464	0.19348164	-0.65249560	-0.17294460	1.51137020	2.28679200
0.15457842	0.46099507	-0.03686490	-1.00120500	-1.64835400	-1.43284700
0.05137878	0.41547911	0.73380859	0.90394104	0.86279221	0.58347956

Exponents for f-functions

5.906600 2.341200 0.927900 0.367800 0.145800 0.057800

Contraction matrix for f-function

4f	5f	6f	7f	8f
0.04103165	-0.11078580	0.24098334	-0.45148900	0.67789259
0.16050066	-0.38304920	0.57916148	-0.36298180	-0.49030530
0.39186678	-0.46986320	-0.26821710	1.09856090	-0.24823550
0.46817414	0.29209866	-0.68232650	-0.89635540	0.97160264
0.23292268	0.51792182	0.64138311	0.00667185	-1.39210200
0.03878760	0.11509426	0.26286929	0.61585876	1.09613420

Exponents for g-functions

3.340600 1.313000 0.516100 0.202800

Contraction matrix for g-function

5g	6g	7g	8g
0.09336339	-0.34102680	0.49376937	-0.20561100
0.31083775	-0.51794230	-0.08196600	0.30412955
0.47448495	0.19167126	-0.53268200	-0.26434240
0.23905823	0.55279659	0.57865717	0.14211497

Cr atom

Exponents for s-functions

6177194. 924929.5 210486.5 59620.05 19450.76 7022.056 2738.763 1135.814
495.0923 224.7487 105.3836 50.19359 22.24957 10.98265 5.383665 2.343685
1.105202 0.487848 0.089599 0.033423 0.013369

Contraction matrix for s-function

1s	2s	3s	4s	5s	6s	7s	8s
0.00000453	-0.00000140	0.00000049	-0.00000010	0.00000022	-0.00000040	0.00000057	-0.00000120
0.00003521	-0.00001060	0.00000382	-0.00000090	0.00000164	-0.00000270	0.00000495	-0.00000570
0.00018515	-0.00005550	0.00002012	-0.00000480	0.00000920	-0.00001470	0.00002201	-0.00005680
0.00078168	-0.00023440	0.00008479	-0.00002000	0.00003566	-0.00005850	0.00011543	-0.00009070
0.00284001	-0.00085460	0.00030979	-0.00007390	0.00014466	-0.00022940	0.00031762	-0.00101630
0.00919119	-0.00277760	0.00100501	-0.00023660	0.00041229	-0.00068230	0.00144524	-0.00057270
0.02681960	-0.00823310	0.00299257	-0.00071610	0.00143310	-0.00225550	0.00281962	-0.01153910
0.07006655	-0.02215430	0.00805281	-0.00189060	0.00319367	-0.00535390	0.01243187	0.00082352
0.15802289	-0.05364420	0.01974039	-0.00475090	0.00983572	-0.01532300	0.01615043	-0.09448890
0.28468010	-0.11084460	0.04123838	-0.00964650	0.01526096	-0.02636230	0.07299220	0.05848109
0.34784190	-0.17981180	0.06982356	-0.01712800	0.03887358	-0.05910420	0.03281594	-0.52732410
0.21469596	-0.15326130	0.06194171	-0.01396960	0.01102886	-0.02750750	0.20421416	0.66490439
0.03639134	0.15704605	-0.07028210	0.01468508	0.01119258	0.00607137	-0.40665110	-1.95251100
-0.00233900	0.55798352	-0.35206530	0.09575892	-0.27550750	0.41885794	-0.00596390	7.62914130
0.00157585	0.40642734	-0.38303600	0.09291531	-0.02447570	0.18358054	-1.93485000	-11.90154000
-0.00070320	0.05485289	0.26660971	-0.06694350	-0.14028950	-0.34679470	6.13937260	10.92015100
0.00028399	-0.00183770	0.70724401	-0.30576810	1.39136390	-1.98221100	-6.58541100	-6.81439800
-0.00010280	0.00145363	0.31331992	-0.17006770	-0.97588370	2.83069160	2.81404490	2.25475520
0.00002443	-0.00007650	0.00785528	0.74527867	-1.41883500	-1.93940600	-0.03754380	-0.40553220
-0.00001690	0.00023542	-0.00362720	0.39684274	1.71845830	0.89050598	-1.11094600	0.09131826
0.00000599	-0.00004620	0.00107928	0.00528540	-0.15218120	0.33550718	1.05236790	0.07126284

Exponents for p-functions

6268.921 1485.118 481.9146 183.5142 77.19005 34.65178 16.14846 7.710939
3.607154 1.667362 0.739088 0.301326 0.120530 0.048212 0.019285

Contraction matrix for p-function

2p	3p	4p	5p	6p	7p	8p
0.00018739	-0.00006560	0.00002114	-0.00004280	0.00004898	-0.00005110	0.00006531
0.00164431	-0.00057560	0.00018614	-0.00036790	0.00041516	-0.00051760	0.00088093
0.00912076	-0.00322040	0.00103814	-0.00210200	0.00240431	-0.00250870	0.00325738
0.03719649	-0.01327760	0.00430205	-0.00850300	0.00960043	-0.01202570	0.02074716
0.11492608	-0.04237710	0.01371148	-0.02787310	0.03196836	-0.03290190	0.04256650
0.25692935	-0.09833830	0.03212876	-0.06332420	0.07142638	-0.09340990	0.17152030
0.38335937	-0.15697670	0.05144403	-0.10828590	0.12916325	-0.12414110	0.14457122
0.30473539	-0.10861110	0.03596735	-0.07062480	0.10060059	-0.21379300	0.39092669
0.08243436	0.18485066	-0.07642230	0.17670897	-0.34212040	0.83665232	-2.42036800
0.00273624	0.47596476	-0.19422200	0.57084961	-0.83549890	0.34600582	3.06951180
0.00145719	0.40672296	-0.18560820	-0.03570800	1.41643780	-2.12483100	-1.59571400
-0.00032910	0.10212740	0.20105820	-1.25601300	-0.04974320	2.48116440	-0.26908320
0.00022833	-0.00155650	0.68652456	0.40458459	-1.33599800	-1.48346900	1.58828110
-0.00010210	0.00275349	0.26067748	0.58709906	0.97815558	-0.10461050	-2.07075200
0.00003224	-0.00077330	0.00171746	0.00688969	0.25778321	0.82880562	1.29901160

Exponents for d-functions

150.8341 44.99723 16.96088 7.040154 3.103878 1.375896 0.592282 0.242138
0.091284 0.036514

Contraction matrix for d-function

3d	4d	5d	6d	7d	8d
0.00118076	-0.00073170	0.00147093	-0.00198190	0.00293042	-0.00365890
0.00966118	-0.00593860	0.01221628	-0.01633860	0.02400180	-0.03901960
0.04140729	-0.02588100	0.05281196	-0.07298360	0.11269289	-0.15934630
0.12131664	-0.07615180	0.16199100	-0.23037030	0.37251217	-0.67852770
0.24095388	-0.15059490	0.29357778	-0.36806240	0.35632893	0.49893128
0.32484954	-0.16871590	0.23847460	0.09367552	-0.97662770	1.00466890
0.32060330	-0.07194640	-0.23308910	0.77748431	0.00841508	-2.05693700
0.23605297	0.19912700	-0.56415040	-0.16503670	1.20105610	1.97008260
0.09618844	0.30980514	-0.18723120	-0.99837170	-1.46416300	-1.33120200
0.02433110	0.61183718	0.71568988	0.83634879	0.77260007	0.56566185

Exponents for f-functions

7.713900 3.057500 1.211900 0.480300 0.190400 0.075500

Contraction matrix for f-function

4f	5f	6f	7f	8f
0.03904982	-0.09216890	0.20473737	-0.37034720	0.61620681
0.16805148	-0.36090680	0.57457543	-0.44508770	-0.20810040
0.40501469	-0.45590560	-0.17144470	0.97410397	-0.66525620
0.45078646	0.24749491	-0.69725310	-0.50845630	1.33086930
0.22761472	0.51827288	0.45746728	-0.45602290	-1.50397300
0.05358525	0.19289890	0.41964846	0.82091235	0.96516122

Exponents for g-functions

4.362700 1.714800 0.674000 0.264900

Contraction matrix for g-function

5g	6g	7g	8g
0.09899293	0.25622855	0.69331465	-0.88396320
0.37757706	0.43342788	-0.05783130	1.28166040
0.52313249	-0.12143690	-0.79726060	-1.10618400
0.29987327	-0.49414150	0.79855974	0.57647738

Mn atom

Exponents for s-functions

3960805. 593115.5 134976.8 38230.67 12471.54 4501.743 1755.212 727.3039
316.3678 143.0098 66.21805 29.91896 14.30318 6.839451 3.012374 1.418808
0.623624 0.134098 0.065548 0.029584 0.011834

Contraction matrix for s-function

1s	2s	3s	4s	5s	6s	7s	8s
0.00000874	-0.00000260	0.00000097	-0.00000020	0.00000035	-0.00000070	0.00000086	-0.00000100
0.00006798	-0.00002050	0.00000754	-0.00000180	0.00000278	-0.00000580	0.00000625	-0.00000740
0.00035740	-0.00010780	0.00003963	-0.00000940	0.00001423	-0.00002880	0.00003619	-0.00004250
0.00150705	-0.00045530	0.00016747	-0.00003980	0.00006222	-0.00012990	0.00013439	-0.00015830
0.00545756	-0.00165520	0.00060841	-0.00014450	0.00021660	-0.00043510	0.00057351	-0.00067290
0.01749973	-0.00535760	0.00197443	-0.00046990	0.00074071	-0.00155900	0.00152212	-0.00179950
0.04993510	-0.01565660	0.00577534	-0.00137120	0.00203365	-0.00404210	0.00567100	-0.00664250
0.12388065	-0.04095100	0.01523348	-0.00363220	0.00580329	-0.01236980	0.01108897	-0.01320330
0.25049690	-0.09287230	0.03492024	-0.00830490	0.01207351	-0.02356150	0.03703101	-0.04346640
0.35895921	-0.16842450	0.06548772	-0.01572940	0.02604552	-0.05741360	0.04081039	-0.05005720
0.27590166	-0.18918780	0.07702395	-0.01842520	0.02385161	-0.04110840	0.11359020	-0.13396720
0.06596040	0.04616512	-0.01954550	0.00436727	0.00485288	-0.03230330	-0.12393240	0.13606088
-0.00123720	0.51471840	-0.30058260	0.07696053	-0.14730130	0.37768105	-0.10939550	0.27189303
0.00195629	0.50418495	-0.45625350	0.12103875	-0.14594950	0.26094306	-1.22496100	1.47458610
-0.00090710	0.09186063	0.12027269	-0.03966160	-0.03547160	-0.00501200	2.76501310	-5.24583100
0.00039751	-0.00258700	0.72812934	-0.26313840	0.77851701	-2.43265200	-1.14813300	6.31715330
-0.00015930	0.00230804	0.40324535	-0.26294560	-0.08070840	2.70448470	-1.32801400	-3.56602700
0.00006825	-0.00059920	0.01779610	0.43299071	-2.04653000	-0.18863590	4.46581210	1.56932110
-0.00006470	0.00056841	-0.01018190	0.54643391	1.23053960	-1.98447500	-6.15458300	0.05076783
0.00003125	-0.00027370	0.00400366	0.19067476	0.54467078	1.81069230	3.05964190	-2.17485400
-0.00000790	0.00006891	-0.00092400	-0.00022150	0.08868424	-0.15215100	-0.17840820	1.72034160

Exponents for p-functions

7048.271 1669.678 541.8571 206.4295 86.89334 39.06309 18.24725 8.741289
4.119332 1.914804 0.857893 0.354950 0.141980 0.056792 0.022717

Contraction matrix for p-function

2p	3p	4p	5p	6p	7p	8p
0.00017838	-0.00006390	0.00001764	-0.00003520	0.00003827	-0.00005470	0.00005396
0.00156682	-0.00056100	0.00015601	-0.00030590	0.00032349	-0.00051490	0.00080032
0.00871540	-0.00314650	0.00086965	-0.00173610	0.00188621	-0.00269970	0.00268301
0.03571612	-0.01303980	0.00363280	-0.00712210	0.00752973	-0.01202360	0.01893382
0.11121532	-0.04192160	0.01162417	-0.02325950	0.02535636	-0.03607640	0.03485681
0.25160511	-0.09857340	0.02770210	-0.05418060	0.05694881	-0.09331070	0.15977682
0.38123080	-0.15962520	0.04470706	-0.09199500	0.10353017	-0.14166600	0.10213504
0.31029020	-0.11507290	0.03304798	-0.06717710	0.07872645	-0.20868190	0.50439901
0.08812067	0.17705150	-0.06260660	0.13777231	-0.19226940	0.67105097	-2.26790500
0.00359901	0.47737788	-0.16108730	0.46888224	-0.69137230	0.84618017	2.31120110
0.00145213	0.41264499	-0.17690520	0.10208168	0.61487765	-2.43522800	-0.39412520
-0.00033420	0.09948657	0.12091273	-1.04596100	0.92077357	1.93810380	-1.48444000
0.00020601	-0.00159780	0.64429185	-0.06945110	-1.51537700	-0.27090800	2.48652390
-0.00009730	0.00267826	0.35827295	0.68819973	0.36824918	-1.06543600	-2.44813000
0.00003032	-0.00071550	0.01972486	0.18214327	0.70160792	0.99859212	1.28274840

Exponents for d-functions

199.8357 59.72176 22.74772 9.565003 4.285499 1.950975 0.872796 0.375621
0.148009 0.059204

Contraction matrix for d-function

3d	4d	5d	6d	7d	8d
0.00086891	-0.00061410	0.00124531	-0.00144350	0.00222581	-0.00235520
0.00740550	-0.00517230	0.01084024	-0.01243060	0.01898880	-0.03388380
0.03343543	-0.02375470	0.04918383	-0.05807330	0.09232563	-0.11399970
0.10222306	-0.07263280	0.16008166	-0.19535270	0.33205016	-0.69995660
0.21763820	-0.15840410	0.32014185	-0.37455660	0.50021708	0.30744285
0.31388649	-0.20224890	0.26650740	0.04875241	-1.01976300	1.41197250
0.32265141	-0.12237590	-0.28152510	0.78022240	-0.16460500	-2.50979900
0.24897735	0.19545298	-0.57570980	-0.11241070	1.43493640	2.26531440
0.11555483	0.39788322	-0.07034260	-1.10424800	-1.56622400	-1.41125700
0.03978048	0.51436971	0.67373316	0.97098943	0.78798753	0.56051661

Exponents for f-functions

9.541300 3.781800 1.499000 0.594100 0.235500 0.093300

Contraction matrix for f-function

4f	5f	6f	7f	8f
0.03498523	-0.08024420	0.16572786	-0.32048120	0.57319223
0.15976609	-0.34830930	0.57437755	-0.55006500	-0.10360680
0.39648688	-0.47839020	-0.10199290	1.01968910	-0.76003690
0.45515610	0.22560179	-0.75240290	-0.48589200	1.37848740
0.23977597	0.52997079	0.45286160	-0.47359720	-1.51873700
0.05663872	0.19214405	0.43555178	0.80734613	0.97413210

Exponents for g-functions

5.396300 2.121000 0.833700 0.327700

Contraction matrix for g-function

5g	6g	7g	8g
0.08170016	-0.30311870	0.64839085	1.01264000
0.34540706	-0.60667150	0.02836825	-1.40696700
0.52930680	0.11185796	-0.84813560	1.17717960
0.34012540	0.65216468	0.79339487	-0.60317130

Fe atom

Exponents for s-functions

4316265.	646342.4	147089.7	41661.52	13590.77	4905.750	1912.746	792.6043
344.8065	155.8999	72.23091	32.72506	15.66762	7.503483	3.312223	1.558471
0.683914	0.146757	0.070583	0.031449	0.012580			

Contraction matrix for s-function

1s	2s	3s	4s	5s	6s	7s	8s
0.00000869	-0.00000260	0.00000085	-0.00000020	0.00000035	-0.00000070	0.00000081	-0.00000100
0.00006755	-0.00002020	0.00000660	-0.00000180	0.00000273	-0.00000570	0.00000587	-0.00000700
0.00035514	-0.00010650	0.00003471	-0.00000940	0.00001401	-0.00002870	0.00003390	-0.00004070
0.00149758	-0.00044950	0.00014670	-0.00003970	0.00006113	-0.00012810	0.00012625	-0.00015070
0.00542368	-0.00163470	0.00053293	-0.00014380	0.00021326	-0.00043330	0.00053681	-0.00064370
0.01739498	-0.00529340	0.00173043	-0.00046800	0.00072769	-0.00153520	0.00143200	-0.00171170
0.04966288	-0.01548620	0.00506478	-0.00136580	0.00200474	-0.00403960	0.00530524	-0.00636670
0.12335573	-0.04059850	0.01338915	-0.00362260	0.00570613	-0.01216330	0.01046250	-0.01252690
0.25002288	-0.09250400	0.03080255	-0.00829640	0.01195172	-0.02374360	0.03466553	-0.04179840
0.35990369	-0.16905000	0.05821825	-0.01577060	0.02569755	-0.05631410	0.03881305	-0.04704460
0.27899279	-0.19228400	0.06938655	-0.01858720	0.02403849	-0.04348580	0.10640664	-0.13008460
0.06684859	0.04532080	-0.01668270	0.00410355	0.00461023	-0.02746690	-0.11425850	0.13536565
-0.00530450	0.52919124	-0.28071900	0.07759402	-0.14507200	0.35854227	-0.08055550	0.16628852
-0.00219420	0.52613699	-0.43502950	0.12054486	-0.14701850	0.29723727	-1.22133900	1.70571700
-0.00156720	0.08634042	0.13102653	-0.04091310	-0.02284040	-0.05560670	2.62540500	-5.39768900
0.00070059	-0.03666660	0.72871523	-0.26246710	0.74958123	-2.35786300	-0.96387930	6.18158200
-0.00001330	-0.01644200	0.39852762	-0.25768170	-0.07729630	2.62219710	-1.39819200	-3.26150500
0.00007584	-0.00138020	0.01733967	0.43339758	-1.92800900	-0.09696180	4.14947270	0.90032804
-0.00006820	0.00098672	-0.00966160	0.54662556	1.06569450	-1.99104900	-5.40974900	0.99723153
0.00003286	-0.00043850	0.00385198	0.18747114	0.60856319	1.72090500	2.35644950	-2.75224800
-0.00000840	0.00010903	-0.00090970	0.00270482	0.09196064	-0.10051950	0.12730233	1.86209100

Exponents for p-functions

7721.489	1829.126	593.6280	226.2054	95.26145	42.85920	20.04971	9.620885
4.541371	2.113500	0.947201	0.391243	0.156497	0.062599	0.025040	

Contraction matrix for p-function

2p	3p	4p	5p	6p	7p	8p
0.00017940	-0.00005530	0.00001827	-0.00003460	0.00003991	-0.00005450	0.00006248
0.00157653	-0.00048580	0.00016138	-0.00030210	0.00034847	-0.00056600	0.00080567
0.00878209	-0.00273220	0.00090232	-0.00170710	0.00197164	-0.00269790	0.00309858
0.03607769	-0.01136920	0.00377265	-0.00706390	0.00815407	-0.01330770	0.01915800
0.11272928	-0.03684800	0.01213515	-0.02300820	0.02661734	-0.03603850	0.04130870
0.25609280	-0.08750780	0.02898861	-0.05424340	0.06262644	-0.10609660	0.16004548
0.38909425	-0.14330720	0.04708145	-0.09111680	0.10665344	-0.13086550	0.14569937
0.31513025	-0.09976090	0.03395627	-0.06773050	0.09339326	-0.27286100	0.46212609
0.07892748	0.18578570	-0.06721070	0.14812742	-0.23558910	0.87476561	-2.46528000
-0.01959520	0.47909012	-0.17287650	0.46037011	-0.68343630	0.58764224	2.86141310
-0.01837930	0.40815100	-0.16620750	0.03915707	0.63114560	-2.29424000	-1.06044600
-0.00505370	0.09750333	0.14589742	-0.91332880	0.89696110	1.92836100	-0.96776360
0.00027944	-0.00155180	0.61178551	-0.15696580	-1.38206000	-0.28128930	2.16152290
-0.00022310	0.00263138	0.35925888	0.64005451	0.16944946	-1.03870800	-2.25377400
0.00006381	-0.00070260	0.04073564	0.28359879	0.76562060	0.93879985	1.18630030

Exponents for d-functions

217.3688 64.99976 24.77314 10.43614 4.679653 2.125622 0.945242 0.402685
0.156651 0.062660

Contraction matrix for d-function

3d	4d	5d	6d	7d	8d
0.00090859	-0.00072370	0.00125891	-0.00161930	0.00209633	-0.00189650
0.00775703	-0.00612900	0.01092111	-0.01394030	0.01981104	-0.03534070
0.03509608	-0.02813160	0.04980135	-0.06542380	0.08767694	-0.09471480
0.10690639	-0.08623050	0.16077486	-0.22105340	0.35342277	-0.75104540
0.22354778	-0.18379140	0.32346144	-0.41836770	0.46566332	0.49963991
0.31482281	-0.22300410	0.24231987	0.18487331	-1.18418500	1.12575900
0.31706314	-0.09948400	-0.34487070	0.78688109	0.22287923	-2.31379000
0.24533968	0.24250462	-0.54964040	-0.34311580	1.12168860	2.24451090
0.11980182	0.42175965	0.03680085	-0.87041820	-1.51115100	-1.50100200
0.04248366	0.43580570	0.65109526	0.90154758	0.84889270	0.63294990

Exponents for f-functions

11.27490 4.469000 1.771300 0.702100 0.278300 0.110300

Contraction matrix for f-function

4f	5f	6f	7f	8f
0.03258762	-0.07378730	0.15048476	-0.32457570	0.57593078
0.15612854	-0.35717230	0.61759584	-0.57365240	-0.17835400
0.40094745	-0.48333090	-0.15246510	1.12688610	-0.62605140
0.45321069	0.23975434	-0.74400380	-0.68332020	1.27788470
0.23899828	0.52100979	0.50331812	-0.28130750	-1.52637500
0.05966161	0.18732479	0.38453654	0.71794260	1.04559300

Exponents for g-functions

6.376800 2.506400 0.985100 0.387200

Contraction matrix for g-function

5g	6g	7g	8g
-0.07181810	-0.29275760	0.59985778	-0.77526150
-0.35672040	-0.60349290	0.01174938	1.06958310
-0.51716410	0.16179085	-0.76182430	-0.90652520
-0.29398480	0.62253897	0.74342225	0.47321069

Co atom

Exponents for s-functions

4676708. 700317.2 159373.0 45140.67 14725.75 5315.448 2072.498 858.8231
373.6437 168.9682 78.31971 35.53724 17.04735 8.175534 3.611578 1.697468
0.743636 0.158325 0.075009 0.033093 0.013237

Contraction matrix for s-function

1s	2s	3s	4s	5s	6s	7s	8s
0.00000862	-0.00000260	0.00000098	-0.00000020	0.00000044	-0.00000070	0.00000067	-0.00000100
0.00006703	-0.00002040	0.00000762	-0.00000170	0.00000347	-0.00000550	0.00000496	-0.00000730
0.00035243	-0.00010750	0.00004004	-0.00000890	0.00001770	-0.00002790	0.00002820	-0.00004220
0.00148616	-0.00045380	0.00016923	-0.00003790	0.00007793	-0.00012220	0.00010728	-0.00015810
0.00538250	-0.00165000	0.00061484	-0.00013730	0.00026886	-0.00042470	0.00044435	-0.00066600
0.01726474	-0.00534190	0.00199594	-0.00044680	0.00093001	-0.00145680	0.00122610	-0.00180440
0.04930401	-0.01562390	0.00584290	-0.00130530	0.00252087	-0.00399180	0.00436638	-0.00656500
0.12253550	-0.04092880	0.01543990	-0.00346240	0.00732687	-0.01146260	0.00906970	-0.01329910
0.24860382	-0.09312740	0.03551543	-0.00794870	0.01498118	-0.02386790	0.02829761	-0.04290580
0.35837905	-0.16965500	0.06696125	-0.01512480	0.03342105	-0.05222480	0.03494891	-0.05088960
0.27841055	-0.19245090	0.07961678	-0.01794030	0.02931208	-0.04836930	0.08403478	-0.13104100
0.06785877	0.04347139	-0.01872100	0.00395775	0.00996532	-0.01193170	-0.08208740	0.13014281
-0.00115750	0.51737043	-0.31042280	0.07479185	-0.19610040	0.30946349	-0.08532520	0.14081641
0.00192304	0.50464645	-0.46054150	0.11490079	-0.17626490	0.39054298	-0.99683840	1.90270160
-0.00088960	0.09201286	0.13587243	-0.04223380	-0.03861910	-0.28532140	2.06965250	-5.66431000
0.00038521	-0.00234550	0.73020264	-0.24686420	1.08415130	-2.05903400	-0.52725830	6.13287560
-0.00015140	0.00224229	0.39330008	-0.24198820	-0.42626710	2.57812780	-1.41835500	-2.89561700
0.00006126	-0.00053850	0.01679521	0.37226088	-1.91956200	-0.61815020	3.49227510	-0.04434280
-0.00005670	0.00050121	-0.00930160	0.56759555	1.37322520	-1.30766700	-4.08162000	2.30677710
0.00002784	-0.00024560	0.00375185	0.21737935	0.27764584	1.32262520	1.06531310	-3.40497900
-0.00000730	0.00006422	-0.00090600	0.00352473	0.13569011	0.10033553	0.75922506	1.87662620

Exponents for p-functions

8421.842 1995.000 647.4855 246.7795 103.9689 46.81052 21.92703 10.53715
4.980678 2.319824 1.039609 0.428921 0.171568 0.068627 0.027451

Contraction matrix for p-function

2p	3p	4p	5p	6p	7p	8p
0.00017491	-0.00006400	0.00001883	-0.00003830	0.00003985	-0.00005370	0.00006911
0.00153773	-0.00056240	0.00016619	-0.00033620	0.00035808	-0.00059270	0.00077512
0.00857464	-0.00316260	0.00093163	-0.00189450	0.00197283	-0.00266360	0.00343876
0.03528967	-0.01316530	0.00389907	-0.00789320	0.00841770	-0.01400160	0.01847170
0.11048562	-0.04258770	0.01259829	-0.02567960	0.02674396	-0.03561910	0.04674610
0.25156273	-0.10095360	0.03016538	-0.06112280	0.06551271	-0.11341290	0.15132134
0.38208843	-0.16409550	0.04922893	-0.10201960	0.10577100	-0.12402180	0.19630074
0.30945671	-0.11461140	0.03475151	-0.07728850	0.10794079	-0.31891370	0.38612866
0.08757280	0.18585070	-0.07188090	0.18257783	-0.29257760	1.05617000	-2.54420900
0.00382659	0.48071243	-0.18284560	0.51785755	-0.65412750	0.30098162	3.24317070
0.00151229	0.40513114	-0.15347360	-0.05554230	0.76754227	-2.12182000	-1.60291700
-0.00028530	0.09651019	0.15599366	-0.93997170	0.67550465	1.98305320	-0.49723420
0.00020138	-0.00155780	0.59752058	-0.05577780	-1.32197400	-0.43478180	1.84870480
-0.00009280	0.00261271	0.36419424	0.61553966	0.22022438	-0.93174570	-2.08922500
0.00002894	-0.00069720	0.04018451	0.23599688	0.76020008	0.91738297	1.13243920

Exponents for d-functions

237.5928 71.08881 27.11903 11.44826 5.139542 2.332694 1.034030 0.437899
0.168963 0.067585

Contraction matrix for d-function

3d	4d	5d	6d	7d	8d
0.00092701	-0.00084720	0.00120627	-0.00171410	0.00205156	-0.00169470
0.00793865	-0.00721600	0.01046468	-0.01490830	0.02182970	-0.03663780
0.03606409	-0.03323240	0.04802992	-0.06950530	0.08697792	-0.08637030
0.10968155	-0.10231590	0.15456282	-0.23750360	0.39857288	-0.79645660
0.22645775	-0.21395030	0.31068293	-0.45108020	0.41507497	0.71535861
0.31367762	-0.24295660	0.20905209	0.26005331	-1.33335300	0.78568134
0.31243547	-0.06620310	-0.35934790	0.80108242	0.58326826	-2.06742900
0.24628330	0.29378188	-0.51288440	-0.47137080	0.79678895	2.20838690
0.12633171	0.41673019	0.07429744	-0.71721040	-1.37039400	-1.60610200
0.03900343	0.37130918	0.68550193	0.82498909	0.82987168	0.72071882

Exponents for f-functions

12.84030 5.089400 2.017200 0.799600 0.316900 0.125600

Contraction matrix for f-function

4f	5f	6f	7f	8f
0.03236906	-0.07453890	0.14591657	-0.33232960	0.60103182
0.15788753	-0.37667740	0.63322144	-0.57727820	-0.26821590
0.41073331	-0.47481310	-0.20378170	1.18471290	-0.50092990
0.45170693	0.27648132	-0.71363400	-0.80309550	1.18335480
0.22855470	0.50315310	0.53295503	-0.15528800	-1.50650700
0.05597529	0.17676002	0.36751161	0.65459913	1.07372280

Exponents for g-functions

7.262100 2.854400 1.121900 0.441000

Contraction matrix for g-function

5g	6g	7g	8g
-0.05941470	0.31279874	-0.69654100	0.99927841
-0.34983510	0.62959057	0.02955342	-1.38401800
-0.50665640	-0.21050110	0.83710582	1.19428590
-0.27189220	-0.60009940	-0.86665030	-0.63699310

Ni atom

Exponents for s-functions

5048010.	755918.1	172026.2	48724.57	15894.89	5737.468	2237.051	927.0302
403.3461	182.4282	84.58917	38.42293	18.46879	8.868190	3.918870	1.839853
0.804663	0.169846	0.079370	0.034700	0.013880			

Contraction matrix for s-function

1s	2s	3s	4s	5s	6s	7s	8s
0.00000859	-0.00000260	0.00000098	-0.00000020	0.00000045	-0.00000070	0.00000086	-0.00000110
0.00006676	-0.00002040	0.00000766	-0.00000170	0.00000355	-0.00000560	0.00000627	-0.00000900
0.00035102	-0.00010760	0.00004028	-0.00000890	0.00001809	-0.00002900	0.00003641	-0.00004420
0.00148024	-0.00045410	0.00017022	-0.00003750	0.00007957	-0.00012620	0.00013477	-0.00020330
0.00536128	-0.00165120	0.00061846	-0.00013620	0.00027478	-0.00044210	0.00057704	-0.00066150
0.01719845	-0.00534630	0.00200801	-0.00044320	0.00094963	-0.00150170	0.00152697	-0.00246440
0.04912754	-0.01564110	0.00587968	-0.00129480	0.00257818	-0.00416600	0.00571489	-0.00610190
0.12216703	-0.04099880	0.01554882	-0.00343810	0.00748691	-0.01179840	0.01115038	-0.01987330
0.24810883	-0.09339290	0.03580902	-0.00790000	0.01536155	-0.02506610	0.03757780	-0.03554580
0.35826234	-0.17040030	0.06764847	-0.01506930	0.03423588	-0.05358670	0.04129612	-0.09667710
0.27910233	-0.19374000	0.08065478	-0.01791070	0.03032359	-0.05236170	0.11727594	-0.05833300
0.06830145	0.04354049	-0.01892620	0.00392193	0.00992020	-0.00783680	-0.12728780	-0.09347020
-0.00118350	0.51950274	-0.31545840	0.07504682	-0.20137340	0.31051000	-0.05821800	0.75915216
0.00191625	0.50372386	-0.46110780	0.11324246	-0.18303880	0.44043500	-1.49958200	1.30065970
-0.00088450	0.09139081	0.14489869	-0.04393570	-0.02175280	-0.39622500	3.49240710	-6.12425400
0.00038171	-0.00227360	0.73044873	-0.24438380	1.09749980	-2.00536500	-2.19076500	8.02386720
-0.00014830	0.00220816	0.38778553	-0.23485420	-0.46797710	2.63047080	-0.54559010	-5.04603200
0.00005854	-0.00051330	0.01622800	0.36865540	-1.85498200	-0.80559900	3.59606440	3.82795330
-0.00005370	0.00047484	-0.00891480	0.57243374	1.32221160	-1.12092700	-5.23758600	-3.83962400
0.00002661	-0.00023480	0.00364398	0.21592434	0.29731170	1.36863090	2.76688540	1.38030780
-0.00000710	0.00006236	-0.00089650	0.00028770	0.11571621	-0.01542830	-0.16839860	0.13715752

Exponents for p-functions

9148.796	2167.171	703.3857	268.1342	113.0078	50.91339	23.87740	11.48924
5.436884	2.533837	1.135309	0.467891	0.187156	0.074862	0.029945	

Contraction matrix for p-function

2p	3p	4p	5p	6p	7p	8p
0.00017357	-0.00006400	0.00001962	-0.00004290	0.00004465	-0.00004950	0.00007492
0.00152657	-0.00056290	0.00017312	-0.00037840	0.00042103	-0.00057910	0.00072143
0.00852129	-0.00316920	0.00097223	-0.00212800	0.00221461	-0.00245930	0.00372753
0.03513410	-0.01321830	0.00407438	-0.00891460	0.00994005	-0.01374210	0.01723879
0.11025027	-0.04287100	0.01321023	-0.02898040	0.03007484	-0.03294680	0.05160920
0.25168061	-0.10196740	0.03171293	-0.06949990	0.07851525	-0.11296890	0.13785585
0.38250457	-0.16592570	0.05192371	-0.11563460	0.11657619	-0.11265270	0.24807384
0.30893669	-0.11411670	0.03605129	-0.09018240	0.15823133	-0.33933110	0.26394793
0.08722897	0.18968805	-0.07725320	0.22442351	-0.46936450	1.23179260	-2.46405900
0.00392062	0.48171716	-0.19414970	0.59429596	-0.66531670	-0.17715500	3.41213180
0.00153919	0.40202033	-0.14772330	-0.16225690	1.24799050	-1.71378400	-2.01147200
-0.00026550	0.09551929	0.17187531	-1.03404300	0.06088248	2.09813720	-0.04219670
0.00019937	-0.00154890	0.60426626	0.15003199	-1.22401600	-0.94192350	1.52019810
-0.00009090	0.00258826	0.35544105	0.61273403	0.59511470	-0.58235760	-1.98531700
0.00002837	-0.00069060	0.02125057	0.09486061	0.50804733	0.95110917	1.17899740

Exponents for d-functions

258.8667 77.49604 29.58972 12.51527 5.624468 2.551303 1.128060 0.475373
0.182128 0.072851

Contraction matrix for d-function

3d	4d	5d	6d	7d	8d
0.00095252	-0.00092610	0.00123665	-0.00177870	0.00201937	-0.00172550
0.00817994	-0.00792440	0.01074816	-0.01571750	0.02331777	-0.03742090
0.03730818	-0.03662670	0.04958935	-0.07273200	0.08728668	-0.08903630
0.11328720	-0.11305370	0.15987740	-0.25411760	0.43666374	-0.83723450
0.23147573	-0.23263250	0.31923224	-0.46309120	0.33746420	0.91659382
0.31613597	-0.24935030	0.17919012	0.36602757	-1.39216000	0.46290674
0.31084320	-0.03532690	-0.41307200	0.75610368	0.84327465	-1.80347100
0.24210237	0.32694740	-0.47494000	-0.60471820	0.52596860	2.11577060
0.12298386	0.41969843	0.17118431	-0.55810490	-1.25860300	-1.65446300
0.03516757	0.31817544	0.63979396	0.78181900	0.83751331	0.78531829

Exponents for f-functions

14.21560 5.634500 2.233300 0.885200 0.350900 0.139100

Contraction matrix for f-function

4f	5f	6f	7f	8f
0.03449541	-0.07796490	0.15327657	-0.35833460	0.66710855
0.16793185	-0.39359110	0.64450372	-0.54220910	-0.41954900
0.42354035	-0.45649420	-0.26415270	1.21175540	-0.31672930
0.44325993	0.31147596	-0.67746640	-0.91050440	1.03355960
0.21579087	0.49201071	0.56328287	-0.03171330	-1.43951900
0.05136224	0.16482549	0.34102044	0.59642445	1.07901770

Exponents for g-functions

8.039900 3.160100 1.242100 0.488200

Contraction matrix for g-function

5g	6g	7g	8g
0.06441670	0.23374941	-0.62261940	-0.53455850
0.39422643	0.43638821	0.07673291	0.75288227
0.54552056	-0.18016960	0.68610126	-0.66399000
0.26876227	-0.40409970	-0.75812330	0.36172785

Cu atom

Exponents for s-functions

9148883. 1369956. 311782.6 88318.80 28815.53 10403.46 4057.791 1682.974
733.7543 333.2677 156.4338 74.69721 33.32262 16.62237 8.208260 3.609400
1.683449 0.733757 0.110207 0.038786 0.015514

Contraction matrix for s-function

1s	2s	3s	4s	5s	6s	7s	8s
0.00000446	-0.00000140	0.00000051	-0.00000010	0.00000023	-0.00000040	0.00000057	-0.00000040
0.00003469	-0.00001070	0.00000399	-0.00000080	0.00000168	-0.00000290	0.00000453	-0.00000230
0.00018239	-0.00005610	0.00002101	-0.00000450	0.00000943	-0.00001540	0.00002305	-0.00002080
0.00077001	-0.00023700	0.00008857	-0.00001870	0.00003654	-0.00006340	0.00010178	-0.00004030
0.00279764	-0.00086380	0.00032360	-0.00006950	0.00014823	-0.00023880	0.00035130	-0.00036510
0.00905596	-0.00280830	0.00105019	-0.00022030	0.00042258	-0.00074630	0.00122040	-0.00031450
0.02644076	-0.00832980	0.00312936	-0.00067530	0.00146999	-0.00232870	0.00335444	-0.00407660
0.06918041	-0.02245400	0.00843864	-0.00176120	0.00328324	-0.00594890	0.00999049	-0.00081870
0.15647987	-0.05456570	0.02077023	-0.00452220	0.01014895	-0.01569050	0.02190012	-0.03274590
0.28318803	-0.11339210	0.04369710	-0.00904300	0.01588483	-0.03044290	0.05407196	0.01311414
0.34834744	-0.18512600	0.07460186	-0.01670180	0.04068724	-0.05907700	0.07563410	-0.17835700
0.21729716	-0.15873810	0.06696043	-0.01288420	0.01192632	-0.04167230	0.10389402	0.21183133
0.03723951	0.16600910	-0.07944260	0.01333561	0.01022034	0.03684613	-0.14016800	-0.65625550
-0.00258070	0.56808838	-0.38487520	0.09790588	-0.29168770	0.38295335	-0.51266650	2.25317130
0.00156037	0.39505047	-0.37246620	0.07249738	-0.02332030	0.36386434	-1.35039800	-2.36524200
-0.00067990	0.05193438	0.31938583	-0.06056550	-0.06553060	-0.83790950	5.69338790	-0.04477630
0.00026190	-0.00105780	0.70435862	-0.29718440	1.32294460	-1.33277500	-6.48947600	2.02007030
-0.00008680	0.00123941	0.27996239	-0.10637610	-1.05594100	2.35852380	2.95092940	-1.74255400
0.00001768	-0.00011970	0.00579101	0.79532714	-1.23087800	-1.82846500	-0.33495160	1.87734720
-0.00001290	0.00008857	-0.00266520	0.30758247	1.65313940	1.20324560	-0.67362260	-3.24805400
0.00000485	-0.00003400	0.00095219	0.01483550	-0.20155160	0.04477909	0.84894095	2.28299140

Exponents for p-functions

9713.253 2300.889 746.7706 284.6806 119.9999 54.07386 25.37321 12.20962
5.757421 2.673402 1.186835 0.481593 0.192637 0.077055 0.030822

Contraction matrix for p-function

2p	3p	4p	5p	6p	7p	8p
0.00017835	-0.00006580	0.00002261	-0.00004700	0.00004948	-0.00004950	0.00008517
0.00156858	-0.00057820	0.00019824	-0.00041560	0.00048665	-0.00057500	0.00066685
0.00875434	-0.00325660	0.00112044	-0.00232770	0.00245539	-0.00245860	0.00423607
0.03608107	-0.01357800	0.00466570	-0.00979250	0.01150309	-0.01366260	0.01591961
0.11299149	-0.04399850	0.01521575	-0.03165890	0.03321540	-0.03298940	0.05943582
0.25664086	-0.10418090	0.03608110	-0.07599310	0.09109846	-0.11166080	0.12028889
0.38518747	-0.16768020	0.05925497	-0.12447490	0.12482896	-0.11756650	0.32080284
0.30288080	-0.10714430	0.03709927	-0.09551570	0.19632255	-0.31552630	0.05813442
0.08164476	0.20500459	-0.09339450	0.27896165	-0.67869170	1.38184500	-2.24967500
0.00338807	0.48293963	-0.22900240	0.62767588	-0.49863740	-0.71329270	3.46521320
0.00157696	0.39022329	-0.12323690	-0.32615190	1.47981130	-1.10903600	-2.38153200
-0.00022080	0.09437742	0.23118244	-1.00099000	-0.46342030	1.92129990	0.45280515
0.00021195	-0.00154480	0.60241087	0.33267140	-0.93055400	-1.20000300	1.12676700
-0.00008950	0.00264387	0.30652419	0.54404043	0.69217014	-0.31796600	-1.81213600
0.00002842	-0.00072740	0.01307756	0.05542395	0.36845722	0.93548985	1.16594150

Exponents for d-functions

249.3497 74.63837 28.37641 11.94893 5.317646 2.364417 1.012386 0.406773
0.147331 0.058932

Contraction matrix for d-function

3d	4d	5d	6d	7d	8d
0.00126396	-0.00155310	0.00186923	-0.00233540	0.00250414	-0.00570250
0.01063885	-0.01311300	0.01612505	-0.02290710	0.03579454	-0.03491120
0.04720950	-0.05895500	0.07240919	-0.09394700	0.11182291	-0.24945710
0.13793658	-0.17782060	0.23628626	-0.37675940	0.69073690	-0.91310100
0.26266752	-0.32716810	0.38296124	-0.32713530	-0.47089260	2.14261590
0.33241634	-0.24099740	-0.16793750	0.95009693	-0.93387540	-1.98874600
0.30779901	0.18960651	-0.68246030	-0.04648790	1.66534460	0.90197359
0.21664096	0.50340449	0.08869927	-0.88560220	-1.12144000	0.19401292
0.08407717	0.30703593	0.60278641	0.54282853	0.03505111	-0.91730500
0.00504377	0.03253971	0.14438102	0.32722396	0.52780363	0.85028700

Exponents for f-functions

15.43330 6.117200 2.424600 0.961000 0.380900 0.151000

Contraction matrix for f-function

4f	5f	6f	7f	8f
0.03901817	-0.08437670	0.16168310	-0.38550350	0.77156950
0.18754340	-0.41437330	0.63482614	-0.50202000	-0.60942220
0.44621247	-0.41723570	-0.31075760	1.20543550	-0.11620230
0.42647410	0.35876802	-0.63188760	-0.94520500	0.87171529
0.19155912	0.47774575	0.56734018	0.01430769	-1.33311800
0.04165182	0.15423758	0.35009788	0.57235196	1.03088110

Exponents for g-functions

8.728600 3.430800 1.348500 0.530000

Contraction matrix for g-function

5g	6g	7g	8g
0.06945941	-0.37915410	0.74921737	-0.95084290
0.43698748	-0.59662630	-0.21698810	1.38380490
0.54147510	0.36137813	-0.67135610	-1.27838100
0.21743974	0.51267837	0.87570242	0.73274226

Zn atom

Exponents for s-functions

5820021.	871523.4	198335.0	56176.31	18325.82	6614.955	2579.199	1068.849
465.1045	210.4130	97.61629	44.38020	21.42308	10.30891	4.553645	2.132821
0.929697	0.192147	0.087595	0.037702	0.015081			

Contraction matrix for s-function

1s	2s	3s	4s	5s	6s	7s	8s
0.00000855	-0.00000260	0.00000100	-0.00000020	0.00000034	-0.00000070	0.00000085	-0.00000110
0.00006647	-0.00002050	0.00000775	-0.00000170	0.00000267	-0.00000590	0.00000622	-0.00000870
0.00034950	-0.00010800	0.00004076	-0.00000910	0.00001374	-0.00003010	0.00003546	-0.00004410
0.00147383	-0.00045590	0.00017228	-0.00003860	0.00005977	-0.00013300	0.00013451	-0.00019630
0.00533833	-0.00165780	0.00062593	-0.00013990	0.00020945	-0.00045660	0.00055909	-0.00066710
0.01712708	-0.00536850	0.00203291	-0.00045590	0.00071124	-0.00158960	0.00153646	-0.00235740
0.04894085	-0.01571240	0.00595456	-0.00133090	0.00197453	-0.00428140	0.00550532	-0.00624260
0.12179340	-0.04122570	0.01576693	-0.00354270	0.00559086	-0.01258460	0.01138318	-0.01879910
0.24765887	-0.09406410	0.03637539	-0.00814300	0.01189243	-0.02556620	0.03591618	-0.03741000
0.35824324	-0.17199640	0.06892730	-0.01561320	0.02539154	-0.05827530	0.04414834	-0.08931210
0.27981702	-0.19585000	0.08237327	-0.01853580	0.02475171	-0.05034830	0.10815451	-0.07339220
0.06857579	0.04532437	-0.02009310	0.00413203	0.00312857	-0.02002860	-0.10561150	-0.05598320
-0.00131270	0.52445222	-0.32530080	0.07898844	-0.14558310	0.36143707	-0.11899220	0.69639944
0.00191627	0.50060099	-0.46020860	0.11413160	-0.14872710	0.36964339	-1.30557700	1.27778720
-0.00087910	0.08947690	0.16339078	-0.04867670	0.03235682	-0.27535280	3.03037740	-5.79535100
0.00037780	-0.00217430	0.72999364	-0.25153870	0.66517083	-2.09870600	-1.56620700	7.35018950
-0.00014330	0.00213747	0.37667470	-0.23375600	-0.09666510	2.46453010	-0.95620310	-4.35362100
0.00005411	-0.00046910	0.01508169	0.43801715	-1.65751300	-0.10951070	3.60138580	2.53567550
-0.00004910	0.00043030	-0.00822400	0.55217385	0.75108879	-1.76128800	-4.88296500	-1.74265200
0.00002471	-0.00021650	0.00344838	0.16985732	0.73491842	1.53073600	2.36980120	-0.38523160
-0.00000670	0.00005905	-0.00087620	0.00249733	0.07323193	-0.07747830	-0.03405900	0.89112169

Exponents for p-functions

10684.58	2530.903	821.4820	313.2522	132.1094	59.58751	28.00399	13.50425
6.401881	2.985769	1.336902	0.549961	0.219984	0.087994	0.035198	

Contraction matrix for p-function

2p	3p	4p	5p	6p	7p	8p
0.00017142	-0.00006410	0.00001678	-0.00003600	0.00004200	-0.00005340	0.00007282
0.00150872	-0.00056380	0.00014822	-0.00031830	0.00037878	-0.00055550	0.00073032
0.00843682	-0.00318040	0.00083377	-0.00178740	0.00208761	-0.00265780	0.00363325
0.03489609	-0.01331030	0.00350653	-0.00753410	0.00897607	-0.01321770	0.01751552
0.10993586	-0.04336340	0.01141348	-0.02449690	0.02862580	-0.03621650	0.05048068
0.25205643	-0.10373190	0.02756400	-0.05930450	0.07089196	-0.10721320	0.14163669
0.38327840	-0.16900020	0.04514618	-0.09830750	0.11494808	-0.13684650	0.23802269
0.30782595	-0.11286720	0.03039094	-0.07579650	0.11746305	-0.28150200	0.29538670
0.08651147	0.19638977	-0.06646510	0.18815812	-0.33659140	1.01539170	-2.38916100
0.00408215	0.48297949	-0.16153150	0.46903915	-0.64064250	0.25916244	2.97771040
0.00158570	0.39676171	-0.13642790	-0.03999370	0.74529538	-1.95908200	-1.23898700
-0.00023230	0.09411042	0.11657871	-0.81822090	0.70157209	1.69317510	-0.86403040
0.00019582	-0.00153060	0.54683596	-0.22067370	-1.15028400	-0.04944150	2.10218020
-0.00008780	0.00254793	0.41490791	0.53820718	-0.05687820	-1.23518600	-2.15106500
0.00002741	-0.00067970	0.07954381	0.36284882	0.84283006	1.00611850	1.08537290

Exponents for d-functions

305.0115 91.40003 34.95829 14.83697 6.680748 3.029026 1.334839 0.558608
0.211743 0.084697

Contraction matrix for d-function

3d	4d	5d	6d	7d	8d
0.00102503	-0.00138600	0.00152391	-0.00179460	0.00178499	-0.00182560
0.00884669	-0.01201630	0.01363618	-0.01752960	0.02611879	-0.03485880
0.04068306	-0.05596400	0.06257503	-0.07605900	0.08325371	-0.09373970
0.12323994	-0.17605410	0.21698562	-0.30775460	0.52970352	-0.83688540
0.24793304	-0.34913890	0.40159133	-0.40478260	-0.04624890	1.19455540
0.33086676	-0.27309330	-0.16958970	0.86315706	-1.22731000	-0.16757340
0.31736352	0.21104719	-0.70399180	0.12409936	1.44555740	-1.14560800
0.22301484	0.51804313	0.13084194	-0.93622630	-0.44625940	1.79902380
0.08092209	0.26108135	0.59401254	0.39627951	-0.72163950	-1.78877200
0.00354324	0.02024492	0.18018634	0.51834504	0.92500468	1.06945330

Exponents for f-functions

16.57440 6.569500 2.603900 1.032100 0.409100 0.162100

Contraction matrix for f-function

4f	5f	6f	7f	8f
0.04557151	-0.09412220	0.18733416	-0.42218380	0.74333209
0.21536031	-0.43664550	0.65450531	-0.39617700	-0.62344920
0.46964768	-0.37405330	-0.44338020	1.17297040	-0.04339050
0.40406899	0.42861552	-0.54524920	-1.07698300	0.77437899
0.16303648	0.47241447	0.66776628	0.21013259	-1.28830900
0.02361615	0.09871225	0.24004604	0.51814434	1.09101730

Exponents for g-functions

9.374000 3.684400 1.448200 0.569200

Contraction matrix for g-function

5g	6g	7g	8g
-0.09254470	0.42041748	-0.75813960	0.92394269
-0.47648320	0.55152456	0.30277636	-1.37279600
-0.50522730	-0.42970440	0.60463461	1.30448750
-0.19574530	-0.47388660	-0.87730740	-0.76219370