TABLE OF LIGAND FIELD INTEGRALS

BY

C. J. BALLHAUSEN AND E. M. ANCMON

Synopsis.

Numerical values of integrals occurring in ligand field calculations are tabulated as functions of the "effective" charges of the wave functions and of the bond lenghts. The integrals fall into three classes: 1: The electronic interaction integral $G^n_{a,b} = \int R(a) \dfrac{r^n_<}{r^{n+1}_>} R(b) r^2 dr$ with α) $a = b = 3d$, $n = 0, 2$ and 4, β) $a = 3d$, $b = 4p$, $n = 1$ and 3, γ) $a = 3d$, $b = 4s$, $n = 2$ and δ) $a = b = 4s$, $n = 0$. 2: The first derivatives $B^i_{a,b} = \dfrac{d}{dr_0} G^n_{a,b}$ with respect to the bond length r_0. Tabulated are α) $a = b = 3d$, $n = 0, 2$ and 4, and β) $a = 3d$, $b = 4p$, $n = 1$ and 3. 3: The second derivatives $C^n_{a,b} = \dfrac{d^2}{dr^2_0} G^n_{a,b}$. Tabulated are α) $a = b = 3d$, $n = 0, 2$ and 4. All the integrals are evaluated using hydrogenlike wavefunctions.

§ I. Introduction.

In calculations using the ligand field theory very little numerical work is required in order to evaluate the angular parts of the various matrix elements, especially if the tables given by CONDON and SHORTLEY[1] are utilized. The remaining part of the problem, that is the calculation of the radial integrals, is certainly not difficult, but only tedious when hydrogenlike wave functions[2] are used. Thus in order to facilitate ligand field calculations the following radial integrals were calculated by use of an I. B. M. 650 magnetic drum data-processing machine. Hydrogenlike wave functions were used in all the calculations.

§ 2. Table I.

Table I gives values of the integrals

$$G_{3d,\,3d}^n = \int R\,(3\,d)\,\frac{r_<^n}{r_>^{n+1}}\,R\,(3\,d)\,r^2\,dr$$

$$= \int_0^{r_0} R^2\,(3\,d)\,\frac{r^{n+2}}{r_0^{n+1}}\,dr + \int_{r_0}^\infty R^2\,(3\,d)\,\frac{r_0^n}{r^{n-1}}\,dr$$

with $n = 0$, 2 and 4.

$R\,(3\,d)$ is the usual hydrogenlike $3\,d$ wave function[2] having the "effective" charge Z_{3d}, and r_0 is the bond distance, that is the distance from the metal ion to the ligand. These integrals are the basic ones, used in ligand field theory to calculate the splitting of the d-levels in fields of various symmetries.[3, 4, 5, 6, 7]

The same table further tabulates the integrals defined as $\dfrac{d}{dr_0}\,G_{3d,\,3d}^n = B_{3d,\,3d}^n$ and $\dfrac{d}{dr_0}\,B_{3d,\,3d}^n = C_{3d,\,3d}^n$. The $B_{3d,\,3d}^n$ integrals are used to obtain the splitting of the $3\,d$-orbitals,[6, 7] if a dipole model is assumed for the com-

1*

plex, and are further useful in calculations of the Jahn-Teller effect.[8, 9, 10] The $C_{3d,\,3d}^n$ integrals occur likewise in Jahn-Teller calculations.[10]

By use of the integrals[11] $A_n(\alpha) = \int_1^\infty e^{-\alpha t}\, t^n\, dt$ we obtain as our master formulae:

$$G_{3d,\,3d}^n = \frac{Z_{3d}}{1080\,a_0}\left[\frac{(n+6)!}{y^{n+1}} - y^6\left(A_{6+n}(y) - A_{5-n}(y)\right)\right]$$

$$B_{3d,\,3d}^n = \frac{Z_{3d}^2}{1620\,a_0^2}\left[-\frac{(n+6)!\,(n+1)}{y^{n+2}} - 6\,y^5\left(A_{6+n}(y) - A_{5-n}(y)\right)\right.$$
$$\left. - y^6\left(A_{6-n}(y) - A_{7+n}(y)\right)\right]$$

and

$$C_{3d,\,3d}^n = \frac{Z_{3d}^3}{2430\,a_0^3}\left[\frac{(n+6)!\,(n+1)\,(n+2)}{y^{n+3}} - 30y^4\left(A_{6+n}(y) - A_{5-n}(y)\right)\right.$$
$$\left. + 12y^5\left(A_{7+n}(y) - \left(A_{6-n}(y)\right) - y^6\,A_{8+n}(y) - A_{7-n}(y)\right)\right].$$

Here $y = \dfrac{2r_0 Z_{3d}}{3a_0}$, a_0 being the Bohr-radii and Z_{3d} the "effective" charge on the $3d$ wave function. Values of these functions are given in Table I for $Z_{3d} = 3.65$ to 7.85 and $r = \dfrac{r_0}{a_0}$ going from 3.40 to 4.20.

The factor $\dfrac{1}{a_0}$ in $G_{3d,\,3d}^n$, $\dfrac{1}{a_0^2}$ in $B_{3d,\,3d}^n$ and $\dfrac{1}{a_0^3}$ in $C_{3d,\,3d}^n$ have been omitted from the tables.

§ 3. Table II.

This Table records values of the integral $G_{3d,\,4s}^2 = \int R(3d)\,\dfrac{r_<^2}{r_>^3}\,R(4s)\,r^2\,dr$. We have for the master formula:

$$G_{3d,\,4s}^2 = \frac{1}{24\cdot 81\cdot\sqrt{30}}\,\frac{(Z_{4s}\cdot Z_{3d})^{3/2}\,Z_{3d}^2}{a_0}\left[24\,r^4\left(\frac{6!}{b^7} - A^6(b)\right)\right.$$

$$-18\,Z_{4s}\,r^5\left(\frac{7!}{b^8} - A_7(b)\right) + 3\,Z_{4s}^2\,r^6\left(\frac{8!}{b^9} - A_8(b)\right) - \frac{1}{8}\,Z_{4s}^3\,r^7\left(\frac{9!}{b^{10}} - A_9(b)\right)$$

$$\left. + 24\,r^4\,A_1(b) - 18\,Z_{4s}\,r^5\,A_2(b) + 3\,Z_{4s}^2\,r^6\,A_3(b) - \frac{1}{8}\,Z_{4s}^3\,r^7\,A_4(b)\right]$$

$$b = \frac{4\,Z_{3d} + 3\,Z_{4s}}{12\,a_0}\,r_0$$

Z_{4s} and Z_{3d} are the "effective charges" of the radial wave function. In Table II Z_{4s} goes from 2.5 to 5.0, Z_{3d} from 3.65 to 7.85 and $r = \dfrac{r_0}{a_0}$ from 3.40 to 4.20. The factor $\dfrac{1}{a_0}$ has been left out. These integrals are used [12)] for calculating the interaction between $4\,s$ and $3\,d$.

§ 4. Table III.

Here we tabulate the integrals $G^1_{3d,\ 4p}$, $G^3_{3d,\ 4p}$ $B^1_{3d,\ 4p}$ and $B^3_{3d,\ 4p}$. The master formulae are:

$$G^1_{3d,\ 4p} = \frac{Zd\,(Zd\,Zp)^{5/2}}{19440\,\sqrt{2}\,a_0\,X^2\,b^5}\left[20\,C_6\,(X) - 5\left(\frac{Zp}{b}\right)C_7\,(X) + \frac{1}{4}\cdot\left(\frac{Zp}{b}\right)^2 C_8\,(X)\right]$$

$$+\,\frac{Zd\,(Zd\,Zp)^{5/2}\,X}{19440\,\sqrt{2}\,a_0\,b^5}\left[20\,\bar{A}_3 - 5\left(\frac{Zp}{b}\right)\bar{A}_4\,(X) + \frac{1}{4}\left(\frac{Zp}{b}\right)^2 \bar{A}_5\,(X)\right]$$

$$G^3_{3d,\ 4p} = \frac{Zd\,(Zd\,Zp)^{5/2}}{19440\,\sqrt{2}\,a_0\,X^4\,b^5}\left[20\,C_8\,(X) - 5\left(\frac{Zp}{b}\right)C_9\,(X) + \frac{1}{4}\left(\frac{Zp}{b}\right)^2 C_{10}(X)\right]$$

$$+\,\frac{Zd\,(Zd\,Zp)^{5/2}\,X^3}{19440\,\sqrt{2}\,a_0\,b^5}\left[20\,\bar{A}_1\,(X) - 5\left(\frac{Zp}{b}\right)\bar{A}_2\,(X) + \frac{1}{4}\left(\frac{Zp}{b}\right)^2 \bar{A}_3\,(X)\right]$$

$$B^1_{3d,\ 4p} = -\,\frac{Zd\,(Zd\,Zp)^{5/2}}{9720\,\sqrt{2}\,a_0^2\,X^3\,b^4}\left[20\,C_6\,(X) - 5\left(\frac{Zp}{b}\right)C_7\,(X) + \frac{1}{4}\left(\frac{Zp}{b}\right)^2 C_8\,(X)\right]$$

$$+\,\frac{Zd\,(Zd\,Zp)^{5/2}}{19440\,\sqrt{2}\,a_0^2\,b^4}\left[20\,\bar{A}_3\,(X) - 5\left(\frac{Zp}{b}\right)\bar{A}_4\,(X) + \frac{1}{4}\left(\frac{Zp}{b}\right)^2 \bar{A}_5\,(X)\right]$$

$$B^3_{3d,\ 4p} = -\,\frac{Zd\,(Zd\,Zp)^{5/2}}{4860\,\sqrt{2}\,a_0^2\,b^4\,X^5}\left[20\,C_8\,(X) - 5\left(\frac{Zp}{b}\right)C_9\,(X) + \frac{1}{4}\left(\frac{Zp}{b}\right)^2 C_{10}\,(X)\right]$$

$$+\,\frac{Zd\,(Zd\,Zp)^{5/2}\,X^2}{6480\,\sqrt{2}\,a_0^2\,b_4}\left[20\,\bar{A}_1 - 5\left(\frac{Zp}{b}\right)\bar{A}_2\,(X) + \frac{1}{4}\left(\frac{Zp}{b}\right)^2 \bar{A}_3\,(X)\right]$$

$$\text{with } b = \frac{4\,Z\,d + 3\,Z\,p}{12} \text{ and } X = \frac{r_0\,b}{a_0}$$

$$\text{and } \bar{A}_l\,(X) = X^{l+1}\,A_l\,(X)$$

$$C_l\,(X) = l\,! - \bar{A}_l\,(X)$$

Zd and Zp are the "effective" charges on the wave functions. The integrals are used to calculated interactions between the two wave functions in a suitable ligand field, and are of special value in calculations of band intensities.[13]

In Table III $Zp = 3.0 \rightarrow 4.25$, $Zd = 3.65 \rightarrow 7.85$ and $r = 3.4 \rightarrow 4.2$. The factors $\dfrac{1}{a_0}$ for the G integrals and $\dfrac{1}{a_0^2}$ for the B integrals have been left out.

§ 5. Table IV.

This table tabulates $G^0_{4s,\,4s} = \int R(4s)\,\dfrac{1}{r_>}\,R(4s)\,r^2 dr$. The master formula is:

$$G^0_{4s,\,4s} = \frac{Z_s}{2304 \cdot x \cdot a_0}\left[C_8(X) - 24\,C_7(X) + 216\,C_6(X) - 912\,C_5(X)\right.$$

$$\left. + 1872\,C_4(X) - 1728\,C_3(X) + 576\,C_2(X)\right]$$

$$+ \frac{Z_s}{2304\,a_0}\left[\bar{A}_7(X) - 24\,\bar{A}_6(X) + 216\,\bar{A}_5(X) - 912\,\bar{A}_4(X) + 1872\,\bar{A}_3(X)\right.$$

$$\left. - 1728\,\bar{A}_2(X) + 576\,\bar{A}_1(X)\right].$$

Here C_l and $\bar{A}_l$ are the same functions previously defined, and $X = \dfrac{Z_s}{2\,a_0}\,r_0$

with Z_s the "effective" charge of the $4s$ wave function. The factor $\dfrac{1}{a_0}$ has been left out in the table. The range is $Z_s = 2.5 \rightarrow 5.0$ and $r = 3.20 \rightarrow 4.20$.

In ligand field calculations this table is used to calculate the displacement of the $4s$ level.[12]

§ 6 The Tabulation.

In all the tables the power of ten with which to multiply the tabulated number is given as an upper subscript. This power is the same *down* a column until it changes. E. G. $1.579362^{-3} = 1.579362 \cdot 10^{-3}$ to be multiplied further by the suitable power of a_0 as specified in the explanations to the various tables.

Since the numbers in the tables are taken directly from the output of the IBM 650, the last two figures may be in doubt due to round off error during the computation.

§ 7 Acknowledgments.

We wish to thank Dr. MARION C. GRAY and Dr. ANDREW D. LIEHR for many helpful discussions. Further thanks are due to Mrs. W. S. CADMUS, Mrs. E. JENKINS, Mrs. L. DORAN, Mrs. E. HART, Mrs. R. SCHULER and Mrs. C. GARTLAND for the excellent job they did in preparing the manuscript of the tables. One of us (C. J. B.) further wants to thank Bell Telephone Laboratories, Inc. Murray Hill, New Jersey, where this work was performed, for their hospitality.

References.

1) E. U. CONDON and G. H. SHORTLEY: *The Theory of Atomic Spectra*, Cambridge 1935.
2) L. PAULING and E. B. WILSON: *Intrduction to Quantum Mechanics*. McGraw-Hill 1935.
3) H. BETHE: Ann. d. Physik (5) **3**, 133 (1929).
4) R. SCHLAPP and W. G. PENNEY: Phys. Rev. **42**, 666 (1932).
5) J. H. VANVLECK: J. Chem Phys. **7**, 61 (1939).
6) F. E. ILSE and H. HARTMANN: Z. phys Ch. **197**, 239 (1951).
7) C. J. BALLHAUSEN: Mat. Fys. Medd. Dan. Vid. Selsk. **29**, no. 4 (1954).
8) J. H. VANVLECK: J. Chem. Phys. **7**, 72 (1939).
9) U. ÖPIK and M. H. L. PRYCE: Proc. Roy. Soc. (London) **A 238**, 425 (1957).
10) A. D. LIEHR and C. J. BALLHAUSEN: Ann. of Physics (N.Y.) **3**, 304 (1958)
11) M. KOTANI, A. AMEMIYA, E. ISHIGURO and T. KIMURA: *Table of Molecular Integrals*. Maruzen 1955.
12) A. D. LIEHR and C. J. BALLHAUSEN: Acta. Chem. Scand. **11**, 207 (1957).
13) A. D. LIEHR and C. J. BALLHAUSEN: Phys. Rev. **106**, (1957) 1161.

TABLE I. $G^n_{3d,3d}$, $B^n_{3d,3d}$ and $C^n_{3d,3d}$ $n = 0, 2, 4$

$$Z_{3d} = 3.65 \longrightarrow 7.85 \quad r = 3.40 \longrightarrow 4.20.$$

r = 3.40

$\underline{Zd}$	$G^0_{3d,3d}$ / $C^0_{3d,3d}$	$G^2_{3d,3d}$ / $C^2_{3d,3d}$	$G^4_{3d,3d}$ / $C^4_{3d,3d}$	$B^0_{3d,3d}$	$B^2_{3d,3d}$	$B^4_{3d,3d}$
3.65	2.7934351^{-1} / 1.2650043^{-2}	1.5605660^{-1} / -2.3833079^{-2}	1.0459682^{-1} / -2.2744288^{-3}	-6.2185011^{-2}	-6.5866407^{-2}	-5.4615218^{-2}
4.00	2.8471121^{-1} / 2.0121271^{-2}	1.4780920^{-1} / -1.8484781^{-3}	9.5323033^{-2} / 1.7157523	-6.9137073	-7.6023160	-6.3184111
4.30	2.8783085^{-1} / 2.6137916^{-2}	1.3882109^{-1} / 1.6076041^{-2}	8.5873660 / 3.2255888	-7.3793972	-8.0997174	-6.6501070
4.60	2.8997183^{-1} / 3.1491204^{-2}	1.2900832^{-1} / 3.1609698^{-2}	7.6015456 / 4.4476832	-7.7383170	-8.2994356	-6.6668864
4.95	2.9160612^{-1} / 3.6720488^{-2}	1.1737370^{-1} / 4.5761434^{-2}	6.4847644 / 5.4344947	-8.0448595	-8.2372019	-6.3871942
5.25	2.9250291^{-1} / 4.0311999^{-2}	1.0772814^{-1} / 5.4330975^{-2}	5.6010675 / 5.9081395	-8.2315310	-8.0017899	-5.9765314
5.60	2.9316554^{-1} / 4.3548623^{-2}	9.7206247 / 6.0535551	4.6835034 / 6.0865622	-8.3829021	-7.5918411	-5.3888725
5.90	2.9351836^{-1} / 4.5621999^{-2}	8.8952826 / 6.3133581	4.0009848 / 5.9885829	-8.4708819	-7.1747853	-4.8492708
6.25	2.9377221^{-1} / 4.7383361^{-2}	8.0267818 / 6.3731906	3.3222532 / 5.6707556	-8.5393968	-6.6573251	-4.2269849
6.55	2.9390408^{-1} / 4.8453919^{-2}	7.3614055 / 6.2733039	2.8327094 / 5.2888195	-8.5777761	-6.2129166	-3.7249818
6.90	2.9399691^{-1} / 4.9322982^{-2}	6.6710069 / 6.0404777	2.3557761 / 4.7795821	-8.6067119	-5.7134592	-3.1927807
7.20	2.9404413^{-1} / 4.9829843^{-2}	6.1461033 / 5.7799049	2.0163148 / 4.3270659	-8.6224413	-5.3110150	-2.7879887
7.85	2.9409309^{-1} / 5.0450535^{-2}	5.1896959 / 5.1380657	1.4547823 / 3.3991605	-8.6401143	-4.5367089	-2.0715129

Table I. (cont.).

$r = 3.50$

Zd	$G^0_{3d,3d}$ / $C^0_{3d,3d}$	$G^2_{3d,3d}$ / $C^2_{3d,3d}$	$G^4_{3d,3d}$ / $C^4_{3d,3d}$	$B^0_{3d,3d}$	$B^2_{3d,3d}$	$B^4_{3d,3d}$
3.65	2.7319013^{-1} / 1.3712567^{-2}	1.4947958^{-1} / -1.5711581^{-2}	9.9133823^{-2} / 3.4167520^{-3}	-6.0864826^{-2}	-6.5586388^{-2}	-5.4550317^{-2}
4.00	2.7789913^{-1} / 2.0667431^{-2}	1.4030734^{-1} / 4.9416613^{-3}	8.9097967^{-2} / 2.1408748	-6.7095424	-7.3948989	-6.1246458
4.30	2.8058222^{-1} / 2.6113976^{-2}	1.3089233^{-1} / 2.1059906^{-2}	7.9389320 / 3.4659411	-7.1179303	-7.7540514	-6.3146006
4.60	2.8238999^{-1} / 3.0844432^{-2}	1.2093819^{-1} / 3.4480689^{-2}	6.9571900 / 4.4795217	-7.4264685	-7.8401489	-6.2197154
4.95	2.8374263^{-1} / 3.5351561^{-2}	1.0941578^{-1} / 4.6129663^{-2}	5.8729041 / 5.2298924	-7.6843928	-7.6814146	-5.8534131
5.25	2.8446973^{-1} / 3.8372315^{-2}	1.0003324^{-1} / 5.2744416^{-2}	5.0323389 / 5.5292846	-7.8380691	-7.3934802	-5.4043652
5.60	2.8499615^{-1} / 4.1031083^{-2}	8.9937919 / 5.7052103	4.1741565 / 5.5523868	-7.9600433	-6.9527748	-4.8069474
5.90	2.8527065^{-1} / 4.2694615^{-2}	8.2105067 / 5.8404504	3.5449479 / 5.3655052	-8.0294051	-6.5302964	-4.2818399
6.25	2.8546414^{-1} / 4.4075827^{-2}	7.3932401 / 5.7984865	2.9267517 / 4.9916794	-8.0822788	-6.0243465	-3.6943786
6.55	2.8556254^{-1} / 4.4896166^{-2}	6.7713166 / 5.6444070	2.4854676 / 4.5959527	-8.1112545	-5.6002798	-3.2314110
6.90	2.8563038^{-1} / 4.5547299^{-2}	6.1293175 / 5.3797128	2.0592251 / 4.1007441	-8.1326380	-5.1319613	-2.7495480
7.20	2.8566417^{-1} / 4.5918503^{-2}	5.6431522 / 5.1125318	1.7580279 / 3.6783080	-8.1440106	-4.7595795	-2.3885568
7.85	2.8569821^{-1} / 4.6359495^{-2}	4.7607747 / 4.4983819	1.2636610 / 2.8451416	-8.1564229	-4.0525706	-1.7601368

$r = 3.60$

Zd	$G^0_{3d,3d}$ / $C^0_{3d,3d}$	$G^2_{3d,3d}$ / $C^2_{3d,3d}$	$G^4_{3d,3d}$ / $C^4_{3d,3d}$	$B^0_{3d,3d}$	$B^2_{3d,3d}$	$B^4_{3d,3d}$
3.65	2.6717369^{-1} / 1.4540833^{-2}	1.4295541^{-1} / -8.7264319^{-3}	9.3704208^{-2} / 8.2002084^{-3}	-5.9450303^{-2}	-6.4823740^{-2}	-5.3962145^{-2}
4.00	2.7129352^{-1} / 2.0967009^{-2}	1.3303082^{-1} / 1.0424426^{-2}	8.3086107^{-2} / 2.4606399	-6.5011803	-7.1532089	-5.8937484
4.30	2.7359452^{-1} / 2.5864419^{-2}	1.2331898^{-1} / 2.4740648^{-2}	7.3250695 / 3.6040415	-6.8578692	-7.3903788	-5.9603249
4.60	2.7511642^{-1} / 3.0018369^{-2}	1.1332811^{-1} / 3.6179246^{-2}	6.3575566 / 4.4251433	-7.1220255	-7.3805704	-5.7738518
4.95	2.7623258^{-1} / 3.3880185^{-2}	1.0200432^{-1} / 4.5595205^{-2}	5.3132974 / 4.9692313	-7.3381687	-7.1451910	-5.3430787
5.25	2.7682025^{-1} / 3.6406533^{-2}	9.2929720 / 5.0542600	4.5188817 / 5.1250073	-7.4641704	-6.8194925	-4.8715162
5.60	2.7723715^{-1} / 3.8578741^{-2}	8.3284699 / 5.3303836	3.7203441 / 5.0285242	-7.5620615	-6.3616262	-4.2780444
5.90	2.7745001^{-1} / 3.9906376^{-2}	7.5873454 / 5.3692289	3.1425986 / 4.7799803	-7.6165242	-5.9420830	-3.7749124
6.25	2.7759699^{-1} / 4.0983887^{-2}	6.8198304 / 5.2536957	2.5812185 / 4.3755780	-7.6571611	-5.4538317	-3.2265463
6.55	2.7767017^{-1} / 4.1609305^{-2}	6.2391776 / 5.0647190	2.1842503 / 3.9817016	-7.6789493	-5.0528243	-2.8031681
6.90	2.7771959^{-1} / 4.2094739^{-2}	5.6424148 / 4.7848107	1.8037568 / 3.5118603	-7.6946883	-4.6164596	-2.3696319
7.20	2.7774368^{-1} / 4.2365256^{-2}	5.1920150 / 4.5206870	1.5366029 / 3.1240759	-7.7028774	-4.2733446	-2.0491761
7.85	2.7776729^{-1} / 4.2677110^{-2}	4.3771610 / 3.9436851	1.1010686 / 2.3837699	-7.7115617	-3.6290904	-1.4993983

TABLE I. (cont.).

r = 3.70

Z_d	$q^0_{3d,3d}$ / $c^0_{3d,3d}$	$q^2_{3d,3d}$ / $c^2_{3d,3d}$	$q^4_{3d,3d}$ / $c^4_{3d,3d}$	$B^0_{3d,3d}$	$B^2_{3d,3d}$	$B^4_{3d,3d}$
3.65	2.6130247^{-1} 1.5158818^{-2}	1.3652818^{-1} -2.7893300^{-3}	8.3355891^{-2} 1.2140228	-5.7963665^{-2}	-6.3660316^{-2}	-5.2938376^{-2}
4.00	2.6489741^{-1} 2.1056459^{-2}	1.2600936^{-1} 1.4758869^{-2}	7.7319544^{-2} 2.6884565	-6.2909021	-6.8861575	-5.6355823
4.30	2.6686531^{-1} 2.5433026^{-2}	1.1611476^{-1} 2.7324082^{-2}	6.7471782^{-2} 3.6578304	-6.6012469	-7.0170645	-5.5965991
4.60	2.6814293^{-1} 2.9059691^{-2}	1.0617481^{-1} 3.6937193^{-2}	5.8021198^{-2} 4.3047555	-6.8265417	-6.9276058	-5.3368827
4.95	2.6906128^{-1} 3.2350530^{-2}	9.5117389 4.4391196	4.8033525^{-2} 4.6722145	-7.0069825	-6.6329583	-4.8607749
5.25	2.6953484^{-1} 3.4452306^{-2}	8.6382129 4.7937604	4.0566678^{-2} 4.7122211	-7.1098989	-6.2818330	-4.3796423
5.60	2.6986401^{-1} 3.6218011^{-2}	7.7198951 4.9459441	3.3168355^{-2} 4.5267283	-7.1881628	-5.8176065	-3.8005036
5.90	2.7002857^{-1} 3.7272336^{-2}	7.0203117 4.9119291	2.7880859^{-2} 4.2385427	-7.2307636	-5.4072132	-3.3243709
6.25	2.7013986^{-1} 3.8108873^{-2}	6.3005561 4.7453753	2.2794943^{-2} 3.8228761	-7.2618766	-4.9407988	-2.8171462
6.55	2.7019411^{-1} 3.8583427^{-2}	5.7587889 4.5361842	1.9229119^{-2} 3.4417714	-7.2781976	-4.5642347	-2.4325911
6.90	2.7023000^{-1} 3.8943640^{-2}	5.2040727 4.2530238	1.5834747^{-2} $3,0041355$	-7.2897382	-4.1595635	-2.0444704
7.20	2.7024713^{-1} 3.9139877^{-2}	4.7865757 3.9983570	1.3464879^{-2} 2.6527142	-7.2956125	-3.8443629	-1.7609799
7.85	2.7026345^{-1} 3.9359440^{-2}	4.0332133 3.4633080	9.6237867^{-3} 2.0001550^{-2}	-7.3016663	-3.2579671	-1.2807935

r = 3.80

Z_d	$q^0_{3d,3d}$ / $c^0_{3d,3d}$	$q^2_{3d,3d}$ / $c^2_{3d,3d}$	$q^4_{3d,3d}$ / $c^4_{3d,3d}$	$B^0_{3d,3d}$	$B^2_{3d,3d}$	$B^4_{3d,3d}$
3.65	2.5558269^{-1} 1.5590173^{-2}	1.3023421^{-1} 2.1928733^{-3}	8.3128347^{-2} 1.5309326	-5.6424760^{-2}	-6.2170575^{-2}	-5.1559801^{-2}
4.00	2.5871172^{-1} 2.0969382^{-2}	1.1926439^{-1} 1.8096287^{-2}	7.1821167^{-2} 2.8373065	-6.0806394	-6.6014261	-5.3586870
4.30	2.6039034^{-1} 2.4858338^{-2}	1.0928577^{-1} 2.8995630^{-2}	6.2058110^{-2} 3.6435218	-6.3496860	-6.6409577	-5.2310287
4.60	2.6145998^{-1} 2.8007737^{-2}	9.9468923 3.6954233	5.2896917^{-2} 4.1356384	-6.5411421	-6.4865278	-4.9145226
4.95	2.6221347^{-1} 3.0797793^{-2}	8.8729432 4.2708606	4.3401127^{-2} 4.3546227	-6.6912344	-6.1476028	-4.4093179
5.25	2.6259399^{-1} 3.2537797^{-2}	8.0353700 4.5095015	3.6415800^{-2} 4.3035527	-6.7749910	-5.7811977	-3.9289306
5.60	2.6285313^{-1} 3.3966276^{-2}	7.1634329 4.5641520	2.9586179^{-2} 4.0546545	-6.8373369	-5.3190121	-3.3717045
5.90	2.6297997^{-1} 3.4799687^{-2}	6.5042393 4.4766125	2.4759975^{-2} 3.7442254	-6.8705388	-4.9222280	-2.9256305
6.25	2.6306401^{-1} 3.5446216^{-2}	5.8299236 4.2767312	2.0160505^{-2} 3.3315078	-6.8942758	-4.4801883	-2.4599252
6.55	2.6310411^{-1} 3.5804696^{-2}	5.3245703 4.0582567	1.6960491^{-2} 2.9703851	-6.9064570	-4.1284687	-2.1125287
6.90	2.6313008^{-1} 3.6070824^{-2}	4.8087752 3.7801619	1.3932939^{-2} 2.5684639	-6.9148879	-3.7544964	-1.7664035
7.20	2.6314221^{-1} 3.6212259^{-2}	4.4214718 3.5389260	1.1829596^{-2} 2.2531532	-6.9190864	-3.4655251	-1.5162410
7.85	2.6315346^{-1} 3.6366495^{-2}	3.7240622 3.0474460	8.4374395^{-3} 1.6814097^{-2}	-6.9232909	-2.9320366	-1.0972071

TABLE I. (cont.).

r = 3.90

Zd	$G^0_{3d,3d}$ $C^0_{3d,3d}$	$G^2_{3d,3d}$ $C^2_{3d,3d}$	$G^4_{3d,3d}$ $C^4_{3d,3d}$	$B^0_{3d,3d}$	$B^2_{3d,3d}$	$B^4_{3d,3d}$
3.65	2.5001868^{-1} 1.5857694^{-2}	1.2410271^{-1} 6.3145805^{-3}	7.8053316^{-2} 1.7784129	-5.4851095^{-2}	-6.0421358^{-2}	-4.9899669^{-2}
4.00	2.5273558^{-1} 2.0736245^{-2}	1.1281021^{-1} 2.0577731^{-2}	6.6605970 2.9194354	-5.8720010	-6.3055475	-5.0703432
4.30	2.5416384^{-1} 2.4173795^{-2}	1.0283193^{-1} 2.9919845^{-2}	5.7008313 3.5754844	-6.1044462	-6.2675594	-4.8696852
4.60	2.5505704^{-1} 2.6895163^{-2}	9.3196486 3.6399971	4.8185903 3.9322895	-6.2665888	-6.0612268	-4.5108940
4.95	2.5567363^{-1} 2.9249464^{-2}	8.2812665 4.0701459	3.9204124 4.0288034	-6.3910113	-5.6907761	-3.9901216
5.25	2.5597857^{-1} 3.0683383^{-2}	7.4807483 4.2141688	3.2695387 3.9080915	-6.4589418	-5.3173021	-3.5184886
5.60	2.5618202^{-1} 3.1833928^{-2}	6.6546548 4.1936240	2.6409764 3.6168008	-6.5084384	-4.8635365	-2.9884290
5.90	2.5627951^{-1} 3.2489855^{-2}	6.0343272 4.0681882	2.2013915 3.2975315	-6.5342263	-4.4834057	-2.5739365
6.25	2.5634279^{-1} 3.2987411^{-2}	5.4029371 3.8486067	1.7859693 2.8978336	-6.5522730	-4.0670469	-2.1489208
6.55	2.5637234^{-1} 3.3257074^{-2}	4.9315239 3.6287838	1.4989412 2.5610522	-6.5613334	-3.7398706	-1.8364459
6.90	2.5639108^{-1} 3.3452887^{-2}	4.4516508 3.3612933	1.2288504 2.1959678	-6.5674721	-3.3951311	-1.5286725
7.20	2.5639965^{-1} 3.3554845^{-2}	4.0920100 3.1357065	1.0420142 1.9152375	-6.5704627	-3.1305366	-1.3082956
7.85	2.5640738^{-1} 3.3662356^{-2}	3.4455054 2.6873055	7.4196833^{-3} 1.4165498^{-2}	-6.5733736	-2.6451424	-9.4271713^{-3}

r = 4.00

Zd	$G^0_{3d,3d}$ $C^0_{3d,3d}$	$G^2_{3d,3d}$ $C^2_{3d,3d}$	$G^4_{3d,3d}$ $C^4_{3d,3d}$	$B^0_{3d,3d}$	$B^2_{3d,3d}$	$B^4_{3d,3d}$
3.65	2.4461312^{-1} 1.5983000^{-2}	1.1815660^{-1} 9.6688336^{-3}	7.3155608^{-2} 1.9642437	-5.3257963^{-2}	-5.8471998^{-2}	-4.8023526^{-2}
4.00	2.4696671^{-1} 2.0384348^{-2}	1.0665516^{-1} 2.2332497^{-2}	6.1682252 2.9461271	-5.6663094	-6.0040005	-4.7766479
4.30	2.4817900^{-1} 2.3408089^{-2}	9.6748280 3.0240766	5.2315723 3.4662382	-5.8664796	-5.9012036	-4.5173023
4.60	2.4892301^{-1} 2.5748719^{-2}	8.7340273 3.5416645	4.3867930 3.7066622	-6.0033506	-5.6544486	-4.1288037
4.95	2.4942631^{-1} 2.7726542^{-2}	7.7338135 3.8492097	3.5410013 3.7041780	-6.1061597	-5.2631679	-3.6035149
5.25	2.4967005^{-1} 2.8903156^{-2}	6.9707176 3.9172604	2.9365945 3.5320748	-6.1610754	-4.8891481	-3.1466618
5.60	2.4982936^{-1} 2.9825993^{-2}	6.1893788 3.8401324	2.3595334 3.2152808	-6.2002438	-4.4484999	-2.6471319
5.90	2.4990409^{-1} 3.0340133^{-2}	5.6061467 3.6892332	1.9597995 2.8972294	-6.2202080	-4.0869473	-2.2645770
6.25	2.4995159^{-1} 3.0721516^{-2}	5.0150886 3.4602459	1.5849108 2.5173157	-6.2338840	-3.6966623	-1.8785858
6.55	2.4997330^{-1} 3.0923568^{-2}	4.5751972 3.2446580	1.3274900 2.2071066	-6.2406012	-3.3932406	-1.5984716
6.90	2.4998680^{-1} 3.1067087^{-2}	4.1284089 2.9912294	1.0864123 1.8783305	-6.2450566	-3.0759866	-1.3253819
7.20	2.4999285^{-1} 3.1140150^{-2}	3.7940882 2.7822642	9.2026500^{-3} 1.6298771^{-2}	-6.2471798	-2.8338628	-1.1314429
7.85	2.4999814^{-1} 3.1214963^{-2}	3.1939095 2.3751287	6.5439541^{-3} 1.1963151^{-2}	-6.2491890	-2.3920052	-8.1241141^{-3}

TABLE I. (cont.).

$r = 4.10$

Z_d	$G^0_{3d,3d}$ / $C^0_{3d,3d}$	$G^2_{3d,3d}$ / $C^2_{3d,3d}$	$G^4_{3d,3d}$ / $C^4_{3d,3d}$	$B^0_{3d,3d}$	$B^2_{3d,3d}$	$B^4_{3d,3d}$
3.65	2.3936729^{-1}	1.1241323^{-1}	6.8453874^{-2}	-5.1658561^{-2}	-5.6374575^{-2}	-4.5989181^{-2}
	1.5986260^{-2}	1.2345265^{-2}	2.0960633			
4.00	2.4140163^{-1}	1.0080259^{-1}	5.7052781	-5.4646294	-5.7013154	-4.4826247
	1.9937836^{-2}	2.3477439^{-2}	2.9275989			
4.30	2.4242823^{-1}	9.1026059	4.7969518	-5.6364738	-5.5452124	-4.1774511
	2.2585515^{-2}	3.0082900	3.3265081			
4.60	2.4304649^{-1}	8.1880810	3.9920530	-5.7516553	-5.2679963	-3.7699794
	2.4589968^{-2}	3.4121972	3.4684326			
4.95	2.4345630^{-1}	7.2276599	3.1986387	-5.8363433	-4.8647300	-3.2490117
	2.6244630^{-2}	3.6176074	3.3877167			
5.25	2.4365062^{-1}	6.5017760	2.6389907	-5.8806006	-4.4952432	-2.8112906
	2.7206226^{-2}	3.6257044	3.1794799			
5.60	2.4377505^{-1}	5.7637020	2.1102729	-5.9114997	-4.0710321	-2.3441478
	2.7943526^{-2}	3.5072753	2.8504703			
5.90	2.4383219^{-1}	5.2156499	1.7472161	-5.9269080	-3.7291142	-1.9930253
	2.8344979^{-2}	3.3406429	2.5408975			
6.25	2.4386778^{-1}	4.6623269	1.4090661	-5.9372410	-3.3646272	-1.6438509
	2.8636221^{-2}	3.1098488	2.1850016			
6.55	2.4388369^{-1}	4.2516350	1.1781511	-5.9422055	-3.0838550	-1.3933955
	2.8787056^{-2}	2.9022697	1.9020502			
6.90	2.4389337^{-1}	3.8352756	9.6279680^{-3}	-5.9454287	-2.7921986	-1.1514315
	2.8891858^{-2}	2.6648345	1.6079684^{-2}			
7.20	2.4389762^{-1}	3.5241224	8.1485160^{-3}	-5.9469315	-2.5706643	-9.8083597^{-3}
	2.8944023^{-2}	2.4726092	1.3890812^{-2}			
7.85	2.4390124^{-1}	2.9661303	5.7881616^{-3}	-5.9483138	-2.1681059	-7.0222589
	2.8995900^{-2}	2.1041558	1.0129679^{-2}			

$r = 4.20$

Z_d	$G^0_{3d,3d}$ / $C^0_{3d,3d}$	$G^2_{3d,3d}$ / $C^2_{3d,3d}$	$G^4_{3d,3d}$ / $C^4_{3d,3d}$	$B^0_{3d,3d}$	$B^2_{3d,3d}$	$B^4_{3d,3d}$
3.65	2.3428124^{-1}	1.0688511^{-1}	6.3961356^{-2}	-5.0064155^{-2}	-5.4174301^{-2}	-4.3846954^{-2}
	1.5886062^{-2}	1.4428691^{-2}	2.1811934			
4.00	2.3603584^{-1}	9.5251681	5.2715752	-5.2677976	-5.4011703	-4.1923300
	1.9417824^{-2}	2.4116828	2.8729558			
4.30	2.3690326^{-1}	8.5653580	4.3955779	-5.4148911	-5.2020490	-3.8527136
	2.1726380^{-2}	2.9552631	3.1653386			
4.60	2.3741585^{-1}	7.6797158	3.6319924	-5.5115352	-4.9029082	-3.4352800
	2.3435979^{-2}	3.2612102	3.2252680			
4.95	2.3774877^{-1}	6.7599143	2.8901643	-5.5810928	-4.4948647	-2.9255323
	2.4814897^{-2}	3.3826610	3.0843788			
5.25	2.3790334^{-1}	6.0705881	2.3732032	-5.6166557	-4.1337688	-2.5099093
	2.5597794^{-2}	3.3443759	2.8525345			
5.60	2.3800029^{-1}	5.3740172	1.8895477	-5.6409606	-3.7282085	-2.0758414
	2.6184692^{-2}	3.1970193	2.5215179			
5.90	2.3804387^{-1}	4.8591561	1.5600761	-5.6528175	-3.4063183	-1.7550334
	2.6497022^{-2}	3.0221358	2.2254819			
6.25	2.3807045^{-1}	4.3410210	1.2551070	-5.6606008	-3.0668805	-1.4401468
	2.6718633^{-2}	2.7949913	1.8958594			
6.55	2.3808209^{-1}	3.9573273	1.0478678	-5.6642593	-2.8074610	-1.2166367
	2.6830836^{-2}	2.5978205	1.6397667			
6.90	2.3808902^{-1}	3.5689343	8.5529480^{-3}	-5.6665845	-2.5394751	-1.0024392
	2.6907106^{-2}	2.3772189	1.3781069^{-2}			
7.20	2.3809202^{-1}	3.2789806	7.2336034^{-3}	-5.6676454	-2.3367244	-8.5237322^{-3}
	2.6944225^{-2}	2.2012875	1.1859216^{-2}			
7.85	2.3809447^{-1}	2.7594432	5.1339206^{-3}	-5.6685936	-1.9695788	-6.0880359
	2.6980082^{-2}	1.8685471	8.6008320			

TABLE II. $G^2_{3d, 4s}$ $Z_{3d} = 3.65 \longrightarrow 7.85$

$$r = 3.40 \longrightarrow 4.20.$$

$$G^2_{3d, 4s}$$
$$r = 3.40$$

$Z_{3d}\backslash Z_{4s}$	2.5	3.0	3.5	4.0	4.5	5.0
3.65	2.8236570^{-2}	4.6623955^{-2}	4.7730543^{-2}	3.3147247^{-2}	7.8207401^{-3}	-2.2722074^{-2}
4.00	2.3140754	4.2791826	4.7046683	3.6395632	1.4851669^{-2}	-1.2650428
4.30	1.8712124	3.8690211	4.5078120	3.7565517	1.9370026	-5.1566985^{-3}
4.60	1.4467943	3.4211036	4.2212532	3.7509961	2.2571823	1.1455436
4.95	9.9391264^{-3}	2.8869969	3.8151113	3.6243397	2.4834167	6.9807547
5.25	6.5091625	2.4417060	3.4345461	3.4405936	2.5709096	1.0758544^{-2}
5.60	3.0768787	1.9550459	2.9802381	3.1682062	2.5739864	1.3895808
5.90	6.1960420^{-4}	1.5749484	2.5983262	2.9049650	2.5110971	1.5647848
6.25	-1.7155328^{-3}	1.1800903	2.1753043	2.5824472	2.3823427	1.6790522
6.55	-3.3023902	8.8442028^{-3}	1.8391411	2.3047285	2.2390662	1.7145811
6.90	-4.7283905	5.8809274	1.4826407	1.9898389	2.0481772	1.6997260
7.20	-5.6351943	3.7329670	1.2092557	1.7336897	1.8737131	1.6504249
7.85	-6.8031325	1.7462468^{-4}	7.1742929^{-3}	1.2369404	1.4911184	1.4689699

<center>TABLE II. (cont.)</center>

$$\sigma^2_{3d,4s}$$
$$4 = 3.50$$

Z3d\Z4s	2.5	3.0	3.5	4.0	4.5	5.0
3.65	2.9538936^{-2}	4.5874993^{-2}	4.4812702^{-2}	2.8616711^{-2}	2.5710436^{-3}	-2.7757030^{-2}
4.00	2.4358193	4.2054848	4.4268704	3.2116071	9.9235700	-1.7338878
4.30	1.9861453	3.7985447	4.2453074	3.3537315	1.4745594^{-2}	-9.5373864^{-3}
4.60	1.5557587	3.3558023	3.9765261	3.3755105	1.8264267	-2.9286232
4.95	1.0971258	2.8298540	3.5933329	3.2823871	2.0901416	3.2539114
5.25	7.5014125^{-3}	2.3929180	3.2336196	3.1279559	2.2094795	7.3165743
5.60	4.0315668	1.9170074	2.8041607	2.8895771	2.2487349	1.0769295^{-2}
5.90	1.5474400	1.5464827	2.4434084	2.6547508	2.2156526	1.2776536
6.25	-8.1500283^{-4}	1.1627074	2.0442790	2.3640077	2.1199414	1.4199378
6.55	-2.4236754^{-3}	8.7613775^{-3}	1.7275589	2.1120127	2.0033393	1.4779958
6.90	-3.8748368	5.8965043	1.3921668	1.8251027	1.8415273	1.4877569
7.20	-4.8038836	3.8246814	1.1353695	1.5910528	1.6901519	1.4581675
7.85	-6.0242473	4.0158649^{-4}	6.7437233^{-3}	1.1360745	1.3518201	1.3152017

$$\sigma^2_{3d,4s}$$
$$r = 3.60$$

Z3d\Z4s	2.5	3.0	3.5	4.0	4.5	5.0
3.65	3.0504347^{-2}	4.4804276^{-2}	4.1732325^{-2}	2.4171540^{-2}	-2.3254998^{-3}	-3.2209296^{-2}
4.00	2.5252763	4.1026110	4.1363003	2.7950387	5.3614712	-2.1451306
4.30	2.0704551	3.7016743	3.9728912	2.9641050	1.0489088^{-2}	-1.3358615
4.60	1.6360215	3.2669184	3.7243890	3.0145006	1.4319372	-6.4679078^{-3}
4.95	1.1739912	2.7522468	3.3666591	2.9557600	1.7317835	2.6521139^{-5}
5.25	8.2505789^{-3}	2.3261085	3.0295225	2.8308577	1.8813292	4.3405224^{-3}
5.60	4.7659422	1.8634257	2.6264451	2.6262416	1.9544858	8.0673708
5.90	2.2734346	1.5042984	2.2877577	2.4192818	1.9490464	1.0294531^{-2}
6.25	-9.6697863^{-5}	1.1333857	1.9132165	2.1593595	1.8837437	1.1957200
6.55	-1.7118810^{-3}	8.5716959^{-3}	1.6162200	1.9320740	1.7915265	1.2730081
6.90	-3.1721615	5.8171375	1.3020393	1.6718305	1.6561282	1.3037542
7.20	-4.1111822	3.8295396	1.0617401	1.4587008	1.5256584	1.2909798
7.85	-5.3613984	5.5443765^{-4}	6.3104450^{-3}	1.0429130	1.2272135	1.1809586

TABLE II. (cont.).

$$a^2_{3d,4s}$$
$$r = 3.70$$

Z3d\Z4s	2.5	3.0	3.5	4.0	4.5	5.0
3.65	3.1157186^{-2}	4.3462808^{-2}	3.8553453^{-2}	1.9869809^{-2}	-6.8340587^{-3}	-3.6079341^{-2}
4.00	2.5852670	3.9757626	3.8390426	2.3949366	1.1910887	-2.4997226
4.30	2.1271825	3.5835600	3.6961964	2.5921339	6.6185560	-1.6637470
4.60	1.6907200	3.1594206	3.4700796	2.6717747	1.0748068^{-2}	-9.4953047^{-3}
4.95	1.2277035	2.6588451	3.1397248	2.6475098	1.4087392	-2.7292122
5.25	8.7881842^{-3}	2.2456107	2.8263674	2.5517776	1.5863756	1.7995777
5.60	5.3106142	1.7982557	2.4506029	2.3800764	1.6906915	5.7579193
5.90	2.8267400	1.4520023	2.1344483	2.1999800	1.7104465	8.1688316
6.25	4.6687829^{-4}	1.0953493	1.7846689	1.9694945	1.6726606	1.0031298^{-2}
6.55	-1.1412424^{-3}	8.3041658^{-3}	1.5073480	1.7656301	1.6024025	1.0964495
6.90	-2.5966974	5.6682873	1.2140988	1.5304807	1.4907144	1.1447241
7.20	-3.5351277	3.7703957	9.8994666^{-3}	1.3369211	1.3789558	1.1460624
7.85	-4.7962213	6.5123456^{-4}	5.8860347	9.5752734^{-3}	1.1161270	1.0638984

$$a^2_{3d,4s}$$
$$r = 3.80$$

Z3d\Z4s	2.5	3.0	3.5	4.0	4.5	5.0
3.65	3.1523802^{-2}	4.1899598^{-2}	3.5332477^{-2}	1.5757726^{-2}	-1.0934152^{-2}	-3.9379445^{-2}
4.00	2.6186982	3.8297944	3.5403476	2.0152140	-2.5754134^{-3}	-2.7998009
4.30	2.1593486	3.4489045	3.4200542	2.2410971	3.1393196	-1.9400854
4.60	1.7229579	3.0377862	3.2179001	2.3499915	7.5499252	-1.2041875
4.95	1.2613372	2.5537509	2.9162471	2.3596517	1.1203965^{-2}	-5.0476867^{-3}
5.25	9.1440397^{-3}	2.1552105	2.6273880	2.2922028	1.3236319	-3.4218817^{-4}
5.60	5.6937607	1.7248700	2.2793480	2.1520805	1.4560702	3.8042850^{-3}
5.90	3.2340819	1.3926383	1.9857646	1.9975122	1.4983883	6.3639655
6.25	9.0024450^{-4}	1.0512512	1.6605273	1.7947607	1.4851419	8.3879485
6.55	-6.8892120	7.9824495^{-3}	1.4025131	1.6128242	1.4343929	9.4511488
6.90	-2.1276087^{-3}	5.4706472	1.1296377	1.4010306	1.3437377	1.0077283^{-2}
7.20	-3.0566278	3.6656854	9.2108124^{-3}	1.2255927	1.2485617	1.0206979
7.85	-4.3129519	7.0634961^{-4}	5.4782021	8.7970865^{-3}	1.0172971	9.6181504^{-3}

Table II. (cont.).

$$G^2_{3d,4s}$$
$$r = 3.90$$

Z3d\Z4s	2.5	3.0	3.5	4.0	4.5	5.0
3.65	3.1632200^{-2}	4.0160845^{-2}	3.2118756^{-2}	1.1870680^{-2}	-1.4616069^{-2}	-4.2132143^{-2}
4.00	2.6285412	3.6691720	3.2446642	1.6587235	-5.9363825^{-3}	-3.0482752
4.30	2.1700118	3.3019584	3.1484653	1.9132541	4.7491096^{-5}	-2.1682301
4.60	1.7357409	2.9059702	2.9713578	2.0508544	4.7162772^{-3}	-1.4143920
4.95	1.2777844	2.4405553	2.6991583	2.0932988	8.6545872	-6.9666725^{-3}
5.25	9.3458894^{-3}	2.0581345	2.4350637	2.0528682	1.0915583^{-2}	-2.1225484
5.60	5.9412900	1.6461099	2.1146894	1.9425849	1.2488894	2.1697297
5.90	3.5194416	1.3287188	1.8433689	1.8119432	1.3110913	4.8443600
6.25	1.2253819	1.0032722	1.5421168	1.6350270	1.3193856	6.9940235
6.55	-3.3494101^{-4}	7.6257837^{-3}	1.3027957	1.4733921	1.2857548	8.1594745
6.90	-1.7468757^{-3}	5.2406994	1.0495037	1.2831236	1.2135473	8.8997863
7.20	-2.6592634	3.5298563	8.5583853^{-3}	1.1243251	1.1329308	9.1236240
7.85	-3.8982215	7.3097379^{-4}	5.0918397	8.0907815^{-3}	9.2944303^{-3}	8.7269919

$$G^2_{3d,4s}$$
$$r = 4.00$$

Z3d\Z4s	2.5	3.0	3.5	4.0	4.5	5.0
3.65	3.1510592^{-2}	3.8289028^{-2}	2.8954053^{-2}	8.2348245^{-3}	-1.7879827^{-2}	-4.4366680^{-2}
4.00	2.6177450	3.4979755	2.9556809	1.3274056^{-2}	-8.8983483^{-3}	-3.2486266
4.30	2.1620875	3.1465152	2.8846143	1.6100034	-2.6682369	-2.3519496
4.60	1.7319348	2.7674467	2.7331781	1.7752793	2.2321515	-1.5840611
4.95	1.2797689	2.3223267	2.4906869	1.8488972	6.4217681	-8.5257811^{-3}
5.25	9.4191752^{-3}	1.9571315	2.2512173	1.8338734	8.8821959	-3.5801120
5.60	6.0764675	1.5643320	1.9580273	1.7514179	1.0671708^{-2}	8.1775982^{-4}
5.90	3.7042095	1.2622997	1.7083817	1.6429316	1.1465643	3.5757889^{-3}
6.25	1.4614574	9.5315892^{-3}	1.4302710	1.4898114	1.1734942	5.8181330
6.55	-6.1760506^{-5}	7.2492880	1.2088615	1.3467873	1.1546764	7.0606621
6.90	-1.4390353^{-3}	4.9914016	9.7420561^{-3}	1.1761897	1.0984860	7.8892456
7.20	-2.3290361	3.3743207	7.9462811	1.0325582	1.0305438	8.1875495
7.85	-3.5407756	7.3386348^{-4}	4.7296978	7.4515522^{-3}	8.5136064^{-3}	7.9477334

Table II. (cont.).

$$G^2_{3d,4s}$$
$$r = 4.10$$

Z3d\Z4s	2.5	3.0	3.5	4.0	4.5	5.0
3.65	3.1187191^{-2}	3.6323183^{-2}	2.5872990^{-2}	4.8673516^{-3}	-2.0733519^{-2}	-4.6117920^{-2}
4.00	2.5891312	3.3197917	2.6763505	1.0223731^{-2}	-1.1475104	-3.4047166
4.30	2.1383746	2.9858737	2.6310105	1.3319681	-5.0254093^{-3}	-2.4952656
4.60	1.7141879	2.6251730	2.5054255	1.5234953	7.7615476^{-5}	-1.7172720
4.95	1.2697471	2.2016407	2.2924146	1.6263009	4.4833954^{-3}	-9.7645393^{-3}
5.25	9.3866680^{-3}	1.8544280	2.0770987	1.6348372	7.1143116	-4.7527914
5.60	6.1198558	1.4814366	1.8102974	1.5779956	9.0873023	-2.8693158^{-4}
5.90	3.8070089	1.1950178	1.5814965	1.4897971	1.0027152^{-2}	2.5258173^{-3}
6.25	1.6249981	9.0228528^{-3}	1.3254794	1.3583670	1.0454939	4.8310784
6.55	1.4541166^{-4}	6.8647762	1.1210590	1.2322649	1.0393415	6.1283261
6.90	-1.1909401^{-3}	4.7327298	9.0397903^{-3}	1.0795140	9.9690592^{-3}	7.0223559
7.20	-2.0541597	3.2077344	7.3762489	9.4961953^{-3}	9.3991747	7.3780384
7.85	-3.2312039	7.2165126^{-4}	4.3929350	6.8740320	7.8191384	7.2645926

$$G^2_{3d,4s}$$
$$r = 4.20$$

Z3d\Z4s	2.5	3.0	3.5	4.0	4.5	5.0
3.65	3.0689241^{-2}	3.4297856^{-2}	2.2904017^{-2}	1.7782986^{-3}	-2.3191307^{-2}	-4.7424297^{-2}
4.00	2.5454056	3.1377813	2.4089744	7.4404047	-1.3685643	-3.5206537
4.30	2.1014240	2.8228675	2.3895185	1.0791853^{-2}	-7.0453551^{-3}	-2.6023362
4.60	1.6849330	2.4816615	2.2895685	1.2951839	-1.7703703	-1.8180844
4.95	1.2499420	2.0806150	2.1054215	1.4249219	2.8163171	-1.0721595
5.25	9.2686649^{-3}	1.7518604	1.9134785	1.4550224	5.5884170	-5.6768631^{-3}
5.60	6.0893715	1.3989209	1.6720029	1.4214691	7.7133712	-1.1773385
5.90	3.8440577	1.1281559	1.4630561	1.3516412	8.7744766	1.6642578
6.25	1.7300797	8.5171037^{-3}	1.2279378	1.2398108	9.3348418	4.0061477
6.55	2.9921753^{-4}	6.4812858	1.0394951	1.1289726	9.3800711	5.3386789
6.90	-9.9157018	4.4721799	8.3887332^{-3}	9.9230406^{-3}	9.0727617	6.2784493
7.20	-1.8247588^{-3}	3.0366076	6.8484919	8.7478432	8.5968875	6.6768974
7.85	-2.9617116	6.9935457^{-4}	4.0816089	6.3526916	7.2005887	6.6638646

TABLE III. $G^n_{3d,\,4p}$ and $B^n_{3d,\,4p}$ $n=1, 3$

$$Z_{3d} = 3.65 \longrightarrow 7.85 \quad Z_{4p} = 3.00 \longrightarrow 4.25$$

$$r = 3.40 \longrightarrow 4.20.$$

$$G^1_{3d,4p}$$
$$r = 3.40$$

$z3d \backslash z4p$	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-5.5826319^{-2}	-5.3556282^{-2}	-4.7018024^{-2}	-3.6898631^{-2}	-2.3958286^{-2}	-8.9582621^{-3}
4.00	-5.3921596	-5.4217042	-5.0383860	-4.2947659	-3.2540377	-1.9828871^{-2}
4.30	-5.0664186	-5.2808202	-5.1057808	-4.5804562	-3.7565744	-2.6916349
4.60	-4.6414699	-5.0065638	-5.0125570	-4.6862804	-4.0683469	-3.2068025
4.95	-4.0724151	-4.5718326	-4.7524544	-4.6285807	-4.2288957	-3.5907773
5.25	-3.5566696	-4.1389167	-4.4385970	-4.4609935	-4.2257404	-3.7617683
5.60	-2.9538004	-3.6001479	-4.0058690	-4.1677217	-4.0963020	-3.8117544
5.90	-2.4540121	-3.1318605	-3.6034695	-3.8598926	-3.9052799	-3.7532612
6.25	-1.9052413	-2.5977446	-3.1213273	-3.4620096	-3.6178862	-3.5961373
6.55	-1.4713957	-2.1614163	-2.7116483	-3.1050116	-3.3355122	-3.4057883
6.90	-1.0123103	-1.6860776	-2.2504673	-2.6859525	-2.9829287	-3.1397324
7.20	-6.6025740^{-3}	-1.3115460	-1.8764366	-2.3341510	-2.6728026	-2.8878458
7.85	-2.4821979^{-4}	-6.1030747^{-3}	-1.1499735	-1.6222606	-2.0124515	-2.3117701

Table III. (cont.).

$$G^1_{3d,4p}$$
$$r = 3.50$$

Z3 d\Z4p	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-5.3929537^{-2}	-5.0865387^{-2}	-4.3668076^{-2}	-3.3059143^{-2}	-1.9816739^{-2}	-4.7068457^{-3}
4.00	-5.2117105	-5.1646869	-4.7177736	-3.9267905	-2.8566932	-1.5746335^{-2}
4.30	-4.8968436	-5.0374872	-4.8010062	-4.2296597	-3.3768773	-2.3006428
4.60	-4.4851194	-4.7794797	-4.7262435	-4.3551983	-3.7085968	-2.8349927
4.95	-3.9338249	-4.3661862	-4.4901829	-4.3228811	-3.8945507	-3.2431120
5.25	-3.4346662	-3.9530935	-4.1983782	-4.1784275	-3.9144002	-3.4358216
5.60	-2.8520051	-3.4383654	-3.7922876	-3.9130043	-3.8125918	-3.5118430
5.90	-2.3697142	-2.9908630	-3.4129174	-3.6292539	-3.6454805	-3.4758974
6.25	-1.8409969	-2.4806249	-2.9572761	-3.2591432	-3.3857372	-3.3449660
6.55	-1.4236691	-2.0640550	-2.5696095	-2.9253117	-3.1265439	-3.1766999
6.90	-9.8272727^{-3}	-1.6105760	-2.1329269	-2.5321850	-2.8000706	-2.9357101
7.20	-6.4507706	-1.2535498	-1.7786618	-2.2014512	-2.5113188	-2.7045333
7.85	-3.6790485^{-4}	-5.8586206^{-3}	-1.0905841	-1.5309819	-1.8935305	-2.1702751

$$G^1_{3d,4p}$$
$$r = 3.60$$

Z3d\Z4p	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-5.1890513^{-2}	-4.8104761^{-2}	-4.0334141^{-2}	-2.9328534^{-2}	-1.5878536^{-2}	-7.4938641^{-4}
4.00	-5.0190270	-4.9026651	-4.4005226	-3.5711158	-2.4806210	1.1961613^{-2}
4.30	-4.7167493	-4.7907176	-4.5008669	-3.8920138	-3.0187836	-1.9392020
4.60	-4.3198466	-4.5503302	-4.4455607	-4.0377697	-3.3703850	-2.4920591
4.95	-3.7879209	-4.1597517	-4.2343236	-4.0310099	-3.5812207	-2.9230956
5.25	-3.3064847	-3.7672989	-3.9649364	-3.9095117	-3.6233323	-3.1361948
5.60	-2.7450461	-3.2772008	-3.5855551	-3.6714121	-3.5479962	-3.2364568
5.90	-2.2808774	-2.8507544	-3.2290320	-3.4110628	-3.4036060	-3.2213939
6.25	-1.7726825	-2.3644397	-2.7994317	-3.0677364	-3.1699973	-3.1146299
6.55	-1.3720757	-1.9674769	-2.4332293	-2.7560990	-2.9326015	-2.9666907
6.90	-9.4934645^{-3}	-1.5355177	-2.0202625	-2.3876705	-2.6305755	-2.7487251
7.20	-6.2603840	-1.1956062	-1.6850198	-2.0769115	-2.3617807	-2.5365443
7.85	-4.4518102^{-4}	-5.6043072^{-3}	-1.0336078	-1.4454844	-1.7835766	-2.0406229

TABLE III. (cont.).

G^1
3d,4p
r = 3.70

z3d\z4p	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-4.9747401^{-2}	-4.5313505^{-2}	-3.7053443^{-2}	-2.5739223^{-2}	-1.2168617^{-2}	2.8988671^{-3}
4.00	-4.8178447	-4.6393463	-4.0900421	-3.2305751	-2.1278212	-8.4846158
4.30	-4.5296873	-4.5439643	-4.2084352	-3.5699604	-2.6838786	-1.6078572^{-2}
4.60	-4.1489765	-4.3222677	-4.1732313	-3.7360495	-3.0548893	-2.1781577
4.95	-3.6377373	-3.9553208	-3.9871843	-3.7545722	-3.2896813	-2.6305012
5.25	-3.1748886	-3.5839891	-3.7402276	-3.6555176	-3.3529737	-2.8623829
5.60	-2.6353771	-3.1187893	-3.3872797	-3.4438716	-3.3026480	-2.9848640
5.90	-2.1897010	-2.7133803	-3.0531405	-3.2059974	-3.1795962	-2.9888722
6.25	-1.7022247	-2.2507498	-2.6488631	-2.8882366	-2.9704192	-2.9041451
6.55	-1.3183478	-1.8730439	-2.3033799	-2.5976604	-2.7533277	-2.7747187
6.90	-9.1368560^{-3}	-1.4620649	-1.9131782	-2.2525729	-2.4740248	-2.5777368
7.20	-6.0450450	-1.1387358	-1.5960982	-1.9606190	-2.2237309	-2.3828724
7.85	-4.9122868^{-4}	-5.3482051^{-3}	-9.7947815^{-3}	-1.3657826	-1.6821563	-1.9219255

G^1
3d,4p
r = 3.80

z3d\z4p	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-4.7534660^{-2}	-4.2525875^{-2}	-3.3856949^{-2}	-2.2316583^{-2}	-8.7041313^{-3}	6.2303138^{-3}
4.00	-4.6114353	-4.3778871	-3.7890821	-2.9072721	-1.7995568^{-2}	-5.3179137
4.30	-4.3387509	-4.3001134	-3.9261316	-3.2652292	-2.3730247	-1.3064890^{-2}
4.60	-3.9753612	-4.0978759	-3.9113237	-3.4514007	-2.7626234	-1.8928401
4.95	-3.4858181	-3.7551126	-3.7504593	-3.4945667	-3.0200670	-2.3645667
5.25	-3.0421566	-3.4051024	-3.5256484	-3.4171507	-3.1032382	-2.6134379
5.60	-2.5249891	-2.9647460	-3.1985372	-3.2308120	-3.0762225	-2.7559499
5.90	-2.0979433	-2.5801234	-2.8861061	-3.0143001	-2.9729847	-2.7771474
6.25	-1.6311448	-2.1407016	-2.5062150	-2.7207058	-2.7864298	-2.7122849
6.55	-1.2638230	-1.7817302	-2.1805716	-2.4499690	-2.5881053	-2.5995847
6.90	-8.7691429^{-3}	-1.3910403	-1.8120570	-2.1267855	-2.3297725	-2.4215815
7.20	-5.8152523	-1.0836578	-1.5122064	-1.8524280	-2.0965486	-2.2424132
7.85	-5.1464554^{-4}	-5.0960466^{-3}	-9.2842415^{-3}	-1.2917294	-1.5887317	-1.8132663

TABLE III. (cont.).

$$G^1$$
$$3d, 4p$$
$$r = 3.90$$

Z_{3d}\\Z_{4p}	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-4.5283013^{-2}	-3.9771085^{-2}	-3.0769875^{-2}	-1.9079235^{-2}	-5.4957742^{-3}	9.2440085^{-3}
4.00	-4.4026870	-4.1209284	-3.4998072	-2.6026777	-1.4964500^{-2}	-2.4581596
4.30	-4.1465831	-4.0615133	-3.6557931	-2.9789470	-2.0865003	-1.0344353^{-2}
4.60	-3.8013992	-3.8792119	-3.6613586	-3.1846268	-2.4935581	-1.6351826
4.95	-3.3342650	-3.5608547	-3.5253123	-3.2514615	-2.7720788	-2.1241496
5.25	-2.9101445	-3.2320947	-3.3221069	-3.1946567	-2.8736174	-2.3880814
5.60	-2.4154653	-2.8162490	-3.0199861	-3.0322551	-2.8680774	-2.5483647
5.90	-2.0069874	-2.4519659	-2.7284080	-2.8358560	-2.7830422	-2.5848415
6.25	-1.5606175	-2.0350878	-2.3718073	-2.5649346	-2.6172536	-2.5377091
6.55	-1.2095340	-1.6942004	-2.0650230	-2.3127479	-2.4361523	-2.4399859
6.90	-8.3992340^{-3}	-1.3229869	-1.7170402	-2.0100036	-2.1970674	-2.2790525
7.20	-5.5789858	-1.0308419	-1.4334432	-1.7520345	-1.9795124	-2.1140486
7.85	-5.2203974^{-4}	-4.8516646^{-3}	-8.8051987^{-3}	-1.2230659	-1.5027135	-1.7137338

$$G^1$$
$$3d, 4p$$
$$r = 4.00$$

Z_{3d}\\Z_{4p}	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-4.3019493^{-2}	-3.7073815^{-2}	-2.7812072^{-2}	-1.6040376^{-2}	-2.5482877^{-3}	1.1944401^{-2}
4.00	-4.1940555	-3.8706152	-3.2238329	-2.3176992	-1.2185778^{-2}	1.0296168^{-4}
4.30	-3.9554202	-3.8300351	-3.3987313	-2.7117146	-1.8240941	-7.9060577^{-3}
4.60	-3.6290650	-3.6678634	-3.4243546	-2.9360614	-2.2472453	-1.4039010^{-2}
4.95	-3.1847692	-3.3738268	-3.3124733	-3.0253235	-2.5450406	-1.9078251
5.25	-2.7803109	-3.0660139	-3.1301144	-2.9879109	-2.6633183	-2.1848317
5.60	-2.3080286	-2.6741220	-2.8519381	-2.8479368	-2.6773168	-2.3606075
5.90	-1.9178774	-2.3295652	-2.5802204	-2.6703137	-2.6088508	-2.4104929
6.25	-1.4915226	-1.9344187	-2.2457091	-2.4205048	-2.4619784	-2.3790169
6.55	-1.1562429	-1.6108641	-1.9567393	-2.1855648	-2.2965839	-2.2946104
6.90	-8.0337162^{-3}	-1.2582419	-1.6280917	-1.9017982	-2.0750827	-2.1489388
7.20	-5.3421216	-9.8058044^{-3}	-1.3597616	-1.6590313	-1.8718605	-1.9966752
7.85	-5.1834776^{-4}	-4.6175185	-8.3573367^{-3}	-1.1594741	-1.4235021	-1.6224579

TABLE III. (cont.).

G^1
3d,4p
r = 4.10

$Z_{3d}\backslash Z_{4p}$	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-4.0767493^{-2}	-3.4454106^{-2}	-2.4998464^{-2}	-1.3208054^{-2}	1.3844558^{-4}	1.4340306^{-2}
4.00	-3.9876342	-3.6286726	-2.9623168	-2.0527950	-9.6558286^{-3}	2.3774660^{-3}
4.30	-3.7671039	-3.6071149	-3.1558094	-2.4637056	-1.5852040	-5.7360614
4.60	-3.4599747	-3.4650127	-3.2009308	-2.7056463	-2.0228941	-1.1974705^{-2}
4.95	-3.0386677	-3.1949344	-3.1123001	-2.8158820	-2.3380194	-1.7139882
5.25	-2.6537935	-2.9075706	-2.9498502	-2.7965233	-2.4713380	-2.0020748
5.60	-2.2036092	-2.5388841	-2.6944223	-2.6773609	-2.5029072	-2.1911109
5.90	-1.8313968	-2.2133155	-2.4414951	-2.5171318	-2.4493839	-2.2525968
6.25	-1.4245034	-1.8389728	-2.1277952	-2.2868579	-2.3196122	-2.2348102
6.55	-1.1044984	-1.5319465	-1.8555641	-2.0678723	-2.1684648	-2.1621590
6.90	-7.6772825^{-3}	-1.1969736	-1.5450461	-1.8016566	-1.9629626	-2.0300783
7.20	-5.1088946	-9.3302083^{-3}	-1.2910049	-1.5729497	-1.7728202	-1.8892415
7.85	-5.0725418^{-4}	-4.3950433	-7.9396457^{-3}	-1.1006061	-1.3505055	-1.5386224

G^1
3d,4p
r = 4.20

$Z_{3d}\backslash Z_{4p}$	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-3.8546836^{-2}	-3.1928281^{-2}	-2.2339754^{-2}	-1.0585924^{-2}	2.5685170^{-3}	1.6444087^{-2}
4.00	-3.7851472	-3.3963914	-2.7159881	-1.8080061	-7.3675941	4.3801872^{-3}
4.30	-3.5831309	-3.3938178	-2.9275217	-2.2347422	-1.3689400^{-2}	-3.8181519
4.60	-3.2953816	-3.2714869	-2.9913553	-2.4930197	-1.8194751	-1.0142002^{-2}
4.95	-2.8969888	-3.0247771	-2.9248654	-2.6226309	-2.1499068	-1.5409417
5.25	-2.5314336	-2.7571991	-2.7812648	-2.6198954	-2.2965282	-1.8381523
5.60	-2.1028723	-2.4108183	-2.5472810	-2.5198784	-2.3437207	-2.0382948
5.90	-1.7480949	-2.1034049	-2.3119975	-2.3756508	-2.3035446	-2.1096612
6.25	-1.3600033	-1.7488670	-2.0178089	-2.1633574	-2.1891444	-2.1037272
6.55	-1.0546809	-1.4575137	-1.7612406	-1.9590653	-2.0508636	-2.0413907
6.90	-7.3332085^{-3}	-1.1392312	-1.4676555	-1.7090292	-1.8598706	-1.9213657
7.20	-4.8822784	-8.8820693^{-3}	-1.2269496	-1.4933032	-1.6816432	-1.7907564
7.85	-4.9144726^{-4}	-4.1849012	-7.5506732^{-3}	-1.0461004	-1.2831551	-1.4614835

TABLE III. (cont.).

$$G^3_{3d,4p}$$
$$r = 3.40$$

z3d\z4p	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-4.8332420^{-2}	-4.5606067^{-2}	-3.9194342^{-2}	-2.9710292^{-2}	-1.7850979^{-2}	-4.3265659^{-3}
4.00	-4.6076452	-4.4623977	-3.9672722	-3.1733705	-2.1414909	-9.3537525
4.30	-4.3243947	-4.2739635	-3.8963332	-3.2339462	-2.3395498	-1.2699453^{-2}
4.60	-3.9891515	-4.0183759	-3.7468405	-3.2088432	-2.4492327	-1.5176568
4.95	-3.5642876	-3.6671247	-3.5023226	-3.0956770	-2.4833931	-1.7070110
5.25	-3.1924781	-3.3428684	-3.2543451	-2.9463809	-2.4484898	-1.7957185
5.60	-2.7687721	-2.9586033	-2.9419862	-2.7321824	-2.3518527	-1.8292035
5.90	-2.4247263	-2.6366167	-2.6682095	-2.5284074	-2.2348264	-1.8105176
6.25	-2.0536721	-2.2800868	-2.3542012	-2.2808185	-2.0726463	-1.7475184
6.55	-1.7650862	-1.9962614	-2.0967401	-2.0685883	-1.9210413	-1.6681476
6.90	-1.4642772	-1.6941412	-1.8156523	-1.8284448	-1.7384790	-1.5561175
7.20	-1.2368355	-1.4611675	-1.5939057	-1.6331521	-1.5826325	-1.4501173
7.85	-8.3361466^{-3}	-1.0370991	-1.1783754	-1.2535274	-1.2629381	-1.2102292

$$G^3_{3d,4p}$$
$$r = 3.50$$

z3d\z4p	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-4.6061200^{-2}	-4.2346736^{-2}	-3.5099511^{-2}	-2.4983398^{-2}	-1.2724854^{-2}	9.5557002^{-4}
4.00	-4.3795213	-4.1431323	-3.5722427	-2.7224635	-1.6571203	-4.4075374^{-3}
4.30	-4.0999366	-3.9651619	-3.5183475	-2.8059640	-1.8829751	-8.0677039
4.60	-3.7720785	-3.7236522	-3.3891540	-2.8064798	-2.0223787	-1.0869375^{-2}
4.95	-3.3596896	-3.3923306	-3.1712232	-2.7252730	-2.0922993	-1.3141403
5.25	-3.0010729	-3.0872641	-2.9475646	-2.6042100	-2.0881094	-1.4345337
5.60	-2.5946877	-2.7268013	-2.6643465	-2.4229887	-2.0265844	-1.5035087
5.90	-2.2664100	-2.4256893	-2.4155078	-2.2468998	-1.9385561	-1.5136602
6.25	-1.9140502	-2.0933089	-2.1298551	-2.0303758	-1.8085096	-1.4822344
6.55	-1.6412407	-1.8295244	-1.8956500	-1.8433722	-1.6827769	-1.4280578
6.90	-1.3580728	-1.5495788	-1.6400966	-1.6307519	-1.5282834	-1.3432141
7.20	-1.1448231	-1.3343334	-1.4386682	-1.4512795	-1.3946184	-1.2586329
7.85	-7.6873759^{-3}	-9.4407095^{-3}	-1.0618094	-1.1191382	-1.1170644	-1.0594267

<p align="center">TABLE III. (cont.).</p>

<p align="center">$a^3_{3d\ 4p}$</p>

<p align="center">r = 3.60</p>

z3d⧵z4p	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-4.3577366^{-2}	-3.8971874^{-2}	-3.1007959^{-2}	-2.0391330^{-2}	-7.8692592^{-3}	5.8355524^{-3}
4.00	-4.1345578	-3.8169469	-3.1820139	-2.2890251	-1.2030235^{-2}	1.1424178^{-4}
4.30	-3.8623416	-3.6530693	-3.1484073	-2.3980568	-1.4584205	-3.8677760^{-3}
4.60	-3.5452915	-3.4288109	-3.0421516	-2.4260316	-1.6284141	-6.9920254
4.95	-3.1488649	-3.1204625	-2.8530794	-2.3780487	-1.7341862	-9.6308284
5.25	-2.8059357	-2.8365947	-2.6550340	-2.2856246	-1.7601215	-1.1135419^{-2}
5.60	-2.4191938	-2.5016181	-2.4017781	-2.1371862	-1.7324168	-1.2156059
5.90	-2.1081894	-2.2223121	-2.1780771	-1.9881618	-1.6718957	-1.2522573
6.25	-1.7757789	-1.9146596	-1.9205443	-1.8015683	-1.5719515	-1.2495010
6.55	-1.5194433	-1.6710495	-1.7090730	-1.6385766	-1.4701852	-1.2179805
6.90	-1.2543755	-1.4131026	-1.4781714	-1.4518745	-1.3414546	-1.1573760
7.20	-1.0554688	-1.2152250	-1.2961505	-1.2987603	-1.2279881	-1.0917736
7.85	-7.0631236^{-3}	-8.5756905^{-3}	-9.5573776^{-3}	-9.9887673^{-3}	-9.8844451^{-3}	-9.2836229^{-3}

<p align="center">$a^3_{3d,4p}$</p>

<p align="center">r = 3.70</p>

z3d⧵z4p	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-4.0938517^{-2}	-3.5542582^{-2}	-2.6979443^{-2}	-1.5987923^{-2}	-3.3274845^{-3}	1.0284213^{-2}
4.00	-3.8783414	-3.4895411	-2.8019271	-1.8775973	-7.8252552	4.1934395^{-3}
4.30	-3.6168946	-3.3429018	-2.7912173	-2.0139881	-1.0683351^{-2}	-1.0859631^{-4}
4.60	-3.3136696	-3.3138514	-2.7098444	-2.0704904	-1.2689889	-3.5451885^{-3}
4.95	-2.9361528	-2.8554773	-2.5510916	-2.0561354	-1.4098287	-6.5308723
5.25	-2.6109148	-2.5942265	-2.3793027	-1.9920838	-1.4646644	-8.3142507
5.60	-2.2455612	-2.2857692	-2.1561454	-1.8755615	-1.4688841	-9.6368001
5.90	-1.9528716	-2.0286918	-1.9572742	-1.7525042	-1.4339777	-1.0241884^{-2}
6.25	-1.6411610	-1.7458193	-1.7271227	-1.5942723	-1.3617483	-1.0469731
6.55	-1.4016247	-1.5221366	-1.5375104	-1.4537821	-1.2818408	-1.0354637
6.90	-1.1547333	-1.2856498	-1.3300628	-1.2911493	-1.1764217	-9.9613980^{-3}
7.20	-9.7004496^{-3}	-1.1045237	-1.1663275	-1.1567857	-1.0811145	-9.4711280
7.85	-6.4716423	-7.7789544^{-3}	-8.5985802^{-3}	-8.9180271^{-3}	-8.7548770^{-3}	-8.1482184

TABLE III. (cont.).

$$a^3_{3d,4p}$$
$$r = 3.80$$

Z3d\Z4p	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-3.8197186^{-2}	-3.2112429^{-2}	-2.3064012^{-2}	-1.1815411^{-2}	8.6975626^{-4}	1.4285449^{-2}
4.00	-3.6158449	-3.1657677	-2.4362919	-1.4915463	-3.9772860^{-3}	7.8244487^{-3}
4.30	-3.3681928	-3.0389892	-2.4504238	-1.6563678	-7.1401847	3.2122587
4.60	-3.0813685	-2.8565102	-2.3952024	-1.7417494	-9.4465366	-5.1950326^{-4}
4.95	-2.7251404	-2.6004481	-2.2675075	-1.7606555	-1.1190595^{-2}	-3.8255769^{-3}
5.25	-2.4191083	-2.3626814	-2.1220313	-1.7241532	-1.2010638	-5.8617133
5.60	-2.0763506	-2.0811854	-1.9285221	-1.6381450	-1.2348483	-7.4537815
5.90	-1.8025871	-1.8463168	-1.7537477	-1.5395840	-1.2233811	-8.2693066
6.25	-1.5118928	-1.5878434	-1.5498353	-1.4078123	-1.1762627	-8.7203867
6.55	-1.2891506	-1.3835299	-1.3809477	-1.2881271	-1.1160060	-8.7790008
6.90	-1.0602012	-1.1676744	-1.1955248	-1.1475657	-1.0314063	-8.5696531
7.20	-8.8938368^{-3}	-1.0024970	-1.0488216	-1.0302827	-9.5223030^{-3}	-8.2221832
7.85	-5.9178497	-7.0505865^{-3}	-7.7364900^{-3}	-7.9683792^{-3}	-7.7657756	-7.1668549

$$a^3_{3d,4p}$$
$$r = 3.90$$

Z3d Z4p	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-3.5400641^{-2}	-2.8727532^{-2}	-1.9302599^{-2}	-7.9055321^{-3}	4.7029167^{-3}	1.7834428^{-2}
4.00	-3.3514058	-2.8496696	-2.0884664	-1.1332050^{-2}	-4.9656385^{-4}	1.1011906
4.30	-3.1201488	-2.7448155	-2.1287353	-1.3268176	-3.9577930^{-3}	6.1063245^{-3}
4.60	-2.8518341	-2.5857171	-2.1003172	-1.4407741	-6.5509343	2.1022609
4.95	-2.5187176	-2.3576630	-2.0037244	-1.4919337	-8.6096446	-1.4929482
5.25	-2.2329433	-2.1437365	-1.8841247	-1.4816900	-9.6801030	-3.7528495
5.60	-1.9134908	-1.8891339	-1.7193230	-1.4243653	-1.0286936^{-2}	-5.5802534
5.90	-1.6588871	-1.6760843	-1.5675792	-1.3485665	-1.0383188	-6.5774667
6.25	-1.3891513	-1.4412719	-1.3884721	-1.2411528	-1.0136046	-7.2198198
6.55	-1.1829316	-1.2555339	-1.2389857	-1.1404589	-9.7076268^{-3}	-7.4265699
6.90	-9.7143197^{-3}	-1.0592707	-1.0740153	-1.0199147	-9.0453050	-7.3735965
7.20	-8.1397380	-9.0910986^{-3}	-9.4301366^{-3}	-9.1803545^{-3}	-8.3953478	-7.1474821
7.85	-5.4041787	-6.3886645	-6.9644863	-7.1285478	-6.9013812	-6.3197583

TABLE III. (cont.).

$$a^3_{3d,4p}$$
$$r = 4.00$$

$z_{3d}\backslash z_{4p}$	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-3.2590447^{-2}	-2.5426687^{-2}	-1.5727322^{-2}	-4.2804641^{-3}	8.1624417^{-3}	2.0935735^{-2}
4.00	-3.0887418	-2.5445233	-1.7609404	-8.0398800	2.6156586	1.3768566
4.30	-2.8760374	-2.4631053	-1.8280260	-1.0261151^{-2}	-1.1312075	8.5921659^{-3}
4.60	-2.6278679	-2.3283272	-1.8264835	-1.1677813	-3.9930263	4.3428863
4.95	-2.3191473	-2.1287220	-1.7604631	-1.2496354	-6.3407967	4.9332794^{-4}
5.25	-2.0542564	-1.9385607	-1.6658807	-1.2640032	-7.6377656	-1.9599202^{-3}
5.60	-1.7583707	-1.7103386	-1.5284579	-1.2332268	-8.4848599	-3.9877150
5.90	-1.5228428	-1.5184128	-1.3984260	-1.1782852	-8.7677371	-5.1381971
6.25	-1.2736875	-1.3062487	-1.2424768	-1.0930006	-8.7175274	-5.9409450
6.55	-1.0835067	-1.1381144	-1.1109547	-1.0094482	-8.4414193	-6.2715981
6.90	-8.8877661^{-3}	-9.6026313^{-3}	-9.6478855^{-3}	-9.0687401^{-3}	-7.9391952	-6.3494419
7.20	-7.4403571	-8.2410624	-8.4813429	-8.1876216	-7.4126092	-6.2250212
7.85	-4.9312570	-5.7898955	-6.2752675	-6.3872993	-6.1468492	-5.5889724

$$a^3_{3d,4p}$$
$$r = 4.10$$

$z_{3d}\backslash z_{4p}$	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-2.9802586^{-2}	-2.2241697^{-2}	-1.2362370^{-2}	-9.5407650^{-4}	1.1246945^{-2}	2.3601659^{-2}
4.00	-2.8309649	-2.2529015	-1.4554364	-5.0451935^{-3}	5.3654221^{-3}	1.6113789
4.30	-2.6385181	-2.1959069	-1.5494422	-7.5433433	1.3508646	1.0693449
4.60	-2.4116727	-2.0858768	-1.5743467	-9.2237144	-1.7574093	6.2291776^{-3}
4.95	-2.1281389	-1.9146410	-1.5378722	-1.0329329^{-2}	-4.3654807	2.1618714
5.25	-1.8843682	-1.7477851	-1.4671115	-1.0699996	-5.8633029	-4.5363608^{-4}
5.60	-1.6119321	-1.5450827	-1.3554449	-1.0634363	-6.9211145	-2.6473865^{-3}
5.90	-1.3951198	-1.3733470	-1.2456304	-1.0273431	-7.3663660	-3.9236765
6.25	-1.1659138	-1.1826137	-1.1110602	-9.6192344^{-3}	-7.4865261	-4.8576876
6.55	-9.9112380^{-3}	-1.0309947	-9.9600855^{-3}	-8.9367606	-7.3418269	-5.2897648
6.90	-8.1233698	-8.7028274^{-3}	-8.6697785	-8.0708273	-6.9775796	-5.4750832
7.20	-6.7959368	-7.4707731	-7.6333414	-7.3117883	-6.5573023	-5.4346506
7.85	-4.4983505	-5.2501802	-5.6612936	-5.7338212	-5.4884892	-4.9583889

TABLE III. (cont.).

$$G^3_{3d,4p}$$
$$r = 4.20$$

Z3d\Z4p	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-2.7067702^{-2}	-1.9197983^{-2}	-9.2248931^{-3}	2.0670699^{-3}	1.3961968^{-2}	2.5850602^{-2}
4.00	-2.5806357	-1.9767277	-1.1729942^{-2}	-2.3479688	7.7646398^{-3}	1.8071412
4.30	-2.4096990	-1.9446449	-1.2935360	-5.1097581	3.5044942	1.2437425
4.60	-2.2049340	-1.8593441	-1.3440152	-7.0366399	1.7489667^{-4}	7.7902344^{-3}
4.95	-1.9469095	-1.7159521	-1.3356564	-8.4062956	-2.6625105^{-3}	3.5426372
5.25	-1.7241654	-1.5716314	-1.2872607	-8.9829942	-4.3347982	7.9556319^{-4}
5.60	-1.4747323	-1.3932991	-1.1995153	-9.1349812	-5.5737625	-1.5308744^{-3}
5.90	-1.2760546	-1.2406431	-1.1083100	-8.9421996	-6.1576884	-2.9071288
6.25	-1.0659779	-1.0699855	-9.9328143^{-3}	-8.4642555	-6.4229486	-3.9453972
6.55	-9.0580802^{-3}	-9.3371629^{-3}	-8.9319134	-7.9170376	-6.3900724	-4.4584738
6.90	-7.4204520	-7.8883530	-7.7965550	-7.1919961	-6.1433224	-4.7302881
7.20	-6.2052660	-6.7752284	-6.8772922	-6.5404166	-5.8137947	-4.7581478
7.85	-4.1038753	-4.7649552	-5.1150977	-5.1580051	-4.9138761	-4.4137619

$$G^3_{3d,4p}$$
$$r = 4.30$$

Z3d\Z4p	3.00	3.25	3.50	3.75	4.00	4.25
3.65	-2.4411217^{-2}	-1.6314773^{-2}	-6.3256273^{-3}	4.7828139^{-3}	1.6318715^{-2}	2.7705399^{-2}
4.00	-2.3397893	-1.7173634	-9.1409413	5.7438302^{-5}	9.8297414^{-3}	1.9668701
4.30	-2.1911886	-1.7102241	-1.0603299^{-2}	-2.9508880^{-3}	5.3492652	1.3853347
4.60	-2.0088583	-1.6492402	-1.1351582	-5.1041843	1.8254946	9.0562406^{-3}
4.95	-1.7762721	-1.5327836	-1.1531708	-6.7126230	-1.2093070	4.6655940
5.25	-1.5741681	-1.4099767	-1.1254983	-7.4733927	-3.0295936	1.8166529
5.60	-1.3470310	-1.2546534	-1.0597050	-7.8181395	-4.4208866	-6.1111160^{-4}
5.90	-1.1657333	-1.1198482	-9.8544890^{-3}	-7.7733844	-5.1209030	-2.0633953^{-3}
6.25	-9.7382110^{-3}	-9.6782520^{-3}	-8.8811100	-7.4500417	-5.5075731	-3.1814184
6.55	-8.2741601	-8.4571165	-8.0150173	-7.0211960	-5.5684395	-3.7571568
6.90	-6.7770208	-7.1534710	-7.0187736	-6.4193886	-5.4206116	-4.0969243
7.20	-5.6661214	-6.1488864	-6.2044055	-5.8617859	-5.1678732	-4.1793376
7.85	-3.7456566	-4.3295158	-4.6295570	-4.6505483	-4.4119251	-3.9426708

<p style="text-align:center">T<small>ABLE</small> III. (cont.).</p>

$$B^1_{3d,4p}$$
$$r = 3.40$$

Z3d Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	1.8121212^{-2}	2.6417281^{-2}	3.3439305^{-2}	3.8813768^{-2}	4.2328404^{-2}	4.3911644^{-2}
4.00	1.7299676	2.5313688	3.2098784	3.7299234	4.0710369	4.2260203
4.30	1.6302100	2.4031431	3.0589034	3.5636430	3.8976621	4.0537255
4.60	1.5065166	2.2484542	2.8804326	3.3703658	3.6993321	3.8600033
4.95	1.3379620	2.0417083	2.6453981	3.1189741	3.4443494	3.6140231
5.25	1.1786294	1.8485530	2.4278197	2.8880281	3.2117474	3.3912636
5.60	9.8273733^{-3}	1.6125125	2.1631936	2.6082099	2.9308152	3.1230198
5.90	8.1175908	1.4068991	1.9330150	2.3650270	2.6867287	2.8898866
6.25	6.1450504	1.1693546	1.6667581	2.0832780	2.4033218	2.6183780
6.55	4.5115178	9.7183537^{-3}	1.4446158	1.8473958	2.1650919	2.3890055
6.90	2.7080112	7.5235621	1.1964756	1.5825577	1.8961259	2.1283125
7.20	1.2701763	5.7587830	9.9557981^{-3}	1.3667602	1.6754644	1.9127539
7.85	-1.4537313	2.3609015	6.0386439	9.4112275^{-3}	1.2351067	1.4769185

$$B^1_{3d,4p}$$
$$r = 3.50$$

Z3d Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	1.9745438^{-2}	2.7327253^{-2}	3.3486657^{-2}	3.7910780^{-2}	4.0446687^{-2}	4.1076984^{-2}
4.00	1.8721945	2.6018410	3.1955589	3.6235914	3.8711131	3.9359900
4.30	1.7546671	2.4567650	3.0302890	3.4469136	3.6922383	3.7637420
4.60	1.6140670	2.2869602	2.8400920	3.2465737	3.4923956	3.5745609
4.95	1.4279553	2.0655595	2.5950507	2.9911366	3.2401786	3.3385462
5.25	1.2559493	1.8627119	2.3720948	2.7600797	3.0132809	3.1274865
5.60	1.0482835	1.6187516	2.1047187	2.4835726	2.7421742	2.8756197
5.90	8.6974776^{-3}	1.4090561	1.8748731	2.2457166	2.5086410	2.6581644
6.25	6.6638421	1.1695333	1.6116396	1.9724767	2.2393363	2.4061267
6.55	4.9981929	9.7232681^{-3}	1.3939069	1.7453742	2.0142360	2.1939555
6.90	3.1766449	7.5506661	1.1525028	1.4919651	1.7612640	1.9534338
7.20	1.7366027	5.8169250	9.5833899^{-3}	1.2865805	1.5545215	1.7549337
7.85	-9.6371942^{-4}	2.5097349	5.8276923	8.8406802^{-3}	1.1437609	1.3543163

Table III. (cont.).

$$B^1_{3d,4p}$$

$$r = 3.60$$

Z3d Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.0971160^{-2}	2.7820489^{-2}	3.3130052^{-2}	3.6647070^{-2}	3.8275360^{-2}	3.8047143^{-2}
4.00	1.9751706	2.6324246	3.1437744	3.4851496	3.6470363	3.6318838
4.30	1.8413125	2.4728767	2.9674153	3.3019496	3.4670021	3.4642738
4.60	1.6858565	2.2908388	2.7690557	3.0985765	3.2699101	3.2838880
4.95	1.4850723	2.0584815	2.5182868	2.8436795	3.0250579	3.0621906
5.25	1.3030788	1.8491876	2.2935202	2.6161580	2.8073596	2.8659395
5.60	1.0868126	1.6009482	2.0272483	2.3467484	2.5495242	2.6333098
5.90	9.0334632^{-3}	1.3900784	1.8006910	2.1169961	2.3289295	2.4333542
6.25	6.9671870	1.1516127	1.5434538	1.8549402	2.0758847	2.2022394
6.55	5.2913629	9.5698091^{-3}	1.3322666	1.6384356	1.8652568	2.0080073
6.90	3.4743144	7.4417541	1.0996153	1.3980657	1.6293215	1.7880118
7.20	2.0486503	5.7549113	9.1354263^{-3}	1.2040879	1.4370154	1.6065226
7.85	-6.0025182^{-4}	2.5633717	5.5605650	8.2585133^{-3}	1.0560362	1.2402224

$$B^1_{3d,4p}$$

$$r = 3.70$$

Z3d Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.1833677^{-2}	2.7947138^{-2}	3.2432854^{-2}	3.5096389^{-2}	3.5894893^{-2}	3.4905208^{-2}
4.00	2.0431087	2.6287151	3.0612760	3.3221814	3.4068237	3.3217253
4.30	1.8947749	2.4573712	2.8771781	3.1362787	3.2297059	3.1628573
4.60	1.7267890	2.2661114	2.6741599	2.9336500	3.0391746	2.9948940
4.95	1.5143623	2.0264525	2.4216809	2.6833991	2.8056236	2.7910067
5.25	1.3250590	1.8137678	2.1983195	2.4625511	2.5999478	2.6118883
5.60	1.1032264	1.5645805	1.9365068	2.2033548	2.3580238	2.4004589
5.90	9.1725558^{-3}	1.3550899	1.7157057	1.9838872	2.1520785	2.2190906
6.25	7.0990941	1.1202669	1.4668624	1.7350056	1.9166944	2.0095709
6.55	5.4322047	9.3007559^{-3}	1.2638617	1.5303615	1.7212895	1.8334193
6.90	3.6386092	7.2350123	1.0414422	1.3040517	1.5028339	1.6337245
7.20	2.2408664	5.6071555	8.6439129^{-3}	1.1220239	1.3250293	1.4687841
7.85	-3.3485572^{-4}	2.5490459	5.2614830	7.6842701^{-3}	9.7327308^{-3}	1.1352467

TABLE III. (cont.).

$B^1_{3d,4p}$

r = 3.80

Z3d Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.2369982^{-2}	2.7756862^{-2}	3.1455180^{-2}	3.3326471^{-2}	3.3376729^{-2}	3.1722500^{-2}
4.00	2.0802322	2.5960769	2.9543083	3.1414730	3.1574093	3.0121993
4.30	1.9195792	2.4157690	2.7657977	2.9564798	2.9868897	2.8656018
4.60	1.7415356	2.2182943	2.5614490	2.7580110	2.8062058	2.7130066
4.95	1.5205071	1.9748112	2.3109167	2.5159707	2.5871588	2.5295637
5.25	1.3264649	1.7615424	2.0917712	2.3043871	2.3956879	2.3691709
5.60	1.1018813	1.5143484	1.8372304	2.0578581	2.1715523	2.1800861
5.90	9.1557914^{-3}	1.3084193	1.6241796	1.8502941	1.9813496	2.0177620
6.25	7.0972945	1.0793701	1.3855708	1.6159521	1.7643748	1.8298583
6.55	5.4554087	8.9509684^{-3}	1.1919522	1.4239498	1.5844565	1.6714694
6.90	3.7007709	6.9610602	9.8076251^{-3}	1.2122202	1.3834281	1.4913955
7.20	2.3416407	5.4009124	8.1329897	1.0423137	1.2198484	1.3422385
7.85	-1.4464374^{-4}	2.4878436	4.9482017	7.1310560^{-3}	8.9620814^{-3}	1.0394761

$B^1_{3d,4p}$

r = 3.90

Z3d Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.2617594^{-2}	2.7297653^{-2}	3.0253140^{-2}	3.1398136^{-2}	3.0783192^{-2}	2.8558933^{-2}
4.00	2.0906805	2.5395536	2.8285374	2.9489671	2.9046604	2.7087189
4.30	1.9200312	2.3531378	2.6388047	2.7681949	2.7439471	2.5773082
4.60	1.7344462	2.1523417	2.4361821	2.5768775	2.5758268	2.4423405
4.95	1.5077629	1.9082523	2.1908149	2.3460158	2.3737782	2.2811655
5.25	1.3113819	1.6968936	1.9782618	2.1457527	2.1980645	2.1404209
5.60	1.0865824	1.4542155	1.7332718	1.9137090	1.9929166	1.9741208
5.90	9.0184904^{-3}	1.2536557	1.5295046	1.7191558	1.8190129	1.8307644
6.25	6.9936465	1.0320727	1.3024638	1.5001803	1.6206484	1.6639885
6.55	5.3899118	8.5483934^{-3}	1.1190250	1.3211859	1.4560802	1.5226786
6.90	3.6864278	6.6439780	9.1965228^{-3}	1.1241473	1.2720491	1.3612265
7.20	2.3740015	5.1573263	7.6203698	9.6624229^{-3}	1.1221526	1.2268809
7.85	-1.1391341^{-5}	2.3957741	4.6333447	6.6070700	8.2514360^{-3}	9.5264056^{-3}

TABLE III. (cont.).

$$B^1_{3d,4p}$$

r = 4.00

Z3d Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.2613609^{-2}	2.6615037^{-2}	2.8878004^{-2}	2.9365454^{-2}	2.8167449^{-2}	2.5463564^{-2}
4.00	2.0784122	2.4637863	2.6890087	2.7497842	2.6534357	2.4155573
4.30	1.9001587	2.2740516	2.5010208	2.5761640	2.5052173	2.3016054
4.60	1.7094945	2.0726374	2.3028449	2.3945296	2.3518064	2.1858665
4.95	1.4799333	1.8308276	2.0653923	2.1772213	2.1685563	2.0480417
5.25	1.2833893	1.6235359	1.8613662	1.9898103	2.0095908	1.9272872
5.60	1.0606008	1.3874754	1.6276923	1.7735026	1.8240211	1.7836171
5.90	8.7904662^{-3}	1.1937236	1.4343180	1.5926161	1.6665249	1.6587329
6.25	6.8146250	9.8089442^{-3}	1.2197314	1.3893672	1.4865297	1.5121954
6.55	5.2594142	8.1149849	1.0469268	1.2234111	1.3368654	1.3870252
6.90	3.6163012	6.3024198	8.5961582^{-3}	1.0408479	1.1691179	1.2429716
7.20	2.3563490	4.8925747	7.1186595	8.9460078^{-3}	1.0321813	1.1223410
7.85	7.9208330^{-5}	2.2848163	4.3255896	6.1169342	7.6008172^{-3}	8.7424858^{-3}

$$B^1_{3d,4p}$$

r = 4.10

Z3d Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.2393807^{-2}	2.5751272^{-2}	2.7375910^{-2}	2.7275294^{-2}	2.5574049^{-2}	2.2475512^{-2}
4.00	2.0471426	2.3729960	2.5401477	2.5482586	2.4076550	2.1359492
4.30	1.8636609	2.1825663	2.3565752	2.3842931	2.2740890	2.0411127
4.60	1.6702676	1.9829927	2.1652023	2.2143952	2.1369717	1.9455923
4.95	1.4403656	1.7459808	1.9379251	2.0124379	1.9736899	1.8315381
5.25	1.2455874	1.5445666	1.7439368	1.8389394	1.8319650	1.7306216
5.60	1.0267125	1.3168108	1.5228635	1.6391024	1.6660536	1.6089507
5.90	8.4966482^{-3}	1.1309654	1.3406216	1.4721528	1.5247053	1.5017145
6.25	6.5819537	9.2780612^{-3}	1.1389807	1.2846085	1.3624862	1.3742405
6.55	5.0830770	7.6677075	9.7697967^{-3}	1.1314531	1.2270498	1.2640960
6.90	3.5068918	5.9504846	8.0169986	9.6290283^{-3}	1.0746741	1.1360908
7.20	2.3032060	4.6187264	6.6364140	8.2780942	9.4985929^{-3}	1.0280160
7.85	1.3829274^{-4}	2.1637585	4.0306247	5.6626820	7.0082147	8.0367950^{-3}

<div align="center">Table III. (cont.).</div>

$$B^1_{3d,4p}$$
$$r = 4.20$$

Z3d Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.1992130^{-2}	2.4745145^{-2}	2.5787764^{-2}	2.5167772^{-2}	2.3039373^{-2}	1.9624801^{-2}
4.00	2.0003032	2.2709326	2.3857668	2.3479658	2.1703953	1.8722278
4.30	1.8138845	2.0822322	2.2089502	2.1957237	2.0531167	1.7975807
4.60	1.6199331	1.8866705	2.0263461	2.0391471	1.9333528	1.7227182
4.95	1.3919664	1.6565951	1.8110343	1.8538054	1.7906435	1.6322943
5.25	1.2006130	1.4625257	1.6281968	1.6948478	1.6662165	1.5506610
5.60	9.8723137^{-3}	1.2443707	1.4205810	1.5117759	1.5196257	1.4499826
5.90	8.1574969	1.0672193	1.2498740	1.3587124	1.3938705	1.3593308
6.25	6.3131556	8.7432540^{-3}	1.0613500	1.1865494	1.2485838	1.2495554
6.55	4.8761832	7.2192941	9.1009208^{-3}	1.0457512	1.1265404	1.1532216
6.90	3.3711899	5.5986039	7.4659388	8.9057140^{-3}	9.8849667^{-3}	1.0398534
7.20	2.2258898	4.3445806	6.1790963	7.6602099	8.7490113	9.4316343^{-3}
7.85	1.7442772^{-4}	2.0388921	3.7519085	5.2445123	6.4703410	7.4025731

$$B^3_{3d,4p}$$
$$r = 3.40$$

Z3d Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.1445857^{-2}	3.1794198^{-2}	4.0740825^{-2}	4.7734434^{-2}	5.2435370^{-2}	5.4697745^{-2}
4.00	2.1769891	3.1369107	3.9537619	4.5781783	4.9804853	5.1488997
4.30	2.1595670	3.0519021	3.8016801	4.3644893	4.7142163	4.8412983
4.60	2.1039947	2.9287939	3.6141186	4.1202590	4.4243989	4.5188529
4.95	1.9984159	2.7469459	3.3623735	3.8100216	4.0704145	4.1376344
5.25	1.8806023	2.5671382	3.1279345	3.5321437	3.7627356	3.8149078
5.60	1.7209382	2.3398365	2.8431618	3.2039735	3.4076004	3.4501662
5.90	1.5724294	2.1375975	2.5967452	2.9258509	3.1118801	3.1514874
6.25	1.3935169	1.9009280	2.3139193	2.6113804	2.7818630	2.8223595
6.55	1.2406526	1.7026391	2.0801580	2.3542618	2.5145919	2.5582861
6.90	1.0679790	1.4814741	1.8217695	2.0721040	2.2231598	2.2721286
7.20	9.2786216^{-3}	1.3034160	1.6149192	1.8472474	1.9918193	2.0458114
7.85	6.5727136	9.6101224^{-3}	1.2183790	1.4171552	1.5500575	1.6141435

TABLE III. (cont.).

$$B^3$$
$$3d \cdot 4p$$
$$r = 3.50$$

z3d\z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.3875140^{-2}	3.3278713^{-2}	4.1039638^{-2}	4.6694161^{-2}	4.9992043^{-2}	5.0871237^{-2}
4.00	2.3752695	3.2374380	3.9360748	4.4303323	4.6990220	4.7381658
4.30	2.3196438	3.1139170	3.7483707	4.1867326	4.4108643	4.4183829
4.60	2.2280665	2.9563708	3.5310312	3.9200157	4.1078447	4.0933734
4.95	2.0850060	2.7406970	3.2524443	3.5925841	3.7482418	3.7192298
5.25	1.9397801	2.5377514	3.0016432	3.3070474	3.4428654	3.4093823
5.60	1.7539820	2.2901637	2.7049138	2.9770454	3.0970798	3.0655144
5.90	1.5879709	2.0758579	2.4536144	2.7023898	2.8137700	2.7882079
6.25	1.3938745	1.8305418	2.1702875	2.3965619	2.5018845	2.4864890
6.55	1.2319454	1.6287692	1.9396832	2.1497995	2.2522514	2.2469768
6.90	1.0525538	1.4072101	1.6881309	1.8820880	1.9827647	1.9897129
7.20	9.0936763^{-3}	1.2312501	1.4890880	1.6708847	1.7706938	1.7877303
7.85	6.3820112	8.9844283^{-3}	1.1129275	1.2718449	1.3698827	1.4055970

$$B^3$$
$$3d, 4p$$
$$r = 3.60$$

z3d\z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.5705480^{-2}	3.4116293^{-2}	4.0691874^{-2}	4.5056936^{-2}	4.7048017^{-2}	4.6680502^{-2}
4.00	2.5146959	3.2767429	3.8596090	4.2308806	4.3774430	4.3023938
4.30	2.4234364	3.1192169	3.6425647	3.9651574	4.0762940	3.9800003
4.60	2.2995626	2.9326609	3.4023452	3.6839361	3.7687197	3.6612839
4.95	2.1242750	2.6900999	3.1051336	3.3483342	3.4127842	3.3032395
5.25	1.9565532	2.4700636	2.8447754	3.0622561	3.1166973	3.0126939
5.60	1.7504545	2.2089935	2.5434028	2.7377443	2.7870995	2.6956001
5.90	1.5717746	1.9880185	2.2927838	2.4718894	2.5209090	2.4434218
6.25	1.3677416	1.7396843	2.0145332	2.1797912	2.2313765	2.1721180
6.55	1.2007953	1.5386105	1.7910571	1.9468217	2.0019900	1.9587223
6.90	1.0188273	1.3207691	1.5500686	1.6965743	1.7564703	1.7311535
7.20	8.7561295^{-3}	1.1498053	1.3613208	1.5008664	1.5646643	1.5535122
7.85	6.0893494	8.3109962^{-3}	1.0090332	1.1349603	1.2051781	1.2193896

TABLE III. (cont.).

B^3
3d,4p
r = 3.70

Z3d\ Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.6984103^{-2}	3.4380364^{-2}	3.9795297^{-2}	4.2941128^{-2}	4.3736100^{-2}	4.2266237^{-2}
4.00	2.6013043	3.2633050	3.7349783	3.9920893	4.0290073	3.8551335
4.30	2.4778340	3.0768980	3.4951887	3.7119446	3.7232559	3.5387644
4.60	2.3259332	2.8670517	3.2389221	3.4237585	3.4189457	3.2339659
4.95	2.1240008	2.6044948	2.9308458	3.0881244	3.0746613	2.8993801
5.25	1.9387226	2.3731227	2.6670983	2.8076574	2.7935870	2.6330481
5.60	1.7179251	2.1047994	2.3674646	2.4946991	2.4854846	2.3468940
5.90	1.5310566	1.8819194	2.1222017	2.2418620	2.2398354	2.1221928
6.25	1.3217796	1.6353625	1.8535259	1.9673079	1.9754511	1.8828276
6.55	1.1533336	1.4384298	1.6402356	1.7505275	1.7678159	1.6959822
6.90	9.7226815^{-3}	1.2275690	1.4125407	1.5196656	1.5471572	1.4978328
7.20	8.3149940	1.0637990	1.2357848	1.3404569	1.3757864	1.3437702
7.85	5.7323146	7.6237436^{-3}	9.0943030^{-3}	1.0083328	1.0566566	1.0549648

B^3
3d,4p
r = 3.80

Z3d\ Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.7763338^{-2}	3.4145998^{-2}	3.8444840^{-2}	4.0456773^{-2}	4.0175875^{-2}	3.7750493^{-2}
4.00	2.6413797	3.2054385	3.5721451	3.7250265	3.6652628	3.4076961
4.30	2.4897023	2.9956059	3.3161976	3.4377926	3.3625522	3.1048897
4.60	2.3143750	2.7682114	3.0503995	3.1495257	3.0682979	2.8203202
4.95	2.0914481	2.4922672	2.7385753	2.8209502	2.7422853	2.5148791
5.25	1.8933842	2.2548569	2.4768512	2.5512288	2.4806967	2.2762511
5.60	1.6631051	1.9848021	2.1843423	2.2546438	2.1979449	2.0236254
5.90	1.4720702	1.7640955	1.9482149	2.0179746	1.9750867	1.8275373
6.25	1.2616352	1.5232745	1.6925731	1.7636048	1.7374137	1.6204011
6.55	1.0946413	1.3332056	1.4916968	1.5645127	1.5521182	1.4596612
6.90	9.1731279^{-3}	1.1317915	1.2791317	1.3540238	1.3563060	1.2898191
7.20	7.8092575	9.7679046^{-3}	1.1153946^{-}	1.1916437	1.2048994	1.1580238
7.85	5.3396273	6.9469164	8.1587268^{-3}	8.9284354^{-3}	9.2418823^{-3}	9.1108213^{-3}

TABLE III. (cont.).

B^3
3d,4p
r = 3.90

Z3d\Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.8098536^{-2}	3.3487490^{-2}	3.6730412^{-2}	3.7704361^{-2}	3.6472447^{-2}	3.3236730^{-2}
4.00	2.6412109	3.1110624	3.3802346	3.4394800	3.2960266	2.9693215
4.30	2.4657035	2.8833504	3.1144853	3.1519019	3.0030896	2.6863907
4.60	2.2716602	2.6439736	2.8451923	2.8696221	2.7245921	2.4270110
4.95	2.0332418	2.3607802	2.5359015	2.5540942	2.4220786	2.1548269
5.25	1.8268640	2.1220569	2.2808081	2.2992191	2.1832470	1.9460797
5.60	1.5918157	1.8550289	1.9998043	2.0226269	1.9283968	1.7282141
5.90	1.4001261	1.6398752	1.7757335	1.8043124	1.7295650	1.5608587
6.25	1.1919856	1.4079304	1.5356475	1.5717591	1.5191315	1.3852612
6.55	1.0288503	1.2267880	1.3486705	1.3910804	1.3560133	1.2495154
6.99	8.5747516^{-3}	1.0365783	1.1523152	1.2012026	1.1843368	1.1062696
7.20	7.2692565	8.9138217^{-3}	1.0020651	1.0554480	1.0519629	9.9506336^{-3}
7.85	4.9327130	6.2971419	7.2935975^{-3}	7.8869489^{-3}	8.0707444^{-3}	7.8609364

B^3
3d,4p
r = 4.00

Z3d\Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.8045734^{-2}	3.2476507^{-2}	3.4735239^{-2}	3.4773632^{-2}	3.2716198^{-2}	2.8810270^{-2}
4.00	2.6069200	2.9875662	3.1674385	3.1438967	2.9294402	2.5472900
4.30	2.4121214	2.7474014	2.8978261	2.8620114	2.6520080	2.2892884
4.60	2.2040133	2.5012733	2.6304427	2.5909019	2.3938562	2.0587751
4.95	1.9553109	2.2163674	2.3290975	2.2932593	2.1187330	1.8224841
5.25	1.7446904	1.9804429	2.0844127	2.0563524	1.9048477	1.6446750
5.60	1.5090136	1.7204018	1.8183249	1.8022806	1.6792839	1.4616387
5.90	1.3196579	1.5134971	1.6084423	1.6036618	1.5048465	1.3223243
6.25	1.1166305	1.2928146	1.3855874	1.3936791	1.3213548	1.1768262
6.55	9.5924612^{-3}	1.1220642	1.2133652	1.2315205	1.1796857	1.0644798
6.90	7.9548920	9.4420376^{-3}	1.0336729	1.0618974	1.0309163	9.4573028^{-3}
7.20	6.7179973	8.0939470	8.9693407^{-3}	9.3216595^{-3}	9.1631914^{-3}	8.5321690
7.85	4.5271202	5.6850802	6.5033987	6.9561600	7.0426820	6.7816030

TABLE III. (cont.).

$$B^3_{3d,4p}$$
$$r = 4.10$$

Z3d\Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.7660162^{-2}	3.1180573^{-2}	3.2534850^{-2}	3.1743096^{-2}	2.8983254^{-2}	2.4539564^{-2}
4.00	2.5443301	2.8416963	2.9409714	2.8454330	2.5720873	2.1471023
4.30	2.3347737	2.5942416	2.6728774	2.5744683	2.3148441	1.9178731
4.60	2.1170444	2.3461355	2.4121172	2.3187955	2.0805268	1.7186849
4.95	1.8628591	2.0643726	2.1232096	2.0427736	1.8354625	1.5196413
5.25	1.6516043	1.8347024	1.8919081	1.8260409	1.6477384	1.3728502
5.60	1.4188474	1.5848463	1.6432484	1.5960483	1.4518714	1.2237928
5.90	1.2342821	1.3882501	1.4489799	1.4177305	1.3015044	1.1111973
6.25	1.0385929	1.1805299	1.2443093	1.2303672	1.1439958	9.9382234^{-3}
6.55	8.8838180^{-3}	1.0211225	1.0871727	1.0863402	1.0226252	9.0296364
6.90	7.3341244	8.5623490^{-3}	9.2409298^{-3}	9.3616975^{-3}	8.9518815^{-3}	8.0638283
7.20	6.1724627	7.3202528	8.0055080	8.2157805	7.9691400	7.3057281
7.85	4.1336510	5.1169109	5.7886430	6.1302555	6.1453044	5.8538825

$$B^3_{3d,4p}$$
$$r = 4.20$$

Z3d\Z4p	3.0	3.25	3.50	3.75	4.00	4.25
3.65	2.6995030^{-2}	2.9662253^{-2}	3.0196800^{-2}	2.8680331^{-2}	2.5336166^{-2}	2.0477317^{-2}
4.00	2.4588578	2.6795016	2.7070529	2.5500177	2.2291154	1.7727257
4.30	2.2389377	2.4295232	2.4452432	2.2943379	1.9957125	1.5749375
4.60	2.0157407	2.1836887	2.1950736	2.0574623	1.7877043	1.4084487
4.95	1.7603642	1.9092123	1.9221961	1.8057652	1.5742454	1.2468859
5.25	1.5515991	1.6886141	1.7064947	1.6105901	1.4130699	1.1304038
5.60	1.3247070	1.4514069	1.4769633	1.4053956	1.2464988	1.0137445
5.90	1.1468887	1.2665983	1.2991200	1.2473868	1.1193253	9.2609946^{-3}
6.25	9.6022400^{-3}	1.0729473	1.1129864	1.0821269	9.8637219^{-3}	8.3451189
6.55	8.1818869	9.2539070^{-3}	9.7084085^{-3}	9.5547098^{-3}	8.8386195	7.6305319
6.90	6.7275756	7.7368054	8.2393814	8.2363503	7.7596056	6.8621911
7.20	5.6447198	6.5999205	7.1302629	7.2311253	6.9245411	6.2512280
7.85	3.7594999	4.5954557	5.1470944	5.4015836	5.3654243	5.0592919

TABLE IV. $G^o_{4s,4s}$ $Z_{4s} = 2.50 \to 5.00$

$r = 3.20 \to 4.20$.

$$G^o_{4s,4s}$$

r\Z4s	2.5	3.0	3.5	4.0	4.5	5.0
3.0	1.2358037^{-1}	1.4507007^{-1}	1.6506257^{-1}	1.8316303^{-1}	1.9988902^{-1}	2.1605411^{-1}
3.1	1.2311615	1.4440270	1.6398410	1.8166741	1.9815977	2.1427314
3.2	1.2266652	1.4371226	1.6287439	1.8018625	1.9651388	2.1260632
3.3	1.2222409	1.4299739	1.6174061	1.7873932	1.9495101	2.1103502
3.4	1.2178476	1.4225474	1.6059515	1.7733079	1.9347736	2.0954624
3.5	1.2134090	1.4148221	1.5944763	1.7597468	1.9208471	2.0811966
3.6	1.2089172	1.4069085	1.5830696	1.7467901	1.9077159	2.0673003
3.7	1.2042900	1.3987990	1.5718371	1.7344026	1.8952514	2.0536707
3.8	1.1995494	1.3905287	1.5608405	1.7226275	1.8832902	2.0400700
3.9	1.1946521	1.3821598	1.5501474	1.7114611	1.8718027	2.0263017
4.0	1.1895853	1.3737227	1.5397784	1.7008505	1.8605703	2.0122518
4.1	1.1843818	1.3652961	1.5298223	1.6907463	1.8495450	1.9977786
4.2	1.1790184	1.3569169	1.5202631	1.6810628	1.8385419	1.9827486
4.3	1.1735384	1.3486560	1.5111100	1.6717511	1.8274220	1.9671792
4.4	1.1679277	1.3405449	1.5023580	1.6627185	1.8161439	1.9509340
4.5	1.1622300	1.3325934	1.4939921	1.6538403	1.8045800	1.9340173
4.6	1.1564406	1.3248458	1.4859816	1.6451154	1.7926855	1.9164152
4.7	1.1506124	1.3173405	1.4783385	1.6364200	1.7803576	1.8981570
4.8	1.1447689	1.3100926	1.4709300	1.6276693	1.7675885	1.8792737
4.9	1.1389117	1.3030827	1.4637955	1.6188378	1.7543392	1.8598124
5.0	1.1330850	1.2963246	1.4568376	1.6098014	1.7406156	1.8398113