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Abstract

Energy optimized, near Hartree–Fock quality Gaussian basis sets ranging in size from (17s12p) to (20s15p) are presented for the ground states of the second-row atoms and for Na (^2P), Na^+, Na^-, Mg (^3P), P^-, S^-, and Cl^-. In addition, optimized supplementary functions are given for the ground state basis sets to describe the negative ions, and the excited Na (^2P) and Mg (^3P) atomic states. The ratios of successive orbital exponents describing the inner part of the 1s and 2p orbitals are found to be nearly independent of both nuclear charge and basis set size. This provides a method of obtaining good starting estimates for other basis set optimizations.

Introduction

Recent studies have demonstrated that approximate solutions of the n-particle problem, particularly multireference singles plus doubles configuration interaction (MRCI), are in excellent agreement with the full CI results [1]. This suggests that incompleteness of the 1-particle basis (the basis set) is a major factor limiting the accuracy of current electronic structure calculations. Recent MRCI calculations on a variety of systems (e.g. N_2 [2], OH [3], and CH_2 [4]) corroborate this conclusion and also show that excellent results are obtained by employing large primitive valence and polarization Gaussian type orbital (GTO) basis sets. For example, Langhoff et al. [2], using a (13s8p6d4f2g) GTO primitive set contracted to [5s4p3d2f1g], obtained a D_e of 5.18 eV for O_2, which is only 0.04 eV less than the accurate experimental value. Large, primitive basis sets can be routinely used owing to the development of new generations of vectorized integral codes that can efficiently treat generalized contractions [5] and to procedures for contracting these basis sets with little contraction error [6] (at either the self-consistent field (SCF) or correlated level). Furthermore, the generalized contraction scheme appears to be sufficiently reliable that, while the primitive sets are considerably larger than are commonly employed, the contracted sets are frequently *smaller*.

There have been several recent reviews discussing GTO basis set selection [7-10] and a recent compendium of basis sets by Poirier et al. [11]. For the first-row systems the most accurate basis sets are the (13s8p) sets of van Duijneveldt [12]. The average error in the SCF energies for the atoms B to Ne is 175 μE_h as compared to 20 μE_h for the Hartree-Fock (HF) quality Slater-type orbitals (STO) basis sets [13] given by Clementi. However, note that Faegri and Almlöf [14] reduced the error in the Ne (14s9p) set from 233 μE_h to 155 μE_h by reoptimizing the basis set. Differences of this magnitude are generally insignificant in molecular calculations with the possible exception of certain properties [15] (such as the charge density) and weakly interacting systems, where minimizing the basis set superposition errors are crucial.

For the second-row atoms there are no energy optimized GTO basis sets comparable to van Duijneveldt's sets. The most comprehensive GTO basis sets for the second-row neutral atoms are the even-tempered sets of Schmidt and Rueden-

berg [16], who present formulas for generating basis sets of arbitrary size which yield energies converging to the numerical HF (NHF) result. To obtain basis sets for the second-row atoms with comparable errors in total energy that would be comparable to the van Duijneveldt sets for the first-row atoms requires a (22s14p) even-tempered set, and a basis comparable to Clementi's HF quality STO sets for the second row requires (24s15p) set (average error in SCF energy of 65 μE_h vs 90 μE_h for Clementi's STO basis sets). In this paper we show that near HF quality results are obtained with an (18s13p) energy optimized set, which results in a significant reduction in the integral computation time compared to using the larger even-tempered sets. We present energy optimized, HF quality basis sets for the ground states of the second-row atoms and for Na (^2P), Na^+ (^1S), Na^- (^1S), Mg (^{3}P), P^- (^3P), S^- (^2P), and Cl^- (^1S). In addition, optimized supplementary functions are given that give HF quality excitation energies for the above systems. All of the basis sets are at least of triple-zeta (TZ) quality in both the s and p spaces. These basis sets are intended to be employed in a generalized contraction scheme, such as the atomic natural orbital (ANO) approach of Almlöf and Taylor [6] or the contraction scheme of Raffenetti [17], since the segmented contractions of large basis sets can introduce quite large errors.

Methods

The orbital exponents were optimized by minimizing the restricted HF energies. The optimizations were performed using a scaled Newton-Raphson scheme developed by Faegri and Almlöf [14] in which the Hessian is evaluated numerically using analytically determined gradients. The starting orbital exponents were either taken from the even-tempered sets of Schmidt and Ruedenberg or were obtained from other optimized sets by increasing or decreasing the number of basis functions in each symmetry by one. The calculations were continued until the energy was stationary to at least 1×10^{-8} E_h and the virial ratio differed from 2.0 by less than 1×10^{-9}. The gradient of the energy with respect to variations of an orbital exponent is generally less than 1×10^{-7}. While a virial ratio of 2.0 is not a sufficient condition for an energy minimum, it is a sensitive measure of convergence in the optimization procedure. The energy stabilized well before the virial ratio and frequently it was necessary to perturb the exponents to get out of local stationary

points where the algorithm stalled. Often the innermost functions would become too compact. In these cases improved convergence was obtained by setting the innermost s (p) exponents so they were a factor of 6.68 (4.22) greater than the next exponents. There was no difficulty with multiple minima and most of the solutions correspond to a positive definite Hessian. However, the energy surface is quite flat for large basis sets and there is a near-linear dependence among the variational parameters resulting in several very small eigenvalues of the Hessian. For several solutions [i.e., Cl^- (19s14p), Cl (20s15p), Mg (19s11p) and Mg (20s12p)], one of the eigenvalues of the Hessian is negative. This appears to be a numerical precision problem and the energies are believed to be converged.

For the tightest s and p functions, the ratios between successive s and successive p functions are nearly independent of the nuclear charge and only slightly dependent on the number of functions. As the basis set gets larger, more functions are approximately given by a predetermined ratio. This is demonstrated in Table I where we compare the ratio between the first seven s functions for the Ar (15s10p), S(19s14p) and H(10s) basis sets. We should emphasize that the magnitude of the innermost function is dependent on Z and the number of functions. The ratios for the first seven s functions and the first three p functions are similar for all of the basis sets derived in this work as well as for the the basis sets optimized by Faegri and Speis [18] for the first-row transition metal atoms. The basis sets optimized by van Duijneveldt [12] and Huzinaga [19] are not optimized sufficiently to discern the pattern. Whereas the H(10s) set of van Duijneveldt differs in energy by only 0.1 μE_h from the 10s set employed in Table I, the exponents differ by 10%. The exponents and the energy for a 1-electron atom scale as Z^2. The variation of the energy and the ratio of the two innermost s functions are given as a function of basis set size for a H-like atom, He and Ar^{16+} in Table II. It appears that the inner part of the 1s function is effectively seeing a charge of Z and is not screened much by the other electrons. If the 1s orbital is doubly occupied, the magnitudes of the orbital exponents are reduced slightly, but the ratios of the innermost functions are the same.

Since the exponents of a H-like atom scale as Z^2, this can be used for obtaining starting basis sets for other systems. The exponents corresponding to the 1s orbital

can be obtained from the corresponding H basis set by scaling the exponents. For at least for the first few iterations these functions may be frozen or scaled as a contracted set. For example, use of the Ar^{17+} (10s) set and the remaining orbitals from the Ar (15s10p) set gives an energy only 70 μE_h above the optimized (15s10p) set. By optimizing the scaling factor, the error is reduced to $2\mu E_h$. Similarly, optimizing the scaling factor for the Ar^{17+}(12s) set gives an energy only $3\mu E_h$ above the optimized Ar(18s13p) set. A procedure based on this method has been used successfully in determining HF quality basis sets for the third-row atoms [20]. Such a scheme would be useful for defining "core deficient" basis sets [21,22], which still employ accurate valence basis sets. Note also that Feller et al. [23] have successfully used scaled, even-tempered, H basis sets to derive near-HF quality basis sets for oxygen atom.

Results

The atomic energies for all of the basis sets generated are compared with the NHF results and Clementi's HF quality STO results in Table III. The (17s12p), (18s13p), (19s14p) and (20s15p) basis sets appear to be balanced in that adding an additional s or p function contributes equally to the lowering of the energy. All of the basis sets that were optimized with 13 or more p functions are quadruple zeta in the p valence space. The 3s space switches from double zeta (DZ) to triple zeta (TZ) at 16 s functions except, for Na where 19s functions are required to have a TZ valance description. The average error in the SCF energy relative to NHF for Al to Ar is 82 μE_h for the (18s13p) set, 38 μE_h for the (19s14p) set, and 17 μE_h for the (20s15p) set. The (17s12p) set has an average error of 200 μE_h which is probably too large to be considered near-HF quality.

The negative ion basis sets have slightly larger errors than the corresponding sets for the neutrals; the (19s14p) sets are comparable to the (18s13p) set for the neutrals. However, for systems with both neutral and negative ion character, however, a balanced description is obtained by supplementing the neutral atom basis sets with both an s and a p function (only an s function for Na). The results and the supplementary functions are presented in Table IV along with the supplementary functions needed to describe Na ^2P and Mg ^3P. In all cases, the excitation energies using the (18s13p) neutral basis sets are within 10 μE_h of the NHF separations.

All of the second-row basis sets optimized in this work are given in Tables VI to LXVI. The basis sets for the (18s13p) sets [Na (19s11p), Mg (18s10p)] have been presented elsewhere [24]. Also given are the basis sets derived for H, He, and Ar^{16+}.

In addition, the (18s13p) ground state sets provide reasonably good description of the positive ions (see Table V). The errors in the computed ionization potentials (IP) decrease as larger neutral basis sets are employed. For example, the Ar (20,15) set has an error of only $4\mu E_h$. The largest error in the HF ionization potential is 22 μE_h. All of the basis sets are TZ in the valence space except for Mg^+. Optimizing an (18s11p) set for Mg^+ results in a basis that is DZ in the 3s space. If the valence space were constrained to be TZ, then the ratios between the valence exponents would be much less than 2.0. This could lead to linear dependency problems in molecular calculations.

Conclusions

Energy optimized, near–HF quality basis sets are presented for the second–row atoms and for Na (^2P), Na^+ (^1S), Na^- (^1S), Mg (^{3}P), P^- (^3P), S^- (^2P), and Cl^- (^1S). In addition, optimized supplementary functions are presented for the ground state basis sets that give HF quality excitation energies. The basis sets given here should be particularly useful when employing a generalized contraction scheme.

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Table I. Log of the ratio of successive s exponents.

	H(10s)	Ar(15s10p)[a]	S (19s14p)
r_1^a	1.89847	1.89845	1.89898
r_2	1.48025	1.48025	1.48031
r_3	1.26162	1.26159	1.26142
r_4	1.12056	1.12047	1.12007
r_5	1.01968	1.01958	1.01877
r_6	0.94318	0.94374	0.94144

[a] $r_i = log(\alpha_i/\alpha_{i+1})$ with α_1 being the most compact exponent.

Table II. Variation of energy and ratio of exponents with number of functions.

	Energy (E_h)		
	Ar^{17+}	Ar^{16+}	He
7s	-161.9945885	-312.8500407	-2.8615142
8s	-161.9982379	-312.8574674	-2.8616248
9s	-161.9993961	-312.8598288	-2.8616607
10s	-161.9997836	-312.8606202	-2.8616729
11s	-161.9999193	-312.8608979	-2.8616773
12s	-161.9999688		-2.8616790
13s	-161.9999876		-2.8616796
14s	-161.9999949	-312.8610528	-2.8616798
15s	-161.9999979	-312.8610589	-2.8616799
16s	-161.9999991	-312.8610614	-2.8616800
NHF	-162.0000000		-2.8616800

	r_1^a		
	Ar^{17+}	Ar^{16+}	He
7s	1.8971	1.8970	1.8966
8s	1.8977	1.8977	1.8974
9s	1.8982	1.8982	1.8980
10s	1.8985	1.8985	1.8983
11s	1.8987	1.8987	1.8986
12s	1.8988		1.8988
13s	1.8989		1.8989
14s	1.8990	1.8990	1.8989
15s	1.8991	1.8991	1.8988
16s	1.8991	1.8993	1.8993

[a] $r_1 = ln(\alpha_1/\alpha_2)$ with α_1 being the most compact function.

Table III. Summary of atomic energies

	NHF	STO[a]	GTO		$\Delta(\mu E_h)$[b]
			Basis	Energy	
$Na(^2S)$	-161.858912	-.85890	20/12	-.858902	10
			19/11	-.858889	23
			19/10	-.858872	40
			18/11	-.858883	29
			18/10	-.858866	46
$Na(^2P)$	-161.786410		18/13	-.786387	23
			16/14	-.786385	25
			16/13	-.786375	35
			15/13	-.786354	54
$Na^-(^1S)$	-161.676963	-.67793	16/11	-.676941	22
			15/10	-.676906	57
$Na^-(^1S)$	-161.855126	-.85466	19/11	-.855092	34
			18/11	-.855073	53
$Mg(^1S)$	-199.614636	-.61461	20/12	-.614626	10
			19/11	-.614611	25
			18/11	-.614594	42
			18/10	-.614575	61
			17/9	-.614477	159
$Mg(^3P)$	-199.546712		19/14	-.546681	22
			19/13	-.546651	32
			18/14	-.546673	39
			18/13	-.546649	43
$Mg^+(^2S)$	-199.371810	-.37042	18/11	-.371780	30
$Al(^2P)$	-241.876707	-.87668	20/15	-.876695	12
			19/14	-.876681	26
			18/13	-.876649	58
			17/12	-.876575	132
$Si(^3P)$	-288.854362	-.85431	20/15	-.854348	14
			19/14	-.854333	29
			18/13	-.854295	67
			17/12	-.854207	155
$P(^4S)$	-340.718780	-.71869	20/15	-.718765	15
			19/14	-.718747	33
			18/13	-.718706	74
			17/12	-.718600	180

$P^-(^3P)$	-340.698873	-.69866	19/14	-.698815	58
			18/13	-.698751	123
$S(^3P)$	-397.504895	-.50485	20/15	-.504877	18
			19/14	-.504856	48
			18/13	-.504809	86
			17/12	-.504682	213
$S^-(^2P)$	-397.538430	-.53820	19/14	-.538367	63
			18/13	-.538292	138
$Cl(^2P)$	-459.482072	-.48187	20/15	-.482052	20
			19/14	-.482027	46
			18/13	-.481973	99
			17/12	-.481828	244
$Cl^-(^1S)$	-459.576925	-.57670	19/14	-.576857	82
			18/13	-.576774	151
$Ar(^1S)$	-526.817513	-.81739	20/15	-.817490	23
			19/14	-.817462	51
			19/13	-.817428	85
			18/13	-.817400	113
			18/12	-.817300	213
			17/12	-.817238	275
			16/11	-.816782	731
			16/10	-.815981	1532
			15/10	-.815610	1903

[a] Ref. 12

[b] Difference between GTO and NHF energies in μE_h.

Table IV. Supplementary functions.

	Basis	suplemental functions	Energy	$\Delta(\mu E_h)^a$
Na^-	Na(19s10p)	α_s =0.005029	-161.855077	16
	Na(19s11p)	α_s =0.005029	-161.855091	15
Na (^{2}P)	Na(19s10p)	α_p =0.080388	-161.786383	-10
		α_p =0.032405		
		α_p =0.013693		
	Na(19s11p)	α_p =0.073912	-161.786385	-1
		α_p =0.030581		
		α_p =0.013192		
Mg (^{3}P)	Mg(18s10p)	α_p =0.100017	-199.546586	68
		α_p =0.034924		
	Mg(18s10p)	α_p =0.132526	-199.546652	5
		α_p =0.057360		
		α_p =0.024530		
	Mg(18s11p)	α_p =0.090644	-199.546634	37
		α_p =0.032883		
	Mg(18s11p)	α_p =0.114446	-199.546670	1
		α_p =0.051399		
		α_p =0.022780		
	Mg(19s11p)	α_p =0.114590	-199.546687	2
		α_p =0.051477		
		α_p =0.022812		
	Mg(20s12p)	α_p =0.095453	-199.546701	1
		α_p =0.044546		
		α_p =0.020652		
P^-	P(17s12p)	α_s =0.034824	-340.698709	22
		α_p =0.025297		
	P(18s13p)	α_s =0.034415	-340.698803	6
		α_p =0.023458		
	P(19s14p)	α_s =0.034103	-340.698842	3
		α_p =0.022285		
S^-	S(17s12p)	α_s =0.042456	-397.538236	-14
		α_p =0.029441		
	S(18s13p)	α_s =0.041938	-397.538352	-6
		α_p =0.027672		
	S(19s14p)	α_s =0.041340	-397.538395	-3

		α_p =0.026477		
	S(20s15p)	α_s =0.039631	-397.538413	2
		α_p =0.025248		
Cl^-	Cl(17s12p)	α_s =0.050758	-459.576704	-17
		α_p =0.035010		
	Cl(18s13p)	α_s =0.050119	-459.576836	-8
		α_p =0.033223		
	Cl(19s14p)	α_s =0.049192	-459.576886	-6
		α_p =0.031673		
	Cl(20s15p)	α_s =0.047027	-459.576907	-2
		α_p =0.030130		

[a]Difference from corresponding NHF separation. The negative sign means the calculated energy separation is less than the NHF result.

Table V. SCF energies for positive ions.

	NHF Energy	SCF Energy[a]	ΔIP[b](μE_h)
Na^+	-161.676963	-.676938	2
Mg^+	-199.371810	-.371746	18
Al^-	-241.674670	-.674617	5
Si^+	-288.573131	-.573057	7
P^+	-340.349775	-.349769	11
S^-	-397.173182	-.173077	19
Cl^-	-459.048590	-.048472	19
Ar^+	-526.274534	-.274399	22

[a] Using (18s13p) basis sets–Na(19s11p), Mg(18s10p).
[b] Error in atomic HF ionization potential in μE_h.

Table VI. Na ^2S (18,10) basis set, orbital energies and eigenvectors. Energy(E_H) = -161.858866

	s space		
Exponent	1s	2s	3s
	-40.478480	-2.797012	-0.182091
1259469.	0.000005	-0.000001	0.000000
188585.0	0.000036	-0.000009	0.000001
42916.43	0.000189	-0.000046	0.000007
12156.01	0.000797	-0.000195	0.000029
3965.814	0.002897	-0.000710	0.000107
1431.702	0.009367	-0.002305	0.000346
558.3654	0.027278	-0.006805	0.001024
231.5007	0.070903	-0.018177	0.002739
100.7917	0.158616	-0.043285	0.006548
45.60650	0.283746	-0.087702	0.013365
21.25913	0.347542	-0.140977	0.021849
10.03045	0.214843	-0.128614	0.020476
4.434134	0.036705	0.081817	-0.014127
2.064841	-0.000252	0.403188	-0.073290
0.927742	0.001397	0.488562	-0.115171
0.408763	-0.000111	0.179857	-0.139504
0.061755	0.000040	0.002685	0.609864
0.024287	-0.000020	-0.000694	0.496746

	p space	
Exponent	2p	3p
	-1.518124	
1119.578	0.000162	
265.3239	0.001408	
85.99553	0.007588	
32.53759	0.029609	
13.51565	0.088498	
5.966856	0.195458	
2.700045	0.306779	
1.218512	0.340870	
0.542187	0.230543	
0.227413	0.052407	

Table VII. Na ^2S (18,11) basis set, orbital energies and eigenvectors. Energy(E_H) = -161.858883

	s space		
Exponent	1s	2s	3s
	-40.478490	-2.797016	-0.182094
1259293.	0.000005	-0.000001	0.000000
188562.4	0.000036	-0.000009	0.000001
42911.82	0.000189	-0.000046	0.000007
12154.79	0.000798	-0.000195	0.000029
3965.434	0.002897	-0.000710	0.000107
1431.569	0.009368	-0.002305	0.000347
558.3144	0.027281	-0.006805	0.001024
231.4818	0.070909	-0.018178	0.002740
100.7844	0.158626	-0.043289	0.006548
45.60303	0.283763	-0.087709	0.013366
21.25730	0.347544	-0.140985	0.021851
10.02949	0.214819	-0.128600	0.020474
4.433432	0.036692	0.081867	-0.014136
2.064627	-0.000255	0.403193	-0.073293
0.927707	0.001397	0.488512	-0.115166
0.408775	-0.000111	0.179857	-0.139498
0.061754	0.000040	0.002686	0.609878
0.024287	-0.000020	-0.000693	0.496728

	p space	
Exponent	2p	3p
	-1.518130	
1774.640	0.000073	
420.3646	0.000640	
136.4821	0.003568	
51.97758	0.014651	
21.78045	0.047151	
9.745674	0.119372	
4.539163	0.225513	
2.137716	0.312485	
1.000488	0.312183	
0.461008	0.184079	
0.197529	0.033749	

Table VIII. Na ^2S (19,10) basis set, orbital energies and eigenvectors. Energy(E_H) = -161.858872

	s space		
Exponent	1s	2s	3s
	-40.478480	-2.797013	-0.182097
1223824.	0.000005	-0.000001	0.000000
183249.7	0.000037	-0.000009	0.000001
41702.81	0.000196	-0.000048	0.000007
11812.37	0.000827	-0.000202	0.000030
3853.719	0.003002	-0.000736	0.000111
1391.236	0.009702	-0.002387	0.000358
542.5841	0.028225	-0.007047	0.001062
224.9563	0.073190	-0.018781	0.002826
97.93848	0.162915	-0.044620	0.006768
44.31314	0.288660	-0.089755	0.013644
20.65334	0.346815	-0.142928	0.022280
9.730428	0.206922	-0.124334	0.019601
4.228692	0.032812	0.099874	-0.016750
1.969339	-0.000644	0.417097	-0.077383
0.889031	0.001457	0.475164	-0.113477
0.396453	-0.000178	0.163279	-0.139153
0.069934	0.000091	0.003122	0.439992
0.032895	-0.000082	-0.001583	0.538920
0.016124	0.000029	0.000569	0.134010

	p space	
Exponent	2p	3p
	-1.518125	
1119.626	0.000162	
265.3364	0.001408	
85.99989	0.007587	
32.53933	0.029606	
13.51630	0.088494	
5.967118	0.195450	
2.700231	0.306754	
1.218673	0.340843	
0.542305	0.230569	
0.227477	0.052450	

Table IX. Na ^2S (19,11) basis set, orbital energies and eigenvectors. Energy(E_H) = -161.858889

	s space		
Exponent	1s	2s	3s
	-40.478490	-2.797017	-0.182100
1223821.	0.000005	-0.000001	0.000000
183243.9	0.000037	-0.000009	0.000001
41700.30	0.000196	-0.000048	0.000007
11811.38	0.000827	-0.000202	0.000030
3853.335	0.003002	-0.000736	0.000111
1391.082	0.009704	-0.002387	0.000359
542.5201	0.028229	-0.007048	0.001062
224.9305	0.073199	-0.018783	0.002827
97.92800	0.162931	-0.044625	0.006769
44.30828	0.288682	-0.089764	0.013646
20.65095	0.346813	-0.142936	0.022282
9.729267	0.206889	-0.124314	0.019599
4.227939	0.032798	0.099939	-0.016763
1.969055	-0.000646	0.417115	-0.077388
0.888957	0.001458	0.475106	-0.113478
0.396443	-0.000178	0.163260	-0.139139
0.069933	0.000091	0.003117	0.440016
0.032893	-0.000082	-0.001574	0.538959
0.016122	0.000029	0.000565	0.133945

	p space	
Exponent	2p	3p
	-1.518131	
1774.857	0.000073	
420.4154	0.000640	
136.4986	0.003567	
51.98394	0.014649	
21.78321	0.047143	
9.746938	0.119357	
4.539640	0.225510	
2.137842	0.312497	
1.000538	0.312176	
0.461070	0.184076	
0.197596	0.033780	

Table X. Na ^2S (20,12) basis set, orbital energies and eigenvectors. Energy(E_H) = -161.858902

	s space		
Exponent	1s	2s	3s
	-40.478490	-2.797022	-0.182102
2185572.	0.000002	-0.000001	0.000000
327228.4	0.000018	-0.000004	0.000001
74466.84	0.000095	-0.000023	0.000004
21093.15	0.000401	-0.000098	0.000015
6881.898	0.001459	-0.000357	0.000054
2484.696	0.004746	-0.001166	0.000175
969.2232	0.014031	-0.003464	0.000520
402.0643	0.037733	-0.009495	0.001431
175.3545	0.090702	-0.023587	0.003554
79.65199	0.186467	-0.052394	0.007954
37.38672	0.301836	-0.098029	0.014954
18.00194	0.323830	-0.143671	0.022472
8.724371	0.168700	-0.102301	0.016204
3.857715	0.023083	0.138034	-0.023549
1.815686	-0.000147	0.428998	-0.080122
0.838254	0.001099	0.447821	-0.112915
0.381935	-0.000101	0.144539	-0.132997
0.071679	0.000061	0.002621	0.417519
0.033916	-0.000053	-0.001196	0.549451
0.016525	0.000018	0.000440	0.148100

	p space	
Exponent	2p	3p
	-1.518136	
2749.971	0.000034	
651.1238	0.000301	
211.5177	0.001713	
80.84058	0.007325	
34.11345	0.024850	
15.38613	0.068751	
7.280423	0.150370	
3.531983	0.248551	
1.718569	0.309745	
0.829935	0.279135	
0.393554	0.142293	
0.169717	0.020481	

Table XI. Na ^2P (15,13) basis set, orbital energies and eigenvectors. Energy(E_H) = -161.786354

	s space		
Exponent	1s	2s	3s
	-40.558260	-2.874268	
646064.2	0.000011	-0.000003	
96748.84	0.000083	-0.000020	
22017.45	0.000435	-0.000106	
6236.113	0.001832	-0.000448	
2034.282	0.006623	-0.001625	
734.2638	0.021126	-0.005241	
286.2328	0.059513	-0.015111	
118.4891	0.143585	-0.038544	
51.38179	0.276397	-0.083196	
23.08383	0.364020	-0.141952	
10.54160	0.238867	-0.139881	
4.479307	0.040950	0.078212	
2.029109	-0.000855	0.425425	
0.882811	0.001539	0.496010	
0.379420	-0.000146	0.152767	
	p space		
Exponent	2p	3p	
	-1.598053	-0.109450	
1359.568	0.000116	-0.000012	
322.1450	0.001012	-0.000100	
104.5127	0.005539	-0.000556	
39.66873	0.022107	-0.002184	
16.54214	0.068390	-0.006957	
7.352832	0.160852	-0.016138	
3.375649	0.273541	-0.028679	
1.555398	0.335582	-0.033282	
0.710640	0.276653	-0.036845	
0.316784	0.104323	-0.005331	
0.089183	0.004448	0.214243	
0.034673	-0.001120	0.563326	
0.014270	0.000385	0.332065	

Table XII. Na ^2P (16,13) basis set, orbital energies and eigenvectors. Energy(E_H) = -161.786375

	s space		
Exponent	1s	2s	3s
	-40.558270	-2.874270	
1161290.	0.000005	-0.000001	
173886.1	0.000040	-0.000010	
39571.43	0.000209	-0.000051	
11208.50	0.000882	-0.000215	
3656.675	0.003204	-0.000785	
1320.096	0.010347	-0.002545	
514.8415	0.030039	-0.007510	
213.4547	0.077542	-0.019927	
92.92676	0.170966	-0.047121	
42.04506	0.297398	-0.093503	
19.59671	0.344322	-0.146026	
9.218754	0.191967	-0.115480	
3.917195	0.026580	0.132978	
1.803327	-0.000615	0.445981	
0.808065	0.001199	0.455788	
0.357042	-0.000103	0.124798	
	p space		
Exponent	2p	3p	
	-1.598054	-0.109450	
1359.756	0.000116	-0.000012	
322.1806	0.001012	-0.000099	
104.5228	0.005538	-0.000556	
39.67232	0.022104	-0.002184	
16.54385	0.068378	-0.006956	
7.354201	0.160801	-0.016133	
3.376570	0.273495	-0.028674	
1.555732	0.335640	-0.033290	
0.710670	0.276720	-0.036850	
0.316764	0.104311	-0.005332	
0.089184	0.004450	0.214245	
0.034673	-0.001121	0.563329	
0.014270	0.000385	0.332062	

Table XIII. Na ^2P (16,14) basis set, orbital energies and eigenvectors. Energy(E_H) = -161.786385

	s space		
Exponent	1s	2s	3s
	-40.558280	-2.874277	
1161342.	0.000005	-0.000001	
173894.1	0.000040	-0.000010	
39573.24	0.000209	-0.000051	
11209.01	0.000882	-0.000215	
3656.840	0.003204	-0.000785	
1320.155	0.010347	-0.002545	
514.8633	0.030037	-0.007509	
213.4636	0.077538	-0.019926	
92.93155	0.170955	-0.047117	
42.04779	0.297383	-0.093497	
19.59815	0.344323	-0.146020	
9.219513	0.191987	-0.115496	
3.917838	0.026589	0.132909	
1.803634	-0.000613	0.445941	
0.808182	0.001198	0.455852	
0.357077	-0.000103	0.124841	
	p space		
Exponent	2p	3p	
	-1.598062	-0.109451	
2109.480	0.000054	-0.000005	
499.5897	0.000476	-0.000048	
162.2537	0.002679	-0.000263	
61.89873	0.011186	-0.001126	
26.01752	0.036794	-0.003640	
11.68392	0.096851	-0.009925	
5.484535	0.194492	-0.019503	
2.620516	0.288897	-0.030585	
1.251456	0.316877	-0.031224	
0.594666	0.229326	-0.034692	
0.276876	0.072120	0.005322	
0.083600	0.002334	0.235978	
0.033072	-0.000443	0.562291	
0.013841	0.000171	0.307345	

Table XIV. Na ^2P (18,13) basis set, orbital energies and eigenvectors. Energy(E_H) = -161.786387

	s space		
Exponent	1s	2s	3s
	-40.558280	-2.874272	
3468994.	0.000001	0.000000	
519709.5	0.000010	-0.000002	
118249.5	0.000053	-0.000013	
33488.56	0.000225	-0.000055	
10927.06	0.000820	-0.000201	
3946.140	0.002674	-0.000654	
1539.749	0.007961	-0.001960	
638.9785	0.021787	-0.005408	
278.8873	0.054366	-0.013848	
126.9074	0.120480	-0.032057	
59.76063	0.224618	-0.065956	
28.95991	0.318326	-0.112220	
14.35704	0.280086	-0.141726	
7.156824	0.110303	-0.056724	
3.255817	0.011056	0.212115	
1.525353	0.000711	0.462363	
0.710507	0.000497	0.393044	
0.325729	0.000015	0.089751	
	p space		
Exponent	2p	3p	
	-1.598055	-0.109450	
1360.579	0.000116	-0.000012	
322.3520	0.001011	-0.000099	
104.5735	0.005534	-0.000555	
39.69061	0.022089	-0.002183	
16.55162	0.068335	-0.006951	
7.357604	0.160741	-0.016128	
3.377785	0.273503	-0.028674	
1.556005	0.335720	-0.033303	
0.710688	0.276758	-0.036845	
0.316765	0.104304	-0.005348	
0.089214	0.004455	0.214102	
0.034685	-0.001122	0.563271	
0.014274	0.000386	0.332269	

Table XV. Na^- ^1S (18,11) basis set, orbital energies and eigenvectors. Energy(E_H) = -161.855073

	s space		
Exponent	1s	2s	3s
	-40.332830	-2.651275	-0.013313
702142.0	0.000010	-0.000002	0.000000
105145.3	0.000074	-0.000018	0.000002
23928.44	0.000392	-0.000096	0.000010
6777.490	0.001652	-0.000404	0.000042
2210.940	0.005975	-0.001468	0.000154
798.0598	0.019104	-0.004731	0.000498
311.1322	0.054104	-0.013719	0.001443
128.8363	0.132116	-0.035167	0.003714
55.91002	0.260396	-0.077317	0.008207
25.16052	0.360370	-0.134794	0.014539
11.56914	0.261086	-0.148423	0.016379
5.165819	0.056523	0.030929	-0.003726
2.303539	0.000763	0.383155	-0.048038
0.997182	0.001488	0.521985	-0.081376
0.425810	-0.000098	0.204544	-0.096640
0.057963	0.000041	0.002787	0.327110
0.018195	-0.000024	-0.001177	0.519700
0.005061	0.000007	0.000333	0.308455

	p space	
Exponent	2p	3p
	-1.372382	
1695.360	0.000079	
401.6069	0.000693	
130.3788	0.003849	
49.62764	0.015730	
20.77829	0.050312	
9.287331	0.125929	
4.316187	0.233785	
2.025512	0.317595	
0.943705	0.308551	
0.431631	0.170944	
0.178544	0.026240	

Table XVI. Na^- ^1S (19,11) basis set, orbital energies and eigenvectors. Energy(E_H) = -161.855092

	s space		
Exponent	1s	2s	3s
	-40.332840	-2.651280	-0.013312
1260332.	0.000005	-0.000001	0.000000
188713.4	0.000036	-0.000009	0.000001
42945.62	0.000189	-0.000046	0.000005
12164.27	0.000797	-0.000195	0.000020
3968.506	0.002894	-0.000709	0.000074
1432.672	0.009359	-0.002303	0.000242
558.7429	0.027256	-0.006799	0.000714
231.6587	0.070849	-0.018163	0.001915
100.8612	0.158514	-0.043257	0.004567
45.63777	0.283632	-0.087658	0.009349
21.27367	0.347554	-0.140941	0.015219
10.03783	0.215021	-0.128710	0.014388
4.439967	0.036801	0.081342	-0.009980
2.067338	-0.000230	0.402949	-0.050548
0.928441	0.001387	0.489171	-0.080892
0.408668	-0.000105	0.180076	-0.090947
0.058618	0.000037	0.002362	0.323454
0.018376	-0.000021	-0.000966	0.521361
0.005093	0.000006	0.000270	0.311427

	p space	
Exponent	2p	3p
	-1.372386	
1695.937	0.000079	
401.7393	0.000692	
130.4211	0.003847	
49.64385	0.015722	
20.78549	0.050286	
9.291061	0.125868	
4.317855	0.233757	
2.025996	0.317650	
0.943829	0.308575	
0.431717	0.170962	
0.178617	0.026268	

Table XVII. Na^+ ^1S (15,10) basis set, orbital energies and eigenvectors. Energy(E_H) = -161.676906

	s space		
Exponent	1s	2s	3s
	-40.759730	-3.073676	
651413.5	0.000011	-0.000003	
97536.27	0.000082	-0.000020	
22194.24	0.000431	-0.000105	
6285.709	0.001814	-0.000444	
2050.342	0.006559	-0.001610	
740.0303	0.020929	-0.005192	
288.4752	0.058988	-0.014978	
119.4197	0.142485	-0.038224	
51.78852	0.274911	-0.082658	
23.26951	0.363832	-0.141331	
10.63248	0.241040	-0.140909	
4.541698	0.042234	0.073249	
2.056141	-0.000733	0.421346	
0.894482	0.001529	0.498881	
0.385055	-0.000134	0.158069	
	p space		
Exponent	2p	3p	
	-1.797180		
1201.441	0.000144		
284.6643	0.001251		
92.28767	0.006782		
34.95602	0.026693		
14.53995	0.080844		
6.435743	0.182831		
2.928093	0.295519		
1.331681	0.340657		
0.599451	0.248771		
0.262061	0.067618		

Table XVIII. Na^+ ^1S (16,11) basis set, orbital energies and eigenvectors. Energy(E_H) = -161.676941

	s space		
Exponent	1s	2s	3s
	-40.759740	-3.073683	
1170270.	0.000005	-0.000001	
175230.5	0.000039	-0.000010	
39877.42	0.000207	-0.000051	
11295.19	0.000874	-0.000213	
3684.958	0.003173	-0.000778	
1330.305	0.010250	-0.002521	
518.8205	0.029766	-0.007441	
215.1038	0.076890	-0.019759	
93.64541	0.169771	-0.046754	
42.36976	0.296145	-0.092973	
19.74711	0.344793	-0.145625	
9.290854	0.194149	-0.116906	
3.962701	0.027399	0.127913	
1.827693	-0.000595	0.441866	
0.819918	0.001210	0.459117	
0.363411	-0.000096	0.130289	
	p space		
Exponent	2p	3p	
	-1.797188		
1949.245	0.000062		
461.6817	0.000546		
149.9238	0.003057		
57.15198	0.012672		
23.98829	0.041285		
10.75412	0.106873		
5.029426	0.208955		
2.385936	0.301022		
1.127438	0.317094		
0.527791	0.209569		
0.239914	0.050077		

Table XIX. Mg ^1S (17,9) basis set, orbital energies and eigenvectors. Energy(E_H) = -199.614477

	s space		
Exponent	1s	2s	3s
	-49.031680	-3.767678	-0.253037
592749.9	0.000015	-0.000004	0.000001
88770.59	0.000115	-0.000029	0.000006
20202.02	0.000603	-0.000152	0.000029
5721.886	0.002538	-0.000644	0.000124
1866.548	0.009148	-0.002322	0.000447
673.7657	0.028923	-0.007490	0.001446
262.6934	0.079837	-0.021164	0.004087
108.7819	0.183945	-0.052912	0.010294
47.24902	0.322441	-0.106465	0.020866
21.32746	0.349063	-0.163983	0.033083
9.779949	0.161926	-0.090844	0.018600
3.750390	0.015040	0.272177	-0.061663
1.606738	-0.000621	0.569687	-0.160042
0.680724	0.000684	0.307176	-0.197886
0.141848	-0.000176	0.013079	0.333509
0.066520	0.000142	-0.006589	0.563959
0.029875	-0.000046	0.001781	0.242677

	p space	
Exponent	2p	3p
	-2.282179	
894.3290	0.000349	
211.9927	0.002978	
68.49909	0.015497	
25.74546	0.057544	
10.61343	0.155957	
4.596185	0.292377	
2.011191	0.371817	
0.874294	0.276886	
0.356318	0.066374	

Table XX. Mg ^1S (18,10) basis set, orbital energies and eigenvectors. Energy(E_H) = -199.614575

	s space		
Exponent	1s	2s	3s
	-49.031710	-3.767703	-0.253045
1015694.	0.000007	-0.000002	0.000000
152096.2	0.000059	-0.000015	0.000003
34613.23	0.000308	-0.000078	0.000015
9803.889	0.001299	-0.000328	0.000063
3198.292	0.004705	-0.001196	0.000231
1154.550	0.015113	-0.003858	0.000743
450.2375	0.043271	-0.011305	0.002186
186.6144	0.108307	-0.029362	0.005673
81.18610	0.223960	-0.066917	0.013073
36.73197	0.341750	-0.122420	0.024079
17.14712	0.302484	-0.160026	0.032719
8.101327	0.104125	-0.041310	0.007976
3.414670	0.007271	0.314129	-0.071266
1.495800	0.000731	0.552763	-0.162492
0.651347	0.000189	0.274118	-0.186875
0.144307	0.000003	0.010710	0.331297
0.066313	-0.000001	-0.004938	0.575705
0.029567	0.000000	0.001322	0.236455

	p space	
Exponent	2p	3p
	-2.282207	
1440.885	0.000152	
341.4284	0.001327	
110.7151	0.007217	
41.96987	0.028532	
17.48596	0.086552	
7.753275	0.194892	
3.533541	0.312210	
1.614324	0.347988	
0.729856	0.219861	
0.302946	0.041290	

Table XXI. Mg ^1S (18,11) basis set, orbital energies and eigenvectors. Energy(E_H) = -199.614594

	s space		
Exponent	1s	2s	3s
	-49.031710	-3.767707	-0.253048
1015599.	0.000007	-0.000002	0.000000
152079.6	0.000059	-0.000015	0.000003
34609.27	0.000308	-0.000078	0.000015
9802.862	0.001299	-0.000328	0.000063
3198.005	0.004705	-0.001196	0.000231
1154.465	0.015114	-0.003858	0.000743
450.2097	0.043274	-0.011306	0.002187
186.6033	0.108314	-0.029364	0.005673
81.18155	0.223968	-0.066920	0.013074
36.73032	0.341749	-0.122422	0.024080
17.14656	0.302473	-0.160025	0.032719
8.101144	0.104118	-0.041299	0.007973
3.414527	0.007271	0.314152	-0.071272
1.495724	0.000731	0.552768	-0.162501
0.651309	0.000189	0.274089	-0.186870
0.144333	0.000003	0.010697	0.331173
0.066322	-0.000001	-0.004925	0.575790
0.029569	0.000000	0.001318	0.236502

	p space	
Exponent	2p	3p
	-2.282214	
2262.857	0.000069	
535.9659	0.000612	
174.0373	0.003431	
66.34299	0.014233	
27.85787	0.046357	
12.49885	0.119021	
5.845407	0.228527	
2.772378	0.320753	
1.313554	0.315382	
0.612590	0.167712	
0.254035	0.024063	

Table XXII. Mg ^1S (19,11) basis set, orbital energies and eigenvectors. Energy(E_H) = -199.614611

	s space		
Exponent	1s	2s	3s
	-49.031720	-3.767715	-0.253048
1708066.	0.000004	-0.000001	0.000000
255748.6	0.000031	-0.000008	0.000002
58200.05	0.000161	-0.000041	0.000008
16485.12	0.000679	-0.000172	0.000033
5378.248	0.002469	-0.000625	0.000120
1941.664	0.007996	-0.002036	0.000393
757.2925	0.023393	-0.006019	0.001159
314.0328	0.061423	-0.016230	0.003144
136.8060	0.140342	-0.039128	0.007566
61.98569	0.261142	-0.081667	0.016029
28.97643	0.345598	-0.136671	0.027014
13.80515	0.247990	-0.146105	0.030324
6.464312	0.059136	0.020730	-0.005724
2.994069	0.001864	0.356433	-0.081486
1.364919	0.001399	0.521901	-0.163799
0.616381	-0.000088	0.235021	-0.172390
0.147513	0.000083	0.008477	0.325007
0.066715	-0.000058	-0.003507	0.585951
0.029514	0.000018	0.000919	0.236253

	p space	
Exponent	2p	3p
	-2.282219	
2263.106	0.000069	
536.0126	0.000612	
174.0500	0.003431	
66.34742	0.014231	
27.85982	0.046351	
12.50059	0.118987	
5.846649	0.228492	
2.772711	0.320819	
1.313476	0.315434	
0.612521	0.167676	
0.254030	0.024058	

Table XXIII. Mg ^1S (20,12) basis set, orbital energies and eigenvectors. Energy(E_H) = -199.614626

	s space		
Exponent	1s	2s	3s
	-49.031730	-3.767718	-0.253050
2967534.	0.000002	-0.000001	0.000000
444290.4	0.000015	-0.000004	0.000001
101102.7	0.000081	-0.000020	0.000004
28637.01	0.000341	-0.000086	0.000017
9342.975	0.001242	-0.000314	0.000061
3373.203	0.004042	-0.001026	0.000197
1315.783	0.011981	-0.003059	0.000591
545.8194	0.032422	-0.008410	0.001619
238.0693	0.078968	-0.021130	0.004099
108.1768	0.166585	-0.047692	0.009231
50.80191	0.282745	-0.092371	0.018209
24.48321	0.332010	-0.142585	0.028296
11.92537	0.203336	-0.126247	0.026523
5.543442	0.038158	0.071715	-0.017247
2.674666	0.000379	0.382883	-0.088553
1.263240	0.001354	0.490104	-0.163851
0.588318	-0.000123	0.204477	-0.159550
0.149616	0.000081	0.007000	0.321626
0.067005	-0.000054	-0.002661	0.591511
0.029515	0.000017	0.000687	0.236826

	p space	
Exponent	2p	3p
	-2.282223	
3477.856	0.000033	
823.3565	0.000291	
267.4546	0.001666	
102.2553	0.007176	
43.20470	0.024592	
19.52643	0.068769	
9.264026	0.152266	
4.512192	0.254873	
2.210683	0.319043	
1.079993	0.276361	
0.515810	0.122109	
0.208679	0.013062	

Table XXIV. Mg ^3P (18,13) basis set, orbital energies and eigenvectors. Energy(E_H) = -199.546662

	s space		
Exponent	1s	2s	3s
	-49.085420	-3.818498	-0.339583
1012585.	0.000008	-0.000002	0.000000
151627.8	0.000059	-0.000015	0.000003
34506.30	0.000309	-0.000078	0.000016
9773.651	0.001303	-0.000329	0.000067
3188.461	0.004723	-0.001199	0.000243
1151.014	0.015169	-0.003869	0.000785
448.8606	0.043425	-0.011338	0.002303
186.0422	0.108655	-0.029435	0.005992
80.93562	0.224519	-0.067068	0.013754
36.61698	0.342100	-0.122542	0.025436
17.09086	0.301921	-0.159929	0.034208
8.071553	0.103327	-0.040134	0.008521
3.399993	0.007152	0.315572	-0.076398
1.488800	0.000744	0.552086	-0.167755
0.649323	0.000178	0.272534	-0.204160
0.143803	0.000001	0.011514	0.368406
0.072072	0.000000	-0.005390	0.565060
0.033761	0.000001	0.001523	0.213645
	p space		
Exponent	2p	3p	
	-2.337479	-0.179639	
1871.833	0.000097	-0.000015	
443.4327	0.000849	-0.000133	
143.9329	0.004704	-0.000750	
54.76049	0.019142	-0.003012	
22.92610	0.060664	-0.009815	
10.24742	0.148105	-0.023801	
4.752136	0.264000	-0.044328	
2.226546	0.338411	-0.054765	
1.043840	0.285793	-0.060238	
0.480340	0.110427	0.003193	
0.167581	0.007258	0.289002	
0.067417	-0.000783	0.552374	
0.027200	0.000226	0.274271	

Table XXV. Mg ^3P (18,14) basis set, orbital energies and eigenvectors. Energy(E_H) = -199.546673

	s space		
Exponent	1s	2s	3s
	-49.085420	-3.818505	-0.339588
1013006.	0.000008	-0.000002	0.000000
151690.8	0.000059	-0.000015	0.000003
34520.66	0.000309	-0.000078	0.000016
9777.720	0.001303	-0.000329	0.000067
3189.791	0.004720	-0.001199	0.000243
1151.495	0.015161	-0.003867	0.000784
449.0496	0.043404	-0.011332	0.002302
186.1203	0.108608	-0.029421	0.005990
80.96915	0.224446	-0.067042	0.013748
36.63212	0.342054	-0.122506	0.025429
17.09818	0.301995	-0.159931	0.034206
8.075333	0.103436	-0.040259	0.008553
3.401170	0.007169	0.315400	-0.076364
1.489322	0.000741	0.552097	-0.167705
0.649538	0.000179	0.272721	-0.204237
0.143863	0.000001	0.011550	0.367679
0.072158	0.000000	-0.005413	0.565019
0.033797	0.000001	0.001528	0.214390

	p space	
Exponent	2p	3p
	-2.337487	-0.179641
2706.008	0.000051	-0.000008
640.8122	0.000450	-0.000071
208.1331	0.002546	-0.000400
79.46091	0.010739	-0.001712
33.46233	0.035765	-0.005663
15.06710	0.095466	-0.015531
7.100984	0.195081	-0.031628
3.414586	0.294892	-0.049699
1.648498	0.323516	-0.053762
0.796906	0.218850	-0.051358
0.378069	0.058955	0.037610
0.147322	0.002481	0.329527
0.061331	0.000107	0.531856
0.025562	-0.000026	0.233399

Table XXVI. Mg ^3P (19,13) basis set, orbital energies and eigenvectors. Energy(E_H) = -199.546680

	s space		
Exponent	1s	2s	3s
	-49.085430	-3.818505	-0.339583
1700188.	0.000004	-0.000001	0.000000
254566.6	0.000031	-0.000008	0.000002
57930.60	0.000162	-0.000041	0.000008
16408.59	0.000683	-0.000173	0.000035
5353.194	0.002483	-0.000628	0.000127
1932.585	0.008042	-0.002046	0.000415
753.7371	0.023526	-0.006049	0.001226
312.5494	0.061754	-0.016307	0.003319
136.1527	0.141006	-0.039296	0.008004
61.68412	0.262036	-0.081966	0.016893
28.83002	0.345846	-0.136924	0.028546
13.72791	0.246824	-0.145698	0.031645
6.414262	0.058112	0.023278	-0.006236
2.969118	0.001731	0.359331	-0.087510
1.352632	0.001417	0.520969	-0.169615
0.611686	-0.000108	0.231198	-0.188655
0.146574	0.000094	0.008674	0.369230
0.071244	-0.000071	-0.003444	0.582429
0.033019	0.000023	0.001015	0.200331

	p space	
Exponent	2p	3p
	-2.337484	-0.179640
1872.188	0.000097	-0.000015
443.5161	0.000849	-0.000133
143.9596	0.004703	-0.000750
54.77049	0.019137	-0.003012
22.92978	0.060653	-0.009813
10.24919	0.148065	-0.023796
4.753622	0.263891	-0.044308
2.227562	0.338364	-0.054762
1.044283	0.285917	-0.060238
0.480465	0.110512	0.003124
0.167613	0.007262	0.288995
0.067415	-0.000783	0.552487
0.027196	0.000226	0.274206

Table XXVII. Mg ^3P (19,14) basis set, orbital energies and eigenvectors. Energy(E_H) = -199.546690

	s space		
Exponent	1s	2s	3s
	-49.085430	-3.818513	-0.339588
1700655.	0.000004	-0.000001	0.000000
254638.6	0.000031	-0.000008	0.000002
57947.86	0.000162	-0.000041	0.000008
16413.69	0.000683	-0.000173	0.000035
5354.908	0.002482	-0.000628	0.000127
1933.217	0.008039	-0.002045	0.000415
753.9876	0.023517	-0.006046	0.001225
312.6563	0.061729	-0.016301	0.003318
136.2018	0.140953	-0.039279	0.008001
61.70766	0.261962	-0.081937	0.016887
28.84161	0.345824	-0.136890	0.028539
13.73403	0.246917	-0.145726	0.031649
6.418292	0.058195	0.023084	-0.006188
2.970780	0.001743	0.359100	-0.087456
1.353369	0.001415	0.521043	-0.169559
0.611985	-0.000107	0.231469	-0.188762
0.146588	0.000093	0.008707	0.368901
0.071287	-0.000070	-0.003467	0.582306
0.033040	0.000023	0.001021	0.200743

	p space	
Exponent	2p	3p
	-2.337493	-0.179642
2708.529	0.000051	-0.000008
641.3995	0.000449	-0.000071
208.3231	0.002542	-0.000399
79.53432	0.010723	-0.001710
33.49429	0.035714	-0.005655
15.08217	0.095351	-0.015512
7.107696	0.194965	-0.031609
3.417445	0.294822	-0.049686
1.650002	0.323468	-0.053748
0.797838	0.219037	-0.051376
0.378598	0.059171	0.037350
0.147477	0.002500	0.329222
0.061372	0.000105	0.532137
0.025569	-0.000026	0.233626

Table XXVIII. Mg^{+} ^2S (18,11) basis set, orbital energies and eigenvectors. Energy(E_H) = -199.371780

	s space		
Exponent	1s	2s	3s
	-49.356350	-4.085612	-0.541431
1716228.	0.000004	-0.000001	0.000000
256961.2	0.000030	-0.000008	0.000002
58474.85	0.000160	-0.000040	0.000009
16562.83	0.000675	-0.000171	0.000039
5403.580	0.002454	-0.000621	0.000141
1950.808	0.007950	-0.002023	0.000463
760.8629	0.023262	-0.005983	0.001360
315.5202	0.061095	-0.016134	0.003708
137.4626	0.139675	-0.038913	0.008873
62.29197	0.260206	-0.081264	0.018960
29.12800	0.345241	-0.136170	0.031641
13.88754	0.249147	-0.146303	0.036453
6.521311	0.060276	0.017884	-0.007112
3.019853	0.002077	0.352539	-0.093701
1.375444	0.001353	0.523698	-0.199048
0.618570	-0.000050	0.239406	-0.211170
0.137048	0.000047	0.007158	0.676583
0.060067	-0.000023	-0.001466	0.485245

	p space	
Exponent	2p	3p
	-2.602934	
2458.756	0.000060	
582.2844	0.000531	
189.0961	0.002991	
72.13612	0.012507	
30.33085	0.041173	
13.63117	0.107740	
6.397635	0.213202	
3.052129	0.310209	
1.456524	0.322042	
0.689163	0.192432	
0.307023	0.035667	

Table XXIX. Al ^2P (17,12) basis set, orbital energies and eigenvectors. Energy(E_H) = -241.876575

	s space		
Exponent	1s	2s	3s
	-58.500950	-4.910609	-0.393381
751932.0	0.000013	-0.000004	0.000001
112608.6	0.000104	-0.000027	0.000006
25627.04	0.000548	-0.000142	0.000033
7258.473	0.002309	-0.000603	0.000139
2367.805	0.008331	-0.002176	0.000502
854.6966	0.026418	-0.007024	0.001627
333.2359	0.073444	-0.019984	0.004620
138.0074	0.171841	-0.050436	0.011785
59.94291	0.310420	-0.103971	0.024383
27.03405	0.356692	-0.165800	0.040318
12.37118	0.183530	-0.110630	0.027109
4.820360	0.019994	0.237258	-0.064021
2.123811	-0.001276	0.569056	-0.198431
0.925412	0.000982	0.339914	-0.240714
0.240543	-0.000301	0.019126	0.308859
0.112700	0.000207	-0.006940	0.604264
0.048331	-0.000062	0.001703	0.258562

	p space	
Exponent	2p	3p
	-3.218241	-0.209933
1489.445	0.000202	-0.000036
352.9742	0.001751	-0.000318
114.3947	0.009442	-0.001690
43.30729	0.036868	-0.006771
18.02528	0.108929	-0.019912
7.966641	0.232659	-0.044532
3.608627	0.346437	-0.064563
1.645418	0.334408	-0.075738
0.738899	0.147849	0.000278
0.257688	0.012093	0.288170
0.097646	-0.000848	0.543314
0.036868	0.000430	0.301345

Table XXX. Al ^2P (18,13) basis set, orbital energies and eigenvectors. Energy(E_H) = -241.876649

	s space		
Exponent	1s	2s	3s
	-58.500990	-4.910640	-0.393398
1328078.	0.000007	-0.000002	0.000000
198873.3	0.000051	-0.000013	0.000003
45258.98	0.000269	-0.000070	0.000016
12819.51	0.001137	-0.000296	0.000068
4182.217	0.004123	-0.001078	0.000249
1509.819	0.013275	-0.003482	0.000803
588.8500	0.038212	-0.010243	0.002377
244.1548	0.096814	-0.026829	0.006203
106.3231	0.205076	-0.062171	0.014585
48.18996	0.328271	-0.117174	0.027559
22.56694	0.320158	-0.164000	0.040375
10.71311	0.133199	-0.072306	0.017237
4.465615	0.012113	0.276561	-0.074852
1.996812	0.000102	0.559569	-0.202955
0.889664	0.000441	0.308687	-0.227837
0.241230	-0.000091	0.016198	0.319182
0.110982	0.000058	-0.005388	0.607753
0.047633	-0.000018	0.001342	0.248338

	p space	
Exponent	2p	3p
	-3.218272	-0.209940
2266.403	0.000097	-0.000018
536.8778	0.000854	-0.000152
174.2806	0.004749	-0.000863
66.35078	0.019444	-0.003493
27.82011	0.062016	-0.011463
12.46120	0.152155	-0.028059
5.796435	0.272046	-0.052459
2.732759	0.345854	-0.065201
1.297110	0.274738	-0.066688
0.605854	0.092187	0.035508
0.226958	0.005840	0.324388
0.088637	0.000082	0.527955
0.034597	0.000134	0.260956

Table XXXI. Al ^2P (19,14) basis set, orbital energies and eigenvectors. Energy(E_H) = -241.876681

	s space		
Exponent	1s	2s	3s
	-58.501010	-4.910659	-0.393411
2203790.	0.000004	-0.000001	0.000000
329944.1	0.000027	-0.000007	0.000002
75081.71	0.000143	-0.000037	0.000009
21266.41	0.000605	-0.000157	0.000036
6938.077	0.002200	-0.000573	0.000132
2504.811	0.007132	-0.001867	0.000432
976.9710	0.020926	-0.005529	0.001274
405.1890	0.055301	-0.014989	0.003484
176.6066	0.128083	-0.036450	0.008437
80.11946	0.244454	-0.077493	0.018266
37.55262	0.339938	-0.133259	0.031512
18.02259	0.268882	-0.155210	0.038847
8.667077	0.079673	-0.014632	0.002036
3.961705	0.004640	0.325486	-0.088956
1.828544	0.001157	0.537157	-0.207344
0.841712	0.000005	0.266742	-0.208685
0.242606	0.000057	0.012938	0.327884
0.109717	-0.000038	-0.003786	0.611401
0.047076	0.000010	0.000956	0.240384

	p space	
Exponent	2p	3p
	-3.218290	-0.209946
3116.242	0.000056	-0.000010
737.9542	0.000493	-0.000089
239.6734	0.002792	-0.000502
91.49985	0.011787	-0.002133
38.54244	0.039280	-0.007147
17.36517	0.104391	-0.019346
8.182553	0.210808	-0.039617
3.930197	0.312844	-0.060030
1.897362	0.325812	-0.066387
0.911690	0.187150	-0.038827
0.411189	0.033723	0.109830
0.175864	0.000402	0.373300
0.073941	0.000724	0.479109
0.030777	-0.000084	0.193269

Table XXXII. Al ^2P (20,15) basis set, orbital energies and eigenvectors. Energy(E_H) = -241.876695

	s space		
Exponent	1s	2s	3s
	-58.501020	-4.910666	-0.393415
3626225.	0.000002	-0.000001	0.000000
542853.7	0.000015	-0.000004	0.000001
123528.5	0.000077	-0.000020	0.000005
34989.18	0.000325	-0.000085	0.000020
11415.51	0.001183	-0.000308	0.000071
4121.529	0.003854	-0.001006	0.000232
1607.711	0.011430	-0.003001	0.000695
666.9412	0.030986	-0.008262	0.001905
290.9281	0.075760	-0.020827	0.004847
132.2357	0.161000	-0.047282	0.010966
62.14103	0.276802	-0.092486	0.021906
29.98422	0.332778	-0.144863	0.034506
14.64881	0.213115	-0.134037	0.034074
6.901022	0.043947	0.056657	-0.017187
3.370289	0.000584	0.375239	-0.105033
1.626973	0.001473	0.496449	-0.210729
0.780997	-0.000191	0.215288	-0.181262
0.242715	0.000102	0.009583	0.339698
0.108230	-0.000062	-0.002374	0.612382
0.046506	0.000017	0.000616	0.232097

	p space	
Exponent	2p	3p
	-3.218297	-0.209948
4692.288	0.000027	-0.000005
1110.726	0.000243	-0.000044
360.8181	0.001397	-0.000251
138.0415	0.006090	-0.001101
58.44202	0.021240	-0.003844
26.49167	0.060753	-0.011163
12.62287	0.139275	-0.025897
6.196135	0.243573	-0.046307
3.072954	0.318716	-0.061164
1.528175	0.287515	-0.062905
0.749864	0.133806	-0.011720
0.328872	0.017161	0.167399
0.146060	-0.000117	0.399026
0.064445	0.000574	0.431631
0.028099	-0.000069	0.148207

Table XXXIII. Si ^3P (17,12) basis set, orbital energies and eigenvectors. Energy(E_H) = -288.854207

	s space		
Exponent	1s	2s	3s
	-68.812370	-6.156468	-0.539792
915136.3	0.000013	-0.000003	0.000001
137046.8	0.000098	-0.000026	0.000007
31188.39	0.000517	-0.000138	0.000035
8833.633	0.002179	-0.000582	0.000149
2881.638	0.007866	-0.002104	0.000538
1040.162	0.024987	-0.006794	0.001747
405.5428	0.069759	-0.019417	0.004978
167.9628	0.164730	-0.049284	0.012790
72.95901	0.302855	-0.103153	0.026843
32.89601	0.360078	-0.167717	0.045394
15.05106	0.196717	-0.123009	0.033582
5.959425	0.023795	0.214934	-0.064206
2.679402	-0.001728	0.568489	-0.225729
1.192164	0.001194	0.359421	-0.269141
0.352512	-0.000396	0.023949	0.297669
0.162695	0.000238	-0.006464	0.630044
0.068471	-0.000069	0.001598	0.266436

	p space	
Exponent	2p	3p
	-4.255983	
1776.719	0.000202	
421.0382	0.001754	
136.4885	0.009504	
51.72592	0.037325	
21.56981	0.110854	
9.560458	0.237566	
4.355018	0.352961	
2.010627	0.328859	
0.923106	0.133124	
0.350629	0.010457	
0.138257	-0.000171	
0.053414	0.000272	

Table XXXIV. Si ^3P (18,13) basis set, orbital energies and eigenvectors. Energy(E_H) = -288.854295

	s space		
Exponent	1s	2s	3s
	-68.812420	-6.156507	-0.539821
1634321.	0.000006	-0.000002	0.000000
244742.0	0.000048	-0.000013	0.000003
55699.34	0.000251	-0.000067	0.000017
15776.92	0.001058	-0.000282	0.000072
5147.070	0.003838	-0.001027	0.000264
1858.148	0.012370	-0.003321	0.000849
724.7153	0.035709	-0.009787	0.002521
300.5200	0.091055	-0.025770	0.006609
130.9134	0.195369	-0.060247	0.015696
59.36738	0.320543	-0.115580	0.030163
27.81705	0.328111	-0.166988	0.045734
13.20936	0.148961	-0.088249	0.023658
5.528180	0.015324	0.256242	-0.077038
2.516762	-0.000313	0.562275	-0.232388
1.143794	0.000607	0.325856	-0.253221
0.350898	-0.000164	0.020320	0.313885
0.159511	0.000089	-0.004939	0.629593
0.067387	-0.000027	0.001262	0.254785

	p space	
Exponent	2p	3p
	-4.256023	-0.297100
2505.780	0.000111	-0.000024
593.5910	0.000974	-0.000208
192.6644	0.005410	-0.001162
73.32723	0.022106	-0.004762
30.74307	0.070105	-0.015365
13.76447	0.169164	-0.037722
6.387656	0.294645	-0.067420
3.003841	0.356462	-0.084539
1.419765	0.244486	-0.063013
0.647454	0.056941	0.096358
0.278197	0.001416	0.384559
0.116691	0.000944	0.484064
0.047757	-0.000084	0.192396

Table XXXV. Si ^3P (19,14) basis set, orbital energies and eigenvectors. Energy(E_H) = -288.854333

	s space		
Exponent	1s	2s	3s
	-68.812440	-6.156525	-0.539832
2707981.	0.000003	-0.000001	0.000000
405228.1	0.000025	-0.000007	0.000002
92186.84	0.000134	-0.000036	0.000009
26107.93	0.000564	-0.000150	0.000039
8516.967	0.002053	-0.000547	0.000140
3074.681	0.006663	-0.001786	0.000459
1199.217	0.019581	-0.005293	0.001353
497.3850	0.051940	-0.014393	0.003713
216.8450	0.121238	-0.035193	0.009037
98.44282	0.234742	-0.075617	0.019795
46.20817	0.335488	-0.132210	0.034705
22.25446	0.279925	-0.160605	0.044729
10.80372	0.092819	-0.032856	0.007510
4.917766	0.006640	0.310441	-0.094654
2.299786	0.000947	0.544340	-0.239823
1.077552	0.000066	0.279920	-0.228826
0.348582	0.000027	0.016091	0.332350
0.156160	-0.000025	-0.003325	0.628045
0.066250	0.000005	0.000895	0.242686

	p space	
Exponent	2p	3p
	-4.256041	-0.297108
3785.985	0.000054	-0.000012
896.4740	0.000479	-0.000102
291.1560	0.002716	-0.000583
111.1984	0.011541	-0.002478
46.89379	0.038769	-0.008427
21.16433	0.103976	-0.022912
9.998535	0.212188	-0.047980
4.823336	0.317749	-0.072743
2.345623	0.327899	-0.082310
1.135399	0.178385	-0.030927
0.505544	0.028378	0.166691
0.227346	-0.000201	0.412061
0.100317	0.000851	0.429210
0.043154	-0.000096	0.144188

Table XXXVI. Si ^3P (20,15) basis set, orbital energies and eigenvectors. Energy(E_H) = -288.854348

	s space		
Exponent	1s	2s	3s
	-68.812450	-6.156532	-0.539836
4200908.	0.000002	-0.000001	0.000000
628873.4	0.000015	-0.000004	0.000001
143100.2	0.000077	-0.000020	0.000005
40532.24	0.000326	-0.000087	0.000022
13223.87	0.001187	-0.000316	0.000081
4774.416	0.003866	-0.001034	0.000264
1862.386	0.011468	-0.003083	0.000792
772.5934	0.031092	-0.008493	0.002174
337.0235	0.076037	-0.021418	0.005530
153.2040	0.161613	-0.048704	0.012551
72.01526	0.277663	-0.095348	0.025087
34.76366	0.332784	-0.149307	0.039656
16.98747	0.212000	-0.136201	0.038600
7.973155	0.043206	0.064332	-0.021417
3.928469	0.000144	0.391384	-0.125331
1.932392	0.001594	0.490512	-0.249258
0.953936	-0.000313	0.198484	-0.176201
0.340751	0.000132	0.009895	0.364555
0.150628	-0.000075	-0.001392	0.620249
0.064493	0.000018	0.000451	0.223992

	p space	
Exponent	2p	3p
	-4.256047	-0.297110
5816.711	0.000025	-0.000005
1376.891	0.000227	-0.000049
447.2925	0.001311	-0.000280
171.1692	0.005749	-0.001236
72.53703	0.020233	-0.004356
32.93644	0.058504	-0.012811
15.73180	0.136081	-0.030207
7.754184	0.242109	-0.055187
3.873014	0.321248	-0.074179
1.948356	0.288673	-0.075477
0.971886	0.131003	-0.003075
0.440860	0.016907	0.208290
0.201728	0.000123	0.421957
0.091415	0.000534	0.392409
0.040475	-0.000033	0.118087

Table XXXVII. P ^4S (17,12) basis set, orbital energies and eigenvectors. Energy(E_H) = -340.718600

	s space		
Exponent	1s	2s	3s
	-79.969630	-7.511023	-0.696364
1087602.	0.000012	-0.000003	0.000001
162874.5	0.000094	-0.000026	0.000007
37066.21	0.000496	-0.000135	0.000037
10498.46	0.002090	-0.000570	0.000157
3424.730	0.007549	-0.002060	0.000565
1236.191	0.024010	-0.006655	0.001836
481.9705	0.067231	-0.019080	0.005246
199.6290	0.159787	-0.048629	0.013542
86.72575	0.297359	-0.102888	0.028729
39.10548	0.361872	-0.169537	0.049318
17.90114	0.206083	-0.132051	0.038842
7.183634	0.026918	0.199193	-0.063765
3.279601	-0.002069	0.568578	-0.247266
1.482407	0.001352	0.372001	-0.289387
0.475975	-0.000472	0.027931	0.295651
0.216657	0.000255	-0.005763	0.646196
0.090385	-0.000074	0.001512	0.269367
	p space		
Exponent	2p	3p	
	-5.400883	-0.391667	
2022.100	0.000214	-0.000051	
479.1779	0.001857	-0.000444	
155.3366	0.010071	-0.002398	
58.88741	0.039605	-0.009608	
24.57418	0.117360	-0.028783	
10.89673	0.249505	-0.063604	
4.968480	0.364213	-0.093714	
2.303074	0.317642	-0.094165	
1.063136	0.108995	0.047495	
0.436791	0.006770	0.371846	
0.178251	0.000422	0.512445	
0.070431	-0.000007	0.217984	

Table XXXVIII. P ^4S (18,13) basis set, orbital energies and eigenvectors. Energy(E_H) = -340.718706

	s space		
Exponent	1s	2s	3s
	-79.969680	-7.511066	-0.696395
1948462.	0.000006	-0.000002	0.000000
291808.8	0.000046	-0.000012	0.000003
66414.49	0.000240	-0.000065	0.000018
18812.82	0.001011	-0.000274	0.000075
6137.677	0.003667	-0.001001	0.000276
2215.792	0.011827	-0.003239	0.000888
864.2240	0.034203	-0.009555	0.002640
358.3963	0.087565	-0.025249	0.006945
156.1584	0.189405	-0.059367	0.016596
70.83940	0.315500	-0.115238	0.032277
33.20326	0.332462	-0.169620	0.049919
15.77306	0.158936	-0.098439	0.028580
6.641184	0.017679	0.244163	-0.078996
3.067501	-0.000625	0.564563	-0.256271
1.416215	0.000726	0.334720	-0.269669
0.470811	-0.000224	0.023480	0.316731
0.211579	0.000106	-0.004239	0.643068
0.088777	-0.000033	0.001179	0.256068

	p space	
Exponent	2p	3p
	-5.400928	-0.391693
2956.262	0.000110	-0.000026
700.2848	0.000969	-0.000231
227.3139	0.005399	-0.001288
86.56184	0.022171	-0.005330
36.33386	0.070711	-0.017233
16.29347	0.171535	-0.042900
7.578966	0.300225	-0.076658
3.578859	0.360617	-0.097701
1.698042	0.235640	-0.059312
0.763358	0.048380	0.139255
0.342119	0.000072	0.413135
0.148620	0.000993	0.448731
0.062345	-0.000187	0.157355

Table XXXIX. P ^4S (19,14) basis set, orbital energies and eigenvectors. Energy(E_H) = -340.718747

	s space		
Exponent	1s	2s	3s
	-79.969700	-7.511082	-0.696405
3213874.	0.000003	-0.000001	0.000000
481206.7	0.000024	-0.000007	0.000002
109508.0	0.000128	-0.000035	0.000010
31018.44	0.000542	-0.000147	0.000041
10119.94	0.001970	-0.000536	0.000147
3653.669	0.006395	-0.001748	0.000482
1425.153	0.018811	-0.005185	0.001422
591.1557	0.050003	-0.014124	0.003907
257.7838	0.117252	-0.034658	0.009547
117.0878	0.228972	-0.074957	0.021054
55.01224	0.332489	-0.132435	0.037333
26.54661	0.286082	-0.164604	0.049261
12.94518	0.100976	-0.043238	0.011386
5.892342	0.007986	0.304177	-0.100383
2.787950	0.000780	0.549025	-0.266692
1.325613	0.000103	0.283821	-0.239199
0.463248	0.000000	0.018265	0.341964
0.205811	-0.000017	-0.002642	0.637694
0.086968	0.000001	0.000820	0.241247
	p space		
Exponent	2p	3p	
	-5.400945	-0.391700	
4590.261	0.000051	-0.000012	
1086.878	0.000454	-0.000108	
353.0188	0.002584	-0.000617	
134.8886	0.011049	-0.002639	
56.95315	0.037433	-0.009064	
25.75100	0.101479	-0.024923	
12.20096	0.209986	-0.053130	
5.915730	0.318852	-0.081855	
2.901045	0.329919	-0.093038	
1.420551	0.176582	-0.027053	
0.643903	0.027882	0.195652	
0.294809	-0.000174	0.427958	
0.132365	0.000664	0.402910	
0.057563	-0.000116	0.124019	

Table XL. P ^4S (20.15) basis set, orbital energies and eigenvectors. Energy(E_H) = -340.718765

	s space		
Exponent	1s	2s	3s
	-79.969700	-7.511089	-0.696410
4754316.	0.000002	-0.000001	0.000000
711807.5	0.000015	-0.000004	0.000001
161983.4	0.000079	-0.000021	0.000006
45882.38	0.000332	-0.000090	0.000025
14969.60	0.001210	-0.000329	0.000090
5404.723	0.003940	-0.001075	0.000295
2108.250	0.011686	-0.003206	0.000883
874.5838	0.031668	-0.008832	0.002427
381.5145	0.077377	-0.022266	0.006163
173.4360	0.164119	-0.050636	0.014022
81.53782	0.280593	-0.098953	0.027934
39.36664	0.332542	-0.154110	0.044168
19.22627	0.207519	-0.136222	0.041481
8.951989	0.040477	0.080389	-0.027891
4.422854	-0.000380	0.419053	-0.150512
2.196486	0.001667	0.480868	-0.283814
1.101012	-0.000444	0.168729	-0.151016
0.437832	0.000167	0.008498	0.397894
0.193112	-0.000090	-0.000311	0.616873
0.083146	0.000021	0.000285	0.210323

	p space	
Exponent	2p	3p
	-5.400952	-0.391704
6965.440	0.000025	-0.000006
1648.816	0.000220	-0.000052
535.6371	0.001272	-0.000302
205.0095	0.005599	-0.001339
86.93168	0.019830	-0.004755
39.51888	0.057756	-0.014087
18.90755	0.135510	-0.033608
9.344997	0.243386	-0.062085
4.690607	0.324563	-0.084470
2.379795	0.287034	-0.083234
1.202373	0.124984	0.007625
0.563374	0.015911	0.236523
0.263037	0.000281	0.431025
0.121093	0.000315	0.365505
0.054091	-0.000035	0.101519

Table XLI. P^- ^3P (18,13) basis set, orbital energies and eigenvectors. Energy(E_H) = -340.698751

	s space		
Exponent	1s	2s	3s
	-79.692810	-7.232521	-0.436648
1860219.	0.000006	-0.000002	0.000000
278524.3	0.000048	-0.000013	0.000004
63375.95	0.000254	-0.000069	0.000018
17948.62	0.001072	-0.000291	0.000077
5854.675	0.003889	-0.001061	0.000284
2113.305	0.012534	-0.003434	0.000912
824.1499	0.036176	-0.010117	0.002714
341.7487	0.092182	-0.026657	0.007097
148.8973	0.197429	-0.062284	0.016929
67.55529	0.322310	-0.119402	0.032354
31.68551	0.326212	-0.170788	0.049124
15.08552	0.145482	-0.086376	0.023594
6.378281	0.014753	0.268553	-0.083551
2.941027	-0.000270	0.567217	-0.259220
1.360365	0.000524	0.310584	-0.240767
0.429533	-0.000138	0.018175	0.393931
0.177964	0.000052	-0.003028	0.614788
0.065004	-0.000018	0.000941	0.212372

	p space	
Exponent	2p	3p
	-5.123795	-0.077140
2352.177	0.000164	-0.000034
557.3088	0.001435	-0.000303
180.7872	0.007870	-0.001654
68.67665	0.031510	-0.006744
28.73619	0.096400	-0.020788
12.81577	0.216564	-0.048528
5.899562	0.341259	-0.076805
2.759996	0.344565	-0.088301
1.291636	0.160009	-0.001253
0.529089	0.016901	0.251927
0.216639	-0.000196	0.432145
0.082697	0.000599	0.369727
0.028186	-0.000004	0.144516

Table XLII. P^- ^3P (19,14) basis set, orbital energies and eigenvectors. Energy(E_H) = -340.698815

	s space		
Exponent	1s	2s	3s
	-79.692870	-7.232585	-0.436709
2295023.	0.000005	-0.000001	0.000000
343621.8	0.000037	-0.000010	0.000003
78197.51	0.000195	-0.000053	0.000014
22148.11	0.000825	-0.000224	0.000060
7225.476	0.002995	-0.000816	0.000217
2608.571	0.009682	-0.002649	0.000707
1017.468	0.028183	-0.007836	0.002089
421.9758	0.073209	-0.020930	0.005606
183.8690	0.163374	-0.050108	0.013468
83.35649	0.289743	-0.101423	0.027678
38.97863	0.346213	-0.161769	0.045125
18.44785	0.205597	-0.134097	0.039327
8.000464	0.032842	0.134625	-0.043695
3.817351	-0.001728	0.497386	-0.185951
1.820878	0.001819	0.443494	-0.297470
0.848190	-0.000680	0.085008	-0.042451
0.371850	0.000280	0.000270	0.494944
0.152901	-0.000116	0.001011	0.554858
0.057533	0.000025	0.000021	0.156574

	p space	
Exponent	2p	3p
	-5.123862	-0.077186
3346.731	0.000089	-0.000019
791.9358	0.000785	-0.000165
256.8851	0.004410	-0.000931
97.84137	0.018364	-0.003889
41.09968	0.059755	-0.012863
18.46267	0.150217	-0.032958
8.632212	0.276073	-0.062277
4.107007	0.356005	-0.083081
1.975683	0.269285	-0.067863
0.935356	0.076961	0.067666
0.416336	0.003980	0.303454
0.176337	0.001004	0.416185
0.069783	0.000056	0.319601
0.024870	0.000108	0.112021

Table XLIII. S ^3P (17,12) basis set, orbital energies and eigenvectors. Energy(E_H) = -397.504682

	s space		
Exponent	1s	2s	3s
	-92.004350	-9.004211	-0.879472
1270413.	0.000012	-0.000003	0.000001
190248.7	0.000091	-0.000025	0.000007
43295.71	0.000481	-0.000133	0.000038
12262.88	0.002026	-0.000561	0.000163
4000.304	0.007319	-0.002032	0.000589
1443.946	0.023301	-0.006566	0.001914
562.9727	0.065386	-0.018871	0.005482
233.1948	0.156145	-0.048247	0.014204
101.3249	0.293186	-0.102915	0.030384
45.69807	0.362879	-0.171268	0.052747
20.93518	0.213069	-0.139051	0.043404
8.493076	0.029498	0.187943	-0.063574
3.924382	-0.002337	0.569305	-0.266729
1.795783	0.001468	0.380152	-0.305690
0.609194	-0.000531	0.031061	0.305443
0.274524	0.000262	-0.005068	0.657507
0.113436	-0.000077	0.001459	0.263661

	p space	
Exponent	2p	3p
	-6.682424	
2199.902	0.000239	
521.3185	0.002077	
168.9647	0.011242	
64.03679	0.044070	
26.71867	0.129187	
11.82811	0.269107	
5.377925	0.378559	
2.481490	0.296922	
1.114796	0.077861	
0.484492	0.002010	
0.200490	0.001444	
0.079451	-0.000062	

Table XLIV. S ^3P (18,13) basis set, orbital energies and eigenvectors. Energy(E_H) = -397.504809

	s space		
Exponent	1s	2s	3s
	-92.004410	-9.004256	-0.879502
2274842.	0.000006	-0.000002	0.000001
340650.2	0.000044	-0.000012	0.000004
77524.87	0.000232	-0.000064	0.000019
21958.96	0.000980	-0.000271	0.000079
7164.041	0.003558	-0.000987	0.000287
2586.393	0.011479	-0.003198	0.000927
1008.801	0.033236	-0.009440	0.002756
418.3794	0.085316	-0.025009	0.007270
182.3255	0.185531	-0.059035	0.017447
82.73415	0.312106	-0.115532	0.034227
38.79145	0.335031	-0.172068	0.053614
18.43911	0.165512	-0.105436	0.032595
7.809316	0.019397	0.237427	-0.081581
3.649862	-0.000864	0.566951	-0.278309
1.706570	0.000808	0.338523	-0.281427
0.599254	-0.000271	0.025725	0.331011
0.267105	0.000115	-0.003529	0.651812
0.111144	-0.000037	0.001120	0.248905

	p space	
Exponent	2p	3p
	-6.682474	-0.437349
3409.886	0.000111	-0.000028
807.7113	0.000981	-0.000251
262.1962	0.005474	-0.001398
99.88313	0.022555	-0.005823
41.96443	0.072166	-0.018856
18.84448	0.175250	-0.047258
8.784542	0.306466	-0.084204
4.166821	0.362435	-0.107678
1.988375	0.224400	-0.049780
0.889997	0.041647	0.184487
0.399230	0.000035	0.426701
0.172546	0.001213	0.414984
0.071738	-0.000064	0.140372

Table XLV. S ^3P (19,14) basis set, orbital energies and eigenvectors. Energy(E_H) = -397.504857

	s space		
Exponent	1s	2s	3s
	-92.004430	-9.004273	-0.879513
3723841.	0.000003	-0.000001	0.000000
557539.5	0.000024	-0.000007	0.000002
126877.3	0.000126	-0.000035	0.000010
35938.26	0.000530	-0.000147	0.000043
11725.10	0.001929	-0.000534	0.000155
4233.234	0.006262	-0.001742	0.000507
1651.239	0.018430	-0.005168	0.001498
684.9535	0.049050	-0.014090	0.004119
298.7111	0.115313	-0.034657	0.010094
135.7104	0.226209	-0.075248	0.022345
63.79220	0.331065	-0.133759	0.039920
30.81179	0.288984	-0.167905	0.053211
15.05720	0.104876	-0.048064	0.013782
6.875340	0.008628	0.305062	-0.107714
3.286845	0.000684	0.552219	-0.291998
1.582565	0.000103	0.280982	-0.243022
0.584575	-0.000017	0.019404	0.362462
0.258294	-0.000017	-0.001924	0.642544
0.108451	-0.000001	0.000758	0.231764

	p space	
Exponent	2p	3p
	-6.682492	-0.437358
5265.683	0.000052	-0.000013
1246.803	0.000464	-0.000118
404.9661	0.002642	-0.000676
154.7606	0.011322	-0.002898
65.37882	0.038457	-0.009995
29.59011	0.104369	-0.027549
14.03998	0.215580	-0.058768
6.826454	0.325199	-0.090353
3.368830	0.326455	-0.100084
1.665416	0.163037	-0.010835
0.767430	0.023897	0.233032
0.350203	0.000441	0.430976
0.155585	0.000748	0.375143
0.066770	0.000019	0.113660

Table XLVI. S ^3P (20,15) basis set, orbital energies and eigenvectors. Energy(E_H) = -397.504877

	s space		
Exponent	1s	2s	3s
	-92.004440	-9.004282	-0.879521
5352410.	0.000002	-0.000001	0.000000
801328.7	0.000015	-0.000004	0.000001
182353.0	0.000080	-0.000022	0.000006
51652.55	0.000337	-0.000093	0.000027
16852.49	0.001228	-0.000339	0.000099
6084.673	0.003998	-0.001110	0.000322
2373.537	0.011855	-0.003309	0.000963
984.6539	0.032115	-0.009117	0.002649
429.5383	0.078420	-0.022984	0.006719
195.2779	0.166077	-0.052278	0.015327
91.82009	0.282866	-0.102057	0.030452
44.33904	0.332270	-0.158212	0.048192
21.65035	0.203957	-0.136281	0.043883
10.02785	0.038407	0.094849	-0.034096
4.954637	-0.000691	0.445537	-0.177188
2.465773	0.001665	0.472370	-0.314532
1.234009	-0.000538	0.141050	-0.116837
0.531535	0.000199	0.006388	0.439645
0.235483	-0.000103	0.000558	0.604595
0.101653	0.000022	0.000178	0.189657

	p space	
Exponent	2p	3p
	-6.682501	-0.437364
7777.460	0.000026	-0.000007
1840.932	0.000236	-0.000060
598.0113	0.001361	-0.000347
228.8665	0.005994	-0.001536
97.04711	0.021233	-0.005467
44.12793	0.061749	-0.016169
21.11828	0.143930	-0.038486
10.43628	0.255466	-0.070228
5.242591	0.332456	-0.094615
2.668014	0.273941	-0.083816
1.354099	0.103603	0.039854
0.652204	0.011314	0.275758
0.305685	0.000930	0.424313
0.140051	0.000367	0.332422
0.062063	0.000079	0.090080

Table XLVII. $S^-\ ^2P$ (18,13 basis set, orbital energies and eigenvectors. Energy(E_H) = -397.538292

	s space		
Exponent	1s	2s	3s
	-91.676280	-8.675611	-0.579708
2156703.	0.000006	-0.000002	0.000001
322953.8	0.000047	-0.000013	0.000004
73495.72	0.000248	-0.000069	0.000019
20816.96	0.001048	-0.000290	0.000082
6791.142	0.003802	-0.001055	0.000299
2451.638	0.012257	-0.003416	0.000961
956.1979	0.035407	-0.010070	0.002861
396.5454	0.090421	-0.026588	0.007503
172.8043	0.194488	-0.062339	0.017953
78.43163	0.319912	-0.120274	0.034582
36.80994	0.328356	-0.173577	0.052965
17.54592	0.150332	-0.091863	0.026931
7.451398	0.015891	0.266533	-0.088710
3.475782	-0.000474	0.570220	-0.283351
1.629429	0.000579	0.309831	-0.248003
0.548946	-0.000176	0.019867	0.402128
0.228276	0.000059	-0.002453	0.622441
0.084253	-0.000021	0.000904	0.210244

	p space	
Exponent	2p	3p
	-6.355371	-0.107717
2759.371	0.000161	-0.000037
653.7488	0.001411	-0.000329
212.0970	0.007767	-0.001804
80.62413	0.031273	-0.007384
33.77725	0.096281	-0.022990
15.09231	0.217794	-0.054000
6.971434	0.344863	-0.086683
3.283612	0.343446	-0.097078
1.553606	0.152708	0.009010
0.662687	0.016105	0.273439
0.276235	0.000485	0.433391
0.107186	0.000685	0.352003
0.037248	0.000113	0.130721

Table XLVIII. S^- ^2P (19,14) basis set, orbital energies and eigenvectors. Energy(E_H) = -397.538367

	s space		
Exponent	1s	2s	3s
	-91.676350	-8.675680	-0.579772
2784727.	0.000004	-0.000001	0.000000
416968.4	0.000034	-0.000010	0.000003
94890.45	0.000180	-0.000050	0.000014
26877.82	0.000762	-0.000211	0.000059
8768.808	0.002768	-0.000767	0.000216
3165.686	0.008959	-0.002493	0.000705
1234.663	0.026144	-0.007382	0.002084
511.9785	0.068296	-0.019822	0.005626
223.0560	0.154196	-0.047788	0.013600
101.1080	0.279470	-0.098384	0.028457
47.27453	0.348077	-0.160758	0.047455
22.41046	0.222484	-0.146678	0.045717
9.962177	0.040959	0.098574	-0.034319
4.803511	-0.001569	0.476369	-0.186620
2.318301	0.001961	0.471775	-0.320704
1.108874	-0.000717	0.109356	-0.063184
0.478163	0.000270	0.002422	0.498386
0.198496	-0.000120	0.001063	0.563175
0.075419	0.000025	0.000089	0.158627
	p space		
Exponent	2p	3p	
	-6.355442	-0.107768	
3898.141	0.000088	-0.000020	
923.2414	0.000779	-0.000181	
299.7695	0.004380	-0.001020	
114.3267	0.018289	-0.004283	
48.11503	0.059743	-0.014193	
21.66395	0.150858	-0.036716	
10.15949	0.278798	-0.069634	
4.855303	0.359393	-0.094242	
2.347403	0.264880	-0.069463	
1.110442	0.070885	0.092733	
0.508450	0.003244	0.324952	
0.219899	0.001406	0.408403	
0.088800	0.000183	0.295612	
0.032431	0.000177	0.097184	

Table XLIX. Cl ^2P (17,12) basis set, orbital energies and eigenvectors. Energy(E_H) = -459.481828

	s space		
Exponent	1s	2s	3s
	-104.884300	-10.607400	-1.072853
1464354.	0.000012	-0.000003	0.000001
219299.6	0.000089	-0.000025	0.000008
49907.83	0.000469	-0.000132	0.000040
14135.80	0.001976	-0.000556	0.000168
4611.304	0.007142	-0.002012	0.000608
1664.496	0.022754	-0.006505	0.001977
648.9663	0.063961	-0.018729	0.005671
268.8316	0.153312	-0.048008	0.014736
116.8292	0.289871	-0.103064	0.031734
52.70434	0.363480	-0.172862	0.055569
24.16458	0.218544	-0.144707	0.047263
9.889574	0.031670	0.179575	-0.063354
4.614575	-0.002558	0.570388	-0.283188
2.132459	0.001557	0.385509	-0.317425
0.753206	-0.000581	0.033675	0.313893
0.336761	0.000266	-0.004391	0.664941
0.138453	-0.000079	0.001418	0.259894

	p space	
Exponent	2p	3p
	-8.072137	-0.506348
2507.025	0.000242	-0.000065
594.0857	0.002108	-0.000568
192.5719	0.011433	-0.003104
73.02404	0.044957	-0.012334
30.49827	0.131976	-0.037220
13.51760	0.274938	-0.079663
6.160296	0.383473	-0.117571
2.850872	0.288717	-0.084354
1.268562	0.068735	0.143901
0.559402	0.001072	0.422525
0.233648	0.001855	0.443514
0.092979	0.000008	0.165633

Table L. Cl ^3P (18.13) basis set, orbital energies and eigenvectors. Energy(E_H) = -459.481973

	s space		
Exponent	1s	2s	3s
	-104.884400	-10.607440	-1.072883
2609488.	0.000006	-0.000002	0.000001
391014.6	0.000043	-0.000012	0.000004
89016.90	0.000228	-0.000064	0.000019
25215.81	0.000961	-0.000269	0.000081
8225.896	0.003488	-0.000983	0.000298
2969.446	0.011261	-0.003184	0.000961
1158.154	0.032629	-0.009402	0.002861
480.3547	0.083891	-0.024949	0.007560
209.3989	0.183008	-0.059039	0.018192
95.07553	0.309702	-0.116132	0.035896
44.61405	0.336395	-0.174243	0.056675
21.23257	0.170008	-0.110434	0.035825
9.034738	0.020710	0.233983	-0.084333
4.265103	-0.001085	0.569271	-0.297315
2.015105	0.000877	0.339339	-0.288269
0.737110	-0.000316	0.027446	0.343498
0.326514	0.000122	-0.002843	0.657009
0.135331	-0.000040	0.001072	0.243661

	p space	
Exponent	2p	3p
	-8.072189	-0.506376
3935.210	0.000111	-0.000030
932.1996	0.000973	-0.000263
302.6459	0.005445	-0.001469
115.3447	0.022519	-0.006154
48.50820	0.072367	-0.020019
21.81634	0.176436	-0.050497
10.19674	0.309542	-0.090429
4.861767	0.363174	-0.115457
2.337857	0.217945	-0.043438
1.056498	0.039105	0.209506
0.474812	0.000500	0.433119
0.205191	0.001363	0.396203
0.085023	0.000052	0.130067

Table LI. Cl ^3P (19,14) basis set, orbital energies and eigenvectors. Energy(E_H) = -459.482027

	s space		
Exponent	1s	2s	3s
	-104.884400	-10.607460	-1.072896
4253216.	0.000003	-0.000001	0.000000
636820.6	0.000023	-0.000007	0.000002
144921.1	0.000124	-0.000035	0.000011
41049.47	0.000523	-0.000147	0.000044
13392.69	0.001904	-0.000534	0.000161
4835.298	0.006180	-0.001745	0.000529
1886.084	0.018195	-0.005178	0.001564
782.3777	0.048466	-0.014128	0.004304
341.2166	0.114133	-0.034809	0.010572
155.0482	0.224560	-0.075794	0.023465
72.90684	0.330239	-0.135293	0.042166
35.23558	0.290721	-0.170791	0.056503
17.24339	0.107179	-0.050828	0.015535
7.898163	0.008985	0.308761	-0.115218
3.807610	0.000614	0.554968	-0.314059
1.851135	0.000089	0.275597	-0.241668
0.713160	-0.000030	0.020043	0.380395
0.314002	-0.000019	-0.001245	0.644055
0.131570	-0.000002	0.000703	0.224353

	p space	
Exponent	2p	3p
	-8.072209	-0.506388
5987.313	0.000053	-0.000014
1417.633	0.000472	-0.000127
460.4456	0.002692	-0.000728
175.9800	0.011561	-0.003133
74.37389	0.039368	-0.010829
33.68659	0.106968	-0.029955
15.99962	0.220714	-0.063874
7.794821	0.330978	-0.098297
3.864784	0.322723	-0.104942
1.924396	0.151079	0.004631
0.903592	0.020945	0.258114
0.414371	0.001027	0.431401
0.184282	0.000840	0.354777
0.078898	0.000124	0.104358

Table LII. Cl ^3P (20,15) basis set, orbital energies and eigenvectors. Energy(E_H) = -459.482052

	s space		
Exponent	1s	2s	3s
	-104.884400	-10.607470	-1.072906
6086151.	0.000002	-0.000001	0.000000
911229.3	0.000015	-0.000004	0.000001
207369.9	0.000079	-0.000022	0.000007
58739.98	0.000334	-0.000094	0.000028
19165.16	0.001218	-0.000342	0.000104
6919.745	0.003967	-0.001117	0.000338
2699.305	0.011764	-0.003333	0.001010
1119.806	0.031883	-0.009186	0.002784
488.5057	0.077921	-0.023182	0.007061
222.1023	0.165284	-0.052819	0.016159
104.4514	0.282172	-0.103416	0.032167
50.45265	0.332564	-0.160707	0.051205
24.64914	0.205273	-0.138953	0.046665
11.43946	0.038983	0.097132	-0.036100
5.663550	-0.000758	0.457868	-0.195662
2.824183	0.001649	0.471145	-0.336423
1.405498	-0.000586	0.129855	-0.092894
0.631179	0.000214	0.005485	0.466840
0.281258	-0.000111	0.001071	0.593313
0.121833	0.000022	0.000137	0.176294

	p space	
Exponent	2p	3p
	-8.072220	-0.506395
8796.819	0.000027	-0.000007
2082.182	0.000242	-0.000065
676.3623	0.001399	-0.000377
258.8527	0.006168	-0.001671
109.7799	0.021893	-0.005971
49.93945	0.063760	-0.017677
23.91250	0.148477	-0.042185
11.82301	0.262707	-0.076719
5.946650	0.337508	-0.103254
3.031694	0.265425	-0.082735
1.537954	0.091054	0.066325
0.753207	0.008884	0.300406
0.356103	0.001379	0.417248
0.163907	0.000474	0.307849
0.072721	0.000151	0.080386

Table LIII. Cl^- ^1S (18,1 basis set, orbital energies and eigenvectors. Energy(E_H) = -459.576774

	s space		
Exponent	1s	2s	3s
	-104.505600	-10.229350	-0.733285
2475703.	0.000006	-0.000002	0.000001
370712.6	0.000046	-0.000013	0.000004
84364.33	0.000243	-0.000068	0.000020
23895.95	0.001028	-0.000288	0.000085
7795.843	0.003728	-0.001050	0.000310
2814.430	0.012024	-0.003401	0.000999
1097.731	0.034762	-0.010030	0.002976
455.2651	0.088940	-0.026531	0.007823
198.4209	0.192004	-0.062396	0.018766
90.08294	0.317880	-0.121051	0.036409
42.29576	0.330145	-0.176072	0.056155
20.17769	0.154424	-0.096508	0.029906
8.598023	0.016869	0.265685	-0.093341
4.048355	-0.000664	0.573189	-0.303831
1.917318	0.000627	0.308071	-0.251725
0.678294	-0.000213	0.021248	0.408762
0.282890	0.000065	-0.001887	0.627047
0.105600	-0.000024	0.000872	0.209833

	p space	
Exponent	2p	3p
	-7.695744	-0.150224
3212.738	0.000158	-0.000039
761.1425	0.001380	-0.000343
246.9721	0.007624	-0.001893
93.93957	0.030861	-0.007779
39.39962	0.095628	-0.024452
17.63367	0.218024	-0.057861
8.169030	0.347557	-0.094293
3.867764	0.343476	-0.103332
1.843638	0.147991	0.017731
0.810741	0.015154	0.287387
0.343983	0.000240	0.433165
0.136075	0.000165	0.339393
0.048473	-0.000021	0.119674

Table LIV. Cl^- ^1S (19,14) basis set, orbital energies and eigenvectors. Energy(E_H) = -459.576857

	s space		
Exponent	1s	2s	3s
	-104.505700	-10.229420	-0.733346
3249104.	0.000004	-0.000001	0.000000
486495.6	0.000033	-0.000009	0.000003
110712.5	0.000173	-0.000049	0.000014
31359.44	0.000732	-0.000205	0.000061
10230.97	0.002661	-0.000748	0.000220
3693.568	0.008614	-0.002433	0.000718
1440.549	0.025169	-0.007207	0.002126
597.3637	0.065925	-0.019401	0.005750
260.2796	0.149684	-0.046944	0.013958
118.0074	0.274135	-0.097479	0.029446
55.20054	0.348259	-0.161145	0.049747
26.21200	0.230761	-0.153358	0.049950
11.81335	0.045673	0.082553	-0.030016
5.718663	-0.001323	0.470994	-0.194629
2.774713	0.001960	0.483644	-0.340005
1.332335	-0.000736	0.116881	-0.062330
0.584347	0.000269	0.003228	0.506464
0.244902	-0.000125	0.001300	0.562432
0.094408	0.000025	0.000109	0.156660

	p space	
Exponent	2p	3p
	-7.695813	-0.150274
4618.003	0.000084	-0.000021
1093.668	0.000740	-0.000183
355.1296	0.004171	-0.001036
135.5096	0.017523	-0.004385
57.09366	0.057716	-0.014644
25.74903	0.147421	-0.038421
12.10980	0.276517	-0.074025
5.814367	0.361077	-0.102103
2.829132	0.267338	-0.072710
1.347763	0.071853	0.104180
0.626745	0.002995	0.335033
0.275482	0.000935	0.404678
0.113358	-0.000183	0.283264
0.042389	0.000060	0.088434

Table LV. Ar ^1S (15,10) basis set, orbital energies and eigenvectors. Energy(E_H) = -526.815610

	s space		
Exponent	1s	2s	3s
	-118.609700	-12.321520	-1.276881
545425.7	0.000045	-0.000013	0.000004
81704.52	0.000354	-0.000100	0.000031
18594.37	0.001855	-0.000529	0.000165
5265.942	0.007763	-0.002213	0.000691
1717.369	0.027431	-0.007970	0.002499
619.5353	0.082546	-0.024633	0.007728
241.1046	0.201891	-0.066001	0.020943
99.49535	0.357530	-0.138399	0.044551
42.99420	0.349216	-0.201705	0.068067
19.05790	0.117158	-0.040136	0.013721
7.480372	0.005462	0.484801	-0.207577
3.205145	0.000513	0.578390	-0.424720
1.200495	-0.000157	0.088116	0.069297
0.521108	0.000033	-0.007087	0.734122
0.195502	-0.000024	0.002301	0.396577

	p space	
Exponent	2p	3p
	-9.570775	-0.590556
1258.411	0.001002	-0.000278
298.2482	0.008364	-0.002367
96.01515	0.041882	-0.011810
35.99376	0.142037	-0.041952
14.71030	0.316022	-0.094349
6.267222	0.421644	-0.141446
2.733425	0.246286	-0.033608
1.031434	0.029102	0.347303
0.393761	-0.001819	0.538356
0.140331	0.000615	0.270685

Table LVI. Ar ^1S (16,10) basis set, orbital energies and eigenvectors. Energy(E_H) = -526.815981

	s space		
Exponent	1s	2s	3s
	-118.609900	-12.321650	-1.276950
901943.1	0.000024	-0.000007	0.000002
135088.9	0.000189	-0.000054	0.000017
30743.17	0.000992	-0.000282	0.000088
8706.985	0.004166	-0.001187	0.000370
2839.882	0.014919	-0.004290	0.001345
1024.715	0.046453	-0.013619	0.004260
399.1070	0.123360	-0.038098	0.012039
164.8535	0.261501	-0.090111	0.028596
71.20951	0.378964	-0.167745	0.055172
31.49795	0.272997	-0.178022	0.060222
12.85603	0.050042	0.104386	-0.036744
5.918585	-0.003617	0.562678	-0.275675
2.675070	0.002202	0.449386	-0.362290
0.940875	-0.000871	0.045885	0.274058
0.423493	0.000410	-0.006000	0.682506
0.171320	-0.000118	0.001879	0.283022

	p space	
Exponent	2p	3p
	-9.570854	
1259.028	0.001002	
298.3944	0.008358	
96.06381	0.041849	
36.01330	0.141941	
14.71791	0.315938	
6.269592	0.421734	
2.733978	0.246410	
1.031371	0.029109	
0.393528	-0.001820	
0.140184	0.000615	

Table LVII. Ar ^1S (16,11) basis set, orbital energies and eigenvectors. Energy(E_H) = -526.816782

	s space		
Exponent	1s	2s	3s
	-118.610100	-12.321920	-1.277183
903124.7	0.000024	-0.000007	0.000002
135265.4	0.000189	-0.000054	0.000017
30783.22	0.000990	-0.000281	0.000088
8718.291	0.004159	-0.001185	0.000370
2843.559	0.014895	-0.004283	0.001342
1026.043	0.046383	-0.013598	0.004253
399.6206	0.123199	-0.038043	0.012022
165.0609	0.261260	-0.090010	0.028563
71.29766	0.378897	-0.167617	0.055130
31.53799	0.273336	-0.178195	0.060275
12.88198	0.050256	0.103377	-0.036354
5.929457	-0.003597	0.562101	-0.275126
2.679522	0.002200	0.450536	-0.362891
0.942572	-0.000871	0.046237	0.271821
0.424622	0.000410	-0.006075	0.682979
0.171652	-0.000117	0.001896	0.284480

	p space	
Exponent	2p	3p
	-9.571201	-0.590854
1869.580	0.000505	-0.000142
443.1443	0.004323	-0.001209
143.2651	0.022627	-0.006411
54.04226	0.083765	-0.024080
22.39138	0.217573	-0.065084
9.745355	0.373971	-0.115274
4.363621	0.365488	-0.123412
1.959873	0.129172	0.064957
0.825975	0.006982	0.403640
0.329748	0.000819	0.490462
0.124250	-0.000148	0.208650

Table LVIII. Ar ^1S (17,12) basis set, orbital energies and eigenvectors. Energy(E_H) = -526.817238

	s space		
Exponent	1s	2s	3s
	-118.610200	-12.322070	-1.277289
1670366.	0.000011	-0.000003	0.000001
250141.2	0.000087	-0.000025	0.000008
56925.56	0.000460	-0.000131	0.000041
16123.34	0.001937	-0.000552	0.000173
5259.645	0.007000	-0.001998	0.000623
1898.516	0.022314	-0.006459	0.002028
740.2106	0.062813	-0.018626	0.005827
306.6452	0.151020	-0.047850	0.015176
133.2833	0.287147	-0.103264	0.032865
60.14317	0.363853	-0.174315	0.057955
27.59682	0.222994	-0.149431	0.050599
11.37590	0.033533	0.173119	-0.063174
5.351630	-0.002746	0.571635	-0.297410
2.492931	0.001628	0.389143	-0.326062
0.908063	-0.000626	0.035909	0.321246
0.403571	0.000269	-0.003761	0.669928
0.165509	-0.000080	0.001386	0.257309

	p space	
Exponent	2p	3p
	-9.571369	-0.590960
2870.502	0.000240	-0.000067
680.1966	0.002090	-0.000584
220.5214	0.011368	-0.003204
83.67863	0.044896	-0.012775
34.98858	0.132358	-0.038835
15.53587	0.277077	-0.083517
7.104168	0.386140	-0.124254
3.304367	0.284953	-0.082067
1.471953	0.064962	0.165352
0.653233	0.000111	0.431300
0.274643	0.001137	0.427941
0.109693	-0.000252	0.153744

Table LIX. Ar ^1S (18,12) basis set, orbital energies and eigenvectors. Energy(E_H) = -526.817300

	s space		
Exponent	1s	2s	3s
	-118.610300	-12.322080	-1.277293
2979618.	0.000005	-0.000002	0.000001
446161.6	0.000042	-0.000012	0.000004
101533.6	0.000223	-0.000063	0.000020
28759.11	0.000942	-0.000267	0.000083
9382.480	0.003418	-0.000975	0.000305
3387.263	0.011037	-0.003161	0.000986
1321.162	0.032006	-0.009339	0.002935
547.9339	0.082459	-0.024830	0.007774
238.8221	0.180607	-0.058948	0.018767
108.4130	0.307693	-0.116645	0.037280
50.86172	0.337999	-0.176338	0.059317
24.20935	0.173976	-0.114914	0.038746
10.34525	0.021803	0.231519	-0.086758
4.922756	-0.001244	0.571723	-0.313860
2.344654	0.000916	0.339328	-0.292346
0.884248	-0.000349	0.028890	0.354289
0.390090	0.000124	-0.002244	0.659822
0.161473	-0.000042	0.001038	0.239860

	p space	
Exponent	2p	3p
	-9.571374	-0.590963
2870.670	0.000240	-0.000067
680.2364	0.002090	-0.000584
220.5344	0.011367	-0.003204
83.68311	0.044893	-0.012774
34.99004	0.132353	-0.038833
15.53676	0.277051	-0.083509
7.104985	0.386099	-0.124239
3.304985	0.284980	-0.082093
1.472417	0.065006	0.165207
0.653485	0.000116	0.431236
0.274727	0.001137	0.428087
0.109703	-0.000252	0.153811

Table LX. Ar ^1S (18,13) basis set, orbital energies and eigenvectors. Energy(E_H) = -526.817400

	s space		
Exponent	1s	2s	3s
	-118.610300	-12.322110	-1.277321
2922053.	0.000005	-0.000002	0.000001
445704.9	0.000042	-0.000012	0.000004
101280.2	0.000224	-0.000064	0.000020
28723.56	0.000940	-0.000267	0.000083
9415.038	0.003387	-0.000966	0.000303
3415.181	0.010883	-0.003116	0.000972
1335.752	0.031528	-0.009198	0.002891
554.6218	0.081317	-0.024466	0.007660
241.7787	0.178641	-0.058219	0.018532
109.7204	0.305957	-0.115574	0.036927
51.44552	0.339327	-0.176040	0.059166
24.45384	0.177486	-0.117394	0.039621
10.38294	0.022621	0.229211	-0.085869
4.935751	-0.001465	0.572290	-0.313480
2.349089	0.001014	0.340685	-0.293513
0.885057	-0.000388	0.029151	0.353614
0.390262	0.000143	-0.002315	0.660325
0.161506	-0.000047	0.001057	0.239965

	p space	
Exponent	2p	3p
	-9.571423	-0.590990
4495.432	0.000110	-0.000031
1064.541	0.000969	-0.000272
345.5496	0.005433	-0.001521
131.7266	0.022546	-0.006394
55.43991	0.072724	-0.020893
24.96524	0.177862	-0.052956
11.69462	0.312700	-0.095322
5.601583	0.363655	-0.120940
2.712658	0.211908	-0.036894
1.240148	0.036682	0.227658
0.559669	0.000012	0.437119
0.242722	0.000623	0.382244
0.100665	-0.000125	0.121628

Table LXI. Ar ^1S (19,13) basis set, orbital energies and eigenvectors. Energy(E_H) = -526.817428

	s space		
Exponent	1s	2s	3s
	-118.610300	-12.322120	-1.277325
4818935.	0.000003	-0.000001	0.000000
721522.6	0.000023	-0.000007	0.000002
164197.0	0.000122	-0.000035	0.000011
46509.55	0.000517	-0.000147	0.000046
15174.12	0.001881	-0.000535	0.000167
5478.469	0.006107	-0.001746	0.000547
2136.963	0.017987	-0.005184	0.001618
886.4458	0.047945	-0.014155	0.004454
386.6163	0.113081	-0.034929	0.010965
175.7020	0.223084	-0.076255	0.024389
82.64155	0.329498	-0.136621	0.044066
39.96008	0.292272	-0.173379	0.059315
19.57890	0.109241	-0.053269	0.017173
8.988502	0.009305	0.312618	-0.122189
4.362390	0.000542	0.557537	-0.333074
2.135958	0.000078	0.270334	-0.238086
0.849671	-0.000044	0.020516	0.395332
0.373438	-0.000020	-0.000659	0.643848
0.156499	-0.000003	0.000662	0.218739

	p space	
Exponent	2p	3p
	-9.571427	-0.590992
4500.972	0.000110	-0.000031
1066.096	0.000967	-0.000271
346.1102	0.005418	-0.001516
131.9542	0.022484	-0.006376
55.53814	0.072548	-0.020841
25.00896	0.177552	-0.052861
11.71484	0.312410	-0.095223
5.611109	0.363765	-0.120957
2.717150	0.212445	-0.037291
1.242119	0.036889	0.227031
0.560618	0.000008	0.436981
0.243087	0.000628	0.382783
0.100766	-0.000126	0.121997

Table LXII. Ar ^1S (19,14) basis set, orbital energies and eigenvectors. Energy(E_H) = -526.817462

	s space		
Exponent	1s	2s	3s
	-118.610300	-12.322130	-1.277336
4812637.	0.000003	-0.000001	0.000000
720569.4	0.000023	-0.000007	0.000002
163977.5	0.000123	-0.000035	0.000011
46446.75	0.000518	-0.000147	0.000046
15153.44	0.001884	-0.000536	0.000167
5470.936	0.006118	-0.001749	0.000548
2134.002	0.018017	-0.005193	0.001621
885.2129	0.048022	-0.014178	0.004461
386.0759	0.113246	-0.034984	0.010982
175.4522	0.223343	-0.076362	0.024424
82.52031	0.329668	-0.136767	0.044116
39.89823	0.292026	-0.173375	0.059320
19.54606	0.108843	-0.052766	0.016993
8.976348	0.009225	0.313422	-0.122554
4.356667	0.000553	0.557423	-0.333334
2.133431	0.000073	0.269571	-0.237409
0.849085	-0.000042	0.020414	0.395962
0.373161	-0.000021	-0.000643	0.643597
0.156409	-0.000003	0.000658	0.218371

	p space	
Exponent	2p	3p
	-9.571446	-0.591004
6770.289	0.000054	-0.000015
1602.972	0.000478	-0.000133
520.6338	0.002727	-0.000765
199.0005	0.011737	-0.003301
84.13351	0.040072	-0.011437
38.13115	0.109060	-0.031772
18.12488	0.225094	-0.067797
8.843640	0.336163	-0.104646
4.399346	0.319695	-0.107543
2.200185	0.141272	0.019295
1.049559	0.018054	0.276722
0.484919	0.000547	0.430477
0.216819	0.000169	0.338324
0.093051	-0.000015	0.096251

Table LXIII. Ar ^1S (20,15) basis set, orbital energies and eigenvectors. Energy(E_H) = -526.817490

	s space		
Exponent	1s	2s	3s
	-118.610300	-12.322150	-1.277347
6928373.	0.000002	-0.000001	0.000000
1037230.	0.000015	-0.000004	0.000001
236034.7	0.000078	-0.000022	0.000007
66858.44	0.000329	-0.000093	0.000029
21813.69	0.001197	-0.000340	0.000106
7875.930	0.003898	-0.001112	0.000347
3072.263	0.011563	-0.003318	0.001039
1274.512	0.031361	-0.009149	0.002865
555.9950	0.076762	-0.023126	0.007275
252.8011	0.163303	-0.052815	0.016703
118.9069	0.280177	-0.103877	0.033382
57.45065	0.333084	-0.162331	0.053551
28.09008	0.208711	-0.142725	0.049558
13.09794	0.040730	0.093518	-0.035751
6.504422	-0.000735	0.462721	-0.208326
3.253226	0.001640	0.473443	-0.352806
1.615179	-0.000616	0.127001	-0.077718
0.740401	0.000218	0.005434	0.483809
0.331507	-0.000116	0.001392	0.585246
0.144030	0.000022	0.000130	0.168188

	p space	
Exponent	2p	3p
	-9.571458	-0.591012
10010.95	0.000027	-0.000008
2369.556	0.000242	-0.000068
769.7255	0.001401	-0.000392
294.6100	0.006189	-0.001738
124.9840	0.022029	-0.006237
56.89169	0.064359	-0.018523
27.26494	0.150258	-0.044435
13.49676	0.266433	-0.081056
6.803179	0.340700	-0.109419
3.477598	0.260939	-0.081310
1.764975	0.084622	0.085234
0.872189	0.007168	0.316060
0.415428	0.000767	0.411680
0.192303	-0.000054	0.290652
0.085567	0.000032	0.073373

Table LXIV. Hydrogen basis sets

7s	8s	9s	10s	11s
190.6877	418.5580	883.5032	1803.494	3575.682
28.60530	62.74535	132.3847	270.1556	535.5113
6.509591	14.27958	30.12829	61.48158	121.8689
1.841251	4.041817	8.530627	17.41122	34.51608
0.598540	1.316389	2.780664	5.677801	11.25832
0.213977	0.473461	1.002138	2.048055	4.062845
0.080316	0.182799	0.389397	0.797488	1.583456
	0.072884	0.159841	0.329563	0.655806
		0.066965	0.142256	0.285079
			0.062126	0.128361
				0.058086

12s	13s	14s	15s	16s
6909.251	13049.07	24142.02	43839.26	78242.24
1034.623	1953.819	3614.500	6562.808	11713.75
235.4512	444.6244	822.5449	1493.461	2665.666
66.68922	125.9390	232.9931	423.0484	755.1177
21.75548	41.08735	76.01846	138.0330	246.3990
7.853013	14.83339	27.44699	49.84036	88.97794
3.062057	5.785359	10.70663	19.44355	34.71598
1.269367	2.399427	4.441639	8.067349	14.40596
0.553063	1.046429	1.937981	3.520895	6.288306
0.250866	0.475795	0.882031	1.603254	2.864083
0.117111	0.223824	0.415967	0.756883	1.352702
0.054654	0.107814	0.201971	0.368476	0.659199
	0.051697	0.100004	0.183967	0.330004
		0.049120	0.093346	0.168881
			0.046850	0.087590
				0.044826

Table LXV. Helium basis sets

7s	8s	9s	10s	11s
529.1919	1144.644	2385.290	4814.103	9448.327
79.42142	171.6457	357.4945	721.2460	1415.193
18.07366	39.06602	81.36230	164.1432	322.0648
5.091303	11.05139	23.03610	46.48338	91.21340
1.610483	3.572555	7.497970	15.15512	29.75039
0.536663	1.242941	2.672134	5.451489	10.73075
0.183374	0.448076	1.000152	2.091377	4.163660
	0.164115	0.384431	0.830293	1.693235
		0.149062	0.336707	0.706113
			0.136951	0.299700
				0.126976

12s	13s	14s	15s	16s
18091.02	33881.84	62208.70	112161.8	199128.1
2709.247	5073.383	9314.775	16795.73	29804.12
616.5502	1154.558	2119.824	3822.594	6780.988
174.6255	327.0232	600.4558	1082.809	1920.636
56.96447	106.6876	195.9047	353.2882	626.6537
20.56074	38.51539	70.73045	127.5587	226.2743
8.009131	15.01941	27.58993	49.76182	88.27902
3.299183	6.218651	11.44180	20.64573	36.63210
1.407378	2.689537	4.979467	9.005021	15.98891
0.612116	1.194470	2.243019	4.085660	7.275507
0.270222	0.538883	1.031317	1.905351	3.420201
0.118607	0.246205	0.480526	0.903111	1.643756
	0.111469	0.226290	0.433058	0.800468
		0.105305	0.209510	0.393863
			0.099922	0.195206
				0.095180

Table LXVI. Ar^{+16} basis sets

7s	8s	9s	10s	11s
59588.86	130630.9	275434.4	561693.3	1112661.
8939.376	19583.22	41272.14	84140.39	166639.3
2034.324	4456.787	9392.792	19148.56	37923.00
575.2504	1261.463	2659.515	5422.758	10740.63
186.5182	410.6126	866.8375	1768.356	3503.339
66.24646	147.2179	312.1154	637.7596	1264.246
24.67150	56.48740	120.8472	248.0161	492.5788
	22.36419	49.31675	102.1066	203.6752
		20.52947	43.83373	88.19606
			19.03134	39.50880
				17.78191

14s	15s	16s
7495203.	13606747	24306045
1122240.	2037070.	3637985.
255389.2	463564.9	827836.2
72340.58	131311.2	234487.0
23602.25	42844.34	76503.68
8521.737	15470.01	27621.96
3324.217	6035.065	10775.45
1379.053	2503.976	4470.907
601.6252	1092.776	1951.415
273.5894	497.4673	888.7062
128.7244	234.5996	419.5832
62.27098	113.9258	204.2195
30.70220	56.67350	101.9715
15.01405	28.64040	52.00105
	14.31440	26.86545
		13.69375

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16. Abstract

Energy optimized, near Hartree–Fock quality Gaussian basis sets ranging in size from (17s12p) to (20s15p) are presented for the ground states of the second-row atoms and for $Na(^2P)$, Na^+, Na^-, $Mg(^3P)$, P^-, S^-, and Cl^-. In addition, optimized supplementary functions are given for the ground state basis sets to describe the negative ions, and the excited $Na(^2P)$ and $Mg(^3P)$ atomic states. The ratios of successive orbital exponents describing the inner part of the 1s and 2p orbitals are found to be nearly independent of both nuclear charge and basis set size. This provides a method of obtaining good starting estimates for other basis set optimizations.

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