ACCURATE GAUSSIAN EXPANSION OF STO'S. TEST OF MANY--CENTER SLATER INTEGRALS

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Dedicated to Dr R. Zahradník on the occasion of his 60th birthday.

The use of large STO-NG expansions for testing algorithms and procedures designed for the calculation of many-center molecular integrals with Slater basis functions was previously proposed. Expansions up to the STO-12G for the 1s and 2s cases and a method for calculating integrals involving higher quantum numbers were there reported. Here, we present the corresponding expansions from STO-13G to STO-27G. Further tests on the convergence in the integral calculations with the new expansions are also included and the results are compared with those obtained previously. These new expansions are necessary when highly accurate comparisons are required.

In a previous paper[1] we have noted that due to the recent advances[2-12] towards the solution of the problem of molecular integrals with Slater orbitals (STO's), a procedure for checking the precision of the new computational algorithms becomes desirable. Therefore we have proposed a procedure based on the use of large NG gaussian expansions of the STO's and we have presented the optimized exponents and coefficients up to the 12G ones. A study of the precision reached with these expansions shows us that any NG expansion must be enlarged with three gaussians in order to gain a next correct figure in the evaluation of integrals, so that the 12G expansion cannot ensure, in general, the fifth significant digit. It is clear that larger expansions are necessary for high precision tests.

In this work we present the optimized exponents and coefficients for the expansions from 13G to 27G and we show the improvement in the accuracy of the integrals.

Gaussian Expansions of the Slater Orbitals

As we have previously remarked[1], any unnormalized real STO can be written as a product of a first factor:

$$r^{2E[(n-l-1)/2]} r^l P_l^m(e^{im\phi} \pm e^{-im\phi})/\sqrt{\pm 1}$$

which is a polynomial of the (x, y, z) cartesian coordinates (with $E(x)$ = Integer part of x) times a second factor which can be, either:

$$f = e^{-r}, \quad \text{if} \quad n - l \quad \text{is odd}$$

or

$$f = r\, e^{-r}, \quad \text{if} \quad n - l \quad \text{is even}.$$

In this way, the expansion of arbitrary STO's in terms of the easy-integrable Gaussian-type functions only requires to obtain two NG expansions of the second factor. These two expansions can be written as:

$$f_N = \sum_{i=1}^{N} c_i\, e^{-\alpha_i r^2},$$

where both the coefficients and exponents are obtained by minimizing the "distance" $f_N - f$ in the least-squares sense. The iterative procedure used for solving this non--linear problem was discussed in detail in our previous paper[1]. Here we only note that although the numerical problems and the convergence difficulties increase with N, both were solved in a similar way to that employed in our previous paper, i.e. the numerical problems were avoided by working in extended precision and the convergence problems by starting near the minimum. As in the previous study, the selection of the starting point was facilitated by the existence of a clear relation between the exponents corresponding to successive values of N. This relation is illustrated in Tables I and II, where the quotients α_i/α_1 for the larger expansions are collected.* As it can be readily noticed, these quotients tend to form a sequence of "magic numbers", which seems to be the same for both the 1s and 2s expansions, except that, in the second one, a gap arises near the middle of the sequence.

The resulting exponents and coefficients are listed in Tables III and IV. We stress that they correspond to the screening constant ζ equal to 1 and that those corresponding to any arbitrary screening constant ζ can be obtained, as usual[13] by the relation $\alpha_i \leftarrow \zeta^2 \alpha_i$.

Accuracy in the Calculation of Many-Center Slater Integrals

We have employed these new expansions for analyzing the convergence in the calculation of many-center integrals. The calculations were performed with the aid of a computer program developed in our laboratory on the basis of the formulas and algorithm described by V. R. Saunders[14]. For comparative purposes, we have chosen the same

* It should be noted that squared roots of the quotients $\sqrt{(\alpha_i/\alpha_1)}$, are given in Table I of ref.[1], while the Tables I and II of the present article contain the quotients α_i/α_1.

TABLE I

Relation between the α-parameters of the STO-NG expansions of STO-1s:
(Each column collects the quotient α_i/α_1 in increasing order of the i-index)

22	23	24	25	26	27
0.10000E+01	0.10000E+01	0.10000E+01	0.10000E+01	0.10000E+01	0.10000E+01
0.18344E+00	0.18344E+00	0.18344E+00	0.18344E+00	0.18344E+00	0.18344E+00
0.51383E-01	0.51383E-01	0.51383E-01	0.51383E-01	0.51383E-01	0.51383E-01
0.17708E-01	0.17708E-01	0.17708E-01	0.17708E-01	0.17708E-01	0.17708E-01
0.69483E-02	0.69483E-02	0.69483E-02	0.69483E-02	0.69483E-02	0.69483E-02
0.29867E-02	0.29867E-02	0.29867E-02	0.29867E-02	0.29867E-02	0.29867E-02
0.13751E-02	0.13751E-02	0.13751E-02	0.13751E-02	0.13751E-02	0.13751E-02
0.66830E-03	0.66830E-03	0.66831E-03	0.66831E-03	0.66831E-03	0.66831E-03
0.33945E-03	0.33945E-03	0.33945E-03	0.33945E-03	0.33945E-03	0.33945E-03
0.17888E-03	0.17889E-03	0.17889E-03	0.17889E-03	0.17889E-03	0.17889E-03
0.97275E-04	0.97278E-04	0.97280E-04	0.97281E-04	0.97282E-04	0.97283E-04
0.54353E-04	0.54355E-04	0.54357E-04	0.54358E-04	0.54359E-04	0.54359E-04
0.31100E-04	0.31103E-04	0.31104E-04	0.31106E-04	0.31106E-04	0.31107E-04
0.18174E-04	0.18176E-04	0.18178E-04	0.18179E-04	0.18179E-04	0.18180E-04
0.10821E-04	0.10823E-04	0.10825E-04	0.10826E-04	0.10827E-04	0.10827E-04
0.65517E-05	0.65547E-05	0.65564E-05	0.65575E-05	0.65582E-05	0.65586E-05
0.40267E-05	0.40303E-05	0.40322E-05	0.40334E-05	0.40341E-05	0.40345E-05
0.25074E-05	0.25120E-05	0.25143E-05	0.25156E-05	0.25164E-05	0.25169E-05
0.15782E-05	0.15844E-05	0.15874E-05	0.15890E-05	0.15899E-05	0.15904E-05
0.10002E-05	0.10090E-05	0.10131E-05	0.10151E-05	0.10162E-05	0.10168E-05
0.63299E-06	0.64631E-06	0.65219E-06	0.65497E-06	0.65636E-06	0.65710E-06
0.39050E-06	0.41308E-06	0.42195E-06	0.42591E-06	0.42780E-06	0.42876E-06
	0.25719E-06	0.27217E-06	0.27812E-06	0.28081E-06	0.28211E-06
		0.17092E-06	0.18094E-06	0.18496E-06	0.18680E-06
			0.11455E-06	0.12130E-06	0.12405E-06
				0.77380E-07	0.81966E-07
					0.52664E-07

TABLE II

Relation between the α-parameters of the STO-NG expansions of STO-2s:
(Each column collects the quotient α_i/α_1 in increasing order of the i-index)

22	23	24	25	26	27
0.10000E+01	0.10000E+01	0.10000E+01	0.10000E+01	0.10000E+01	0.10000E+01
0.18344E+00	0.18344E+00	0.18344E+00	0.18344E+00	0.18344E+00	0.18344E+00
0.51382E-01	0.51383E-01	0.51383E-01	0.51383E-01	0.51383E-01	0.51383E-01
0.17708E-01	0.17708E-01	0.17708E-01	0.17708E-01	0.17708E-01	0.17708E-01
0.69483E-02	0.69483E-02	0.69483E-02	0.69483E-02	0.69483E-02	0.69483E-02
0.29867E-02	0.29867E-02	0.29867E-02	0.29867E-02	0.29867E-02	0.29867E-02
0.13750E-02	0.13750E-02	0.13751E-02	0.13751E-02	0.13751E-02	0.13751E-02
0.66826E-03	0.66825E-03	0.66830E-03	0.66830E-03	0.66830E-03	0.66831E-03
0.33940E-03	0.33938E-03	0.33945E-03	0.33945E-03	0.33945E-03	0.33945E-03
0.17883E-03	0.17879E-03	0.17890E-03	0.17889E-03	0.17889E-03	0.17889E-03
0.97212E-04	0.97139E-04	0.97305E-04	0.97288E-04	0.97281E-04	0.97277E-04
0.54279E-04	0.54175E-04	0.54399E-04	0.54372E-04	0.54359E-04	0.54353E-04
0.31021E-04	0.30886E-04	0.31168E-04	0.31127E-04	0.31108E-04	0.31098E-04
0.18097E-04	0.17937E-04	0.18265E-04	0.18211E-04	0.18184E-04	0.18169E-04
0.10760E-04	0.10584E-04	0.10936E-04	0.10870E-04	0.10834E-04	0.10815E-04
-	0.63384E-05	0.66885E-05	0.66125E-05	0.65691E-05	0.65442E-05
0.40182E-05	-	-	0.40979E-05	0.40488E-05	0.40192E-05
0.25233E-05	0.23808E-05	0.26643E-05	-	0.25350E-05	0.25021E-05
0.16117E-05	0.14960E-05	0.17326E-05	0.16615E-05	-	0.15779E-05
0.10447E-05	0.95559E-06	0.11467E-05	0.10853E-05	0.10401E-05	-
0.68424E-06	0.61927E-06	0.77025E-06	0.71986E-06	0.68109E-06	0.65207E-06
0.44881E-06	0.40545E-06	0.52337E-06	0.48375E-06	0.45213E-06	0.42749E-06
0.28786E-06	0.26585E-06	0.35797E-06	0.32845E-06	0.30380E-06	0.28387E-06
	0.17045E-06	0.24432E-06	0.22433E-06	0.20613E-06	0.19071E-06
		0.16265E-06	0.15283E-06	0.14066E-06	0.12935E-06
			0.10154E-06	0.95728E-07	0.88217E-07
				0.63532E-07	0.60008E-07
					0.39805E-07

TABLE III

α- and c-parameters for the STO-NG expansions of the STO-1S with exponent equal to one. (N = 13 to 16).

STO-13G ε[a] = 6.9(-11)

α_i	c_i
0.1315407025E+04	0.1633693621E−01
0.2412963020E+03	0.2583660675E−01
0.6758712719E+02	0.3933224310E−01
0.2329165930E+02	0.5736417056E−01
0.9138581942E+01	0.8038476703E−01
0.3927673620E+01	0.1078177598E+00
0.1807837198E+01	0.1364781739E+00
0.8781872806E+00	0.1582344586E+00
0.4455908687E+00	0.1590215202E+00
0.2342633181E+00	0.1258397926E+00
0.1266267248E+00	0.6653386136E−01
0.6959022430E−01	0.1756699004E−01
0.3779259742E−01	0.1246786212E−02

STO-14G ε[a] = 2.1(-11)

α_i	c_i
0.2145377075E+04	0.1279323688E−01
0.3935460605E+03	0.2023883927E−01
0.1102331133E+03	0.3084198062E−01
0.3798874530E+02	0.4510326502E−01
0.1490547441E+02	0.6360888319E−01
0.6406579555E+01	0.8651685053E−01
0.2949148146E+01	0.1127068119E+00
0.1432914928E+01	0.1382448991E+00
0.7274236354E+00	0.1545029374E+00
0.3829153388E+00	0.1484819790E+00
0.2076926940E+00	0.1112352941E+00
0.1153107605E+00	0.5508142042E−01
0.6485370488E−01	0.1349273683E−01
0.3594217442E−01	0.8819637529E−03

STO-15G ε[a] = 6.6(-12)

α_i	c_i
0.3446098165E+04	0.1009455830E−01
0.6321504192E+03	0.1597262916E−01
0.1770674923E+03	0.2435557149E−01
0.6102187492E+02	0.3567518010E−01
0.2394328741E+02	0.5050531108E−01
0.1029148520E+02	0.6927061680E−01
0.4737775054E+01	0.9180422181E−01
0.2302229857E+01	0.1164650474E+00
0.1169015323E+01	0.1386988872E+00
0.6157054066E+00	0.1496829642E+00
0.3344122161E+00	0.1378369694E+00
0.1863432414E+00	0.9801977489E−01
0.1059100137E+00	0.4562509752E−01
0.6079710651E−01	0.1041658728E−01
0.3431061600E−01	0.6302861489E−03

STO-16G ε[a] = 2.2(-12)

α_i	c_i
0.5459188399E+04	0.8020447259E−02
0.1001431818E+04	0.1269225302E−01
0.2805052207E+03	0.1936074073E−01
0.9666961441E+02	0.2838682758E−01
0.3793085880E+02	0.4028079449E−01
0.1630404012E+02	0.5552867417E−01
0.7505970039E+01	0.7436539192E−01
0.3647617627E+01	0.9629531104E−01
0.1852402951E+01	0.1191965574E+00
0.9758920644E+00	0.1380320581E+00
0.5303572460E+00	0.1440546701E+00
0.2959603789E+00	0.1273348360E+00
0.1688575914E+00	0.8616339385E−01
0.9798149837E−01	0.3782278426E−01
0.5728186185E−01	0.8080736456E−02
0.3285938681E−01	0.4546331359E−03

[a]Squared error in the norm of the expansion.

TABLE III (cont.)

α- and c-parameters for the STO-NG expansions of the STO-1S with exponent equal to one. (N = 17 to 20).

STO-17G $\varepsilon^a = 7.3(-13)$		STO-18G $\varepsilon^a = 2.5(-13)$	
α_i	c_i	α_i	c_i
0.8539172306E+04	0.6413008737E−02	0.1320178595E+05	0.5157720645E−02
0.1566424260E+04	0.1014923909E−01	0.2421734400E+04	0.8162988751E−02
0.4387626762E+03	0.1548518309E−01	0.6783396976E+03	0.1245645368E−01
0.1512098732E+03	0.2271825177E−01	0.2337752896E+03	0.1828176158E−01
0.5933153450E+02	0.3228344506E−01	0.9172880745E+02	0.2600240414E−01
0.2550311352E+02	0.4464388924E−01	0.3942906888E+02	0.3602871860E−01
0.1174123991E+02	0.6017537819E−01	0.1815277124E+02	0.4875963889E−01
0.5706016136E+01	0.7891316760E−01	0.8822100536E+01	0.6445134741E−01
0.2897941908E+01	0.1000392498E+00	0.4480707497E+01	0.8293546701E−01
0.1526915784E+01	0.1210015151E+00	0.2361048474E+01	0.1030850663E+00
0.8300511623E+00	0.1364191426E+00	0.1283684989E+01	0.1219756236E+00
0.4634981946E+00	0.1378531151E+00	0.7170255073E+00	0.1340179783E+00
0.2648565311E+00	0.1171526209E+00	0.4100116368E+00	0.1312735232E+00
0.1543028324E+00	0.7559633545E−01	0.2392633185E+00	0.1074117308E+00
0.9120776095E−01	0.3138607933E−01	0.1420186437E+00	0.6622659323E−01
0.5420474587E−01	0.6297418650E−02	0.8535567641E−01	0.2607438909E−01
0.3155866745E−01	0.3307382803E−03	0.5148728804E−01	0.4928955972E−02
		0.3038499949E−01	0.2425028725E−03

STO-19G $\varepsilon^a = 8.9(-14)$		STO-20G $\varepsilon^a = 3.2(-14)$	
α_i	c_i	α_i	c_i
0.2019129024E+05	0.4170565421E−02	0.3057377073E+05	0.3389255245E−02
0.3703889506E+04	0.6600834265E−02	0.5608452381E+04	0.5364338691E−02
0.1037478315E+04	0.1007357400E−01	0.1570956734E+04	0.8187028460E−02
0.3575452123E+03	0.1478808191E−01	0.5413978511E+03	0.1202047655E−01
0.1402940314E+03	0.2104528803E−01	0.2124346963E+03	0.1711289568E−01
0.6030481075E+02	0.2919651839E−01	0.9131444574E+02	0.2376001022E−01
0.2776399296E+02	0.3961459898E−01	0.4204087246E+02	0.3229121736E−01
0.1349327060E+02	0.5262695440E−01	0.2043200443E+02	0.4303646818E−01
0.6853346968E+01	0.6836432098E−01	0.1037775161E+02	0.5624657578E−01
0.3611439362E+01	0.8645470922E−01	0.5468807545E+01	0.7192311571E−01
0.1963673492E+01	0.1054813612E+00	0.2973735292E+01	0.8949389001E−01
0.1097018982E+01	0.1222097548E+00	0.1661441902E+01	0.1072759924E+00
0.6275075151E+00	0.1309700827E+00	0.9505256082E+00	0.1217896175E+00
0.3664534072E+00	0.1244762813E+00	0.5552868397E+00	0.1274014187E+00
0.2178937418E+00	0.9819060624E−01	0.3304336002E+00	0.1175916816E+00
0.1315256733E+00	0.5795181774E−01	0.1998230323E+00	0.8953504394E−01
0.8025036185E−01	0.2168836357E−01	0.1224684076E+00	0.5066721317E−01
0.4906875960E−01	0.3873738157E−02	0.7575825322E−01	0.1806363869E−01
0.2931965334E−01	0.1791033810E−03	0.4690146243E−01	0.3056325630E−02
		0.2834749861E−01	0.1331751259E−03

[a]Squared error in the norm of the expansion.

TABLE III (cont.)
α- and c-parameters for the STO-NG expansions of the STO-1S with exponent equal to one. (N = 21 to 24).

STO-21G $\varepsilon^a = 1.2(-14)$		STO-22G $\varepsilon^a = 4.5(-15)$	
α_i	c_i	α_i	c_i
0.4586552246E+05	0.2767175967E−02	0.6820913712E+05	0.2269130318E−02
0.8413572280E+04	0.4379796101E−02	0.1251228636E+05	0.3591533825E−02
0.2356686072E+04	0.6684677252E−02	0.3504758174E+04	0.5481725447E−02
0.8121837107E+03	0.9815656419E−02	0.1207843738E+04	0.8049792527E−02
0.3186864862E+03	0.1397732692E−01	0.4739367865E+03	0.1146454685E−01
0.1369867333E+03	0.1941655541E−01	0.2037210100E+03	0.1593133907E−01
0.6306845709E+02	0.2641634136E−01	0.9379301027E+02	0.2168981239E−01
0.3065166014E+02	0.3528028794E−01	0.4558415680E+02	0.2900744278E−01
0.1556863876E+02	0.4629159929E−01	0.2315332565E+02	0.3815925279E−01
0.8204410653E+01	0.5962049161E−01	0.1220154594E+02	0.4937843550E−01
0.4461384929E+01	0.7513747900E−01	0.6635063999E+01	0.6275154581E−01
0.2492727138E+01	0.9207656424E−01	0.3707350911E+01	0.7801783597E−01
0.1426244965E+01	0.1085159614E+00	0.2121323005E+01	0.9422657980E−01
0.8333490490E+00	0.1207956360E+00	0.1239604636E+01	0.1092470497E+00
0.4960874818E+00	0.1234232933E+00	0.7380730562E+00	0.1193027379E+00
0.3002488344E+00	0.1107240618E+00	0.4468871447E+00	0.1191333640E+00
0.1843711884E+00	0.8146607752E−01	0.2746578538E+00	0.1039557962E+00
0.1145778341E+00	0.4427022162E−01	0.1710287576E+00	0.7398664287E−01
0.7177553011E−01	0.1506497438E−01	0.1076471838E+00	0.3866374389E−01
0.4494734279E−01	0.2420353024E−02	0.6822044693E−01	0.1258140016E−01
0.2745613911E−01	0.9964961123E−04	0.4317573097E−01	0.1923495104E−02
		0.2663534456E−01	0.7500422729E−04

STO-23G $\varepsilon^a = 1.7(-15)$		STO-24G $\varepsilon^a = 6.9(-16)$	
α_i	c_i	α_i	c_i
0.1006133757E+06	0.1868329033E−02	0.1472781066E+06	0.1544231705E−02
0.1845652193E+05	0.2957168952E−02	0.2701670309E+05	0.2444200014E−02
0.5169770882E+04	0.4513574089E−02	0.7567524176E+04	0.3730662211E−02
0.1781656978E+04	0.6628371272E−02	0.2607994568E+04	0.5478791159E−02
0.6990913934E+03	0.9441122057E−02	0.1023332282E+04	0.7804251644E−02
0.3005036235E+03	0.1312249449E−01	0.4398784340E+03	0.1084898255E−01
0.1383518590E+03	0.1787393828E−01	0.2025202140E+03	0.1478177138E−01
0.6724028435E+02	0.2392581481E−01	0.9842686389E+02	0.1979862189E−01
0.3415315612E+02	0.3152810329E−01	0.4999380353E+02	0.2611921184E−01
0.1799846251E+02	0.4092481417E−01	0.2634649139E+02	0.3397427960E−01
0.9787477642E+01	0.5229631975E−01	0.1432720668E+02	0.4357461539E−01
0.5468873619E+01	0.6564333648E−01	0.8005604855E+01	0.5504539891E−01
0.3129359396E+01	0.8057526109E−01	0.4581005748E+01	0.6830020661E−01
0.1828761831E+01	0.9596801419E−01	0.2677182449E+01	0.8282148151E−01
0.1088979866E+01	0.1095136691E+00	0.1594291353E+01	0.9732510294E−01
0.6594911115E+00	0.1173803586E+00	0.9656205117E+00	0.1093586932E+00
0.4054988578E+00	0.1146166867E+00	0.5938595532E+00	0.1150924384E+00
0.2527374992E+00	0.9735064211E−01	0.3703067216E+00	0.1099466758E+00
0.1594071849E+00	0.6708647291E−01	0.2337884595E+00	0.9095658360E−01
0.1015150112E+00	0.3375765019E−01	0.1492052517E+00	0.6074584243E−01
0.6502773634E−01	0.1052188931E−01	0.9605340487E−01	0.2946943207E−01
0.4156159945E−01	0.1533788553E−02	0.6214459394E−01	0.8811754859E−02
0.2587657724E−01	0.5676698346E−04	0.4008427519E−01	0.1226965595E−02
		0.2517262997E−01	0.4318765729E−04

[a] Squared error in the norm of the expansion.

TABLE III (cont.)

α- and c-parameters for the STO-NG expansions of the STO-1S with exponent equal to one. (N = 25 to 27).

STO-25G $\varepsilon^a = 2.7(-16)$		STO-26G $\varepsilon^a = 1.1(-16)$		STO-27G $\varepsilon^a = 4.6(-17)$	
α_i	c_i	α_i	c_i	α_i	c_i
0.2140365093E+06	0.1280966755E−02	0.3089405512E+06	0.1066214253E−02	0.4430575248E+06	0.8903320126E−03
0.3926286867E+05	0.2027510660E−02	0.5667207210E+05	0.1687603650E−02	0.8127449816E+05	0.1409218801E−02
0.1099774175E+05	0.3094678410E−02	0.1587415430E+05	0.2575876273E−02	0.2276542763E+05	0.2150970473E−02
0.3790150266E+04	0.4544883914E−02	0.5470708062E+04	0.3783014416E−02	0.7845647220E+04	0.3159012588E−02
0.1487190177E+04	0.6474247653E−02	0.2146612622E+04	0.5389122555E−02	0.3078498564E+04	0.4500291766E−02
0.6392675550E+03	0.9000999534E−02	0.9227200164E+03	0.7492885510E−02	0.1323290798E+04	0.6257371205E−02
0.2943192396E+03	0.1226642665E−01	0.4248211430E+03	0.1021262345E−01	0.6092444822E+03	0.8529463503E−02
0.1430422752E+03	0.1643625010E−01	0.2064677428E+03	0.1368804426E−01	0.2960996655E+03	0.1143424029E−01
0.7265537703E+02	0.2170001644E−01	0.1048711711E+03	0.1808105907E−01	0.1503980495E+03	0.1510927002E−01
0.3828915019E+02	0.2826548180E−01	0.5526688724E+02	0.2357387503E−01	0.7925957106E+02	0.1971201559E−01
0.2082172409E+02	0.3634251431E−01	0.3005435862E+02	0.3036115370E−01	0.4310177902E+02	0.2541650437E−01
0.1163463921E+02	0.4610668689E−01	0.1679368946E+02	0.3863036069E−01	0.2408438087E+02	0.3240317547E−01
0.6657719270E+01	0.5762607061E−01	0.9609981873E+01	0.4852007328E−01	0.1378207306E+02	0.4083566275E−01
0.3890919796E+01	0.7072667457E−01	0.5616369279E+01	0.6003979656E−01	0.8054745015E+01	0.5081400538E−01
0.2317172254E+01	0.8476828636E−01	0.3344814247E+01	0.7292837476E−01	0.4797056469E+01	0.6228815632E−01
0.1403543061E+01	0.9832166336E−01	0.2026080997E+01	0.8642846632E−01	0.2905832400E+01	0.7491100344E−01
0.8632881011E+00	0.1088230565E+00	0.1246284811E+01	0.9898183275E−01	0.1787514132E+01	0.8781470838E−01
0.5384384197E+00	0.1124976381E+00	0.7774164518E+00	0.1079460889E+00	0.1115111393E+01	0.9932906463E−01
0.3400997599E+00	0.1051867284E+00	0.4911709944E+00	0.1096492611E+00	0.7046229506E+00	0.1067649414E+00
0.2172752700E+00	0.8480938539E−01	0.3139473758E+00	0.1003901333E+00	0.4505011410E+00	0.1065956832E+00
0.1401877273E+00	0.5493958216E−01	0.2027772255E+00	0.7893299409E−01	0.2911317884E+00	0.9560218008E−01
0.9116064440E−01	0.2572507876E−01	0.1321658262E+00	0.4963737552E−01	0.1899640621E+00	0.7334335007E−01
0.5952831221E−01	0.7389969470E−02	0.8675337613E−01	0.2245748270E−01	0.1249889240E+00	0.4480750374E−01
0.3872677142E−01	0.9845578224E−03	0.5714315202E−01	0.6206157721E−02	0.8276409041E−01	0.1960743373E−01
0.2451749147E−01	0.3301888779E−04	0.3747455461E−01	0.7923631302E−03	0.5495976162E−01	0.5219158234E−02
		0.2390588682E−01	0.2536148168E−04	0.3631553319E−01	0.6394872001E−03
				0.2333337459E−01	0.1956566625E−04

[a] Squared error in the norm of the expansion.

TABLE IV

α- and c-parameters for the STO-NG expansions of the STO-2S with exponent equal to one. (N = 13 to 16).

STO-13G $\varepsilon^a = 2.3(-11)$		STO-14G $\varepsilon^a = 1.5(-11)$	
α_i	c_i	α_i	c_i
0.1458954840E+04	-0.1550745821E-01	0.1399260935E+04	-0.1583443828E-01
0.2676246961E+03	-0.2448985649E-01	0.2566751010E+03	-0.2500367733E-01
0.7495944224E+02	-0.3711371385E-01	0.7189394191E+02	-0.3787899802E-01
0.2583091497E+02	-0.5347716052E-01	0.2477748639E+02	-0.5452076166E-01
0.1013424026E+02	-0.7276670166E-01	0.9726114746E+01	-0.7395819807E-01
0.4355827977E+01	-0.9117266576E-01	0.4188287307E+01	-0.9192424136E-01
0.2006308261E+01	-0.9841862791E-01	0.1939499385E+01	-0.9745444059E-01
0.9774261007E+00	-0.7488080784E-01	0.9564053226E+00	-0.7178020653E-01
0.2674098619E+00	0.1127032201E+00	0.2760286501E+00	0.1001724733E+00
0.1488262284E+00	0.1827601110E+00	0.1598935537E+00	0.1648608000E+00
0.8556849963E-01	0.1359699658E+00	0.9635304316E-01	0.1393003881E+00
0.5019852073E-01	0.4110053091E-01	0.5978722240E-01	0.6055116363E-01
0.2918689431E-01	0.2894951563E-02	0.3767840549E-01	0.1079181794E-01
		0.2344691416E-01	0.4405566813E-03

STO-15G $\varepsilon^a = 3.2(-12)$		STO-16G $\varepsilon^a = 7.7(-13)$	
α_i	c_i	α_i	c_i
0.2668209957E+04	-0.1146968696E-01	0.4963957387E+04	-0.8410143140E-02
0.4894508695E+03	-0.1813183276E-01	0.9105827194E+03	-0.1330277748E-01
0.1370949725E+03	-0.2756744374E-01	0.2550558165E+03	-0.2026226361E-01
0.4724631958E+02	-0.4006584048E-01	0.8789820469E+02	-0.2959271999E-01
0.1854018545E+02	-0.5566164455E-01	0.3448960903E+02	-0.4160063418E-01
0.7973683255E+01	-0.7314655515E-01	0.1482686586E+02	-0.5616071625E-01
0.3678341011E+01	-0.8826062952E-01	0.6829816779E+01	-0.7191809466E-01
0.1797917231E+01	-0.9110444891E-01	0.3325072344E+01	-0.8476858468E-01
0.9253704044E+00	-0.6579321921E-01	0.1696621912E+01	-0.8583742287E-01
0.2827056606E+00	0.9248096322E-01	0.9030554321E+00	-0.6132388931E-01
0.1663643802E+00	0.1582065207E+00	0.2871382315E+00	0.8784817452E-01
0.1011367211E+00	0.1430372115E+00	0.1703207165E+00	0.1548228482E+00
0.6294077200E-01	0.6856781070E-01	0.1037800816E+00	0.1455253122E+00
0.3959583435E-01	0.1386893312E-01	0.6450118171E-01	0.7289389238E-01
0.2450262902E-01	0.6610815897E-03	0.4044410509E-01	0.1543713263E-01
		0.2492063724E-01	0.7711338058E-03

[a] Squared error in the norm of the expansion.

TABLE IV (cont.)

α- and c-parameters for the STO-NG expansions of the STO-2S with exponent equal to one. (N = 17 to 20).

STO-17G $\varepsilon^a = 2.5(-13)$		STO-18G $\varepsilon^a = 1.3(-13)$	
α_i	c_i	α_i	c_i
0.9100231387E+04	-0.6211846090E-02	0.1657919196E+05	-0.4602366399E-02
0.1669340908E+04	-0.9828582989E-02	0.3041281668E+04	-0.7283203580E-02
0.4675876893E+03	-0.1498486919E-01	0.8518751782E+03	-0.1110988562E-01
0.1611421815E+03	-0.2194121599E-01	0.2935779466E+03	-0.1628982553E-01
0.6322769953E+02	-0.3103443054E-01	0.1151909831E+03	-0.2311703458E-01
0.2717722791E+02	-0.4247819253E-01	0.4950974208E+02	-0.3187457577E-01
0.1251182289E+02	-0.5603619486E-01	0.2278764707E+02	-0.4270895940E-01
0.6080912564E+01	-0.7033024244E-01	0.1106632213E+02	-0.5535430823E-01
0.3089471258E+01	-0.8156161356E-01	0.5610330874E+01	-0.6854747642E-01
0.1629844563E+01	-0.8176927702E-01	0.2945222473E+01	-0.7888127977E-01
0.8889366427E+00	-0.5835229397E-01	0.1591177552E+01	-0.7900904881E-01
0.2895586862E+00	0.8552057532E-01	0.8813700673E+00	-0.5667177233E-01
0.1723074639E+00	0.1534008923E+00	0.2906592712E+00	0.8452419037E-01
0.1050104459E+00	0.1468348874E+00	0.1731547729E+00	0.1528724649E+00
0.6518333710E-01	0.7486814604E-01	0.1055110399E+00	0.1474065282E+00
0.4079720475E-01	0.1612879364E-01	0.6545199004E-01	0.7566185548E-01
0.2508814423E-01	0.8192752999E-03	0.4093323891E-01	0.1640160609E-01
		0.2515170344E-01	0.8381759095E-03

STO-19G $\varepsilon^a = 4.5(-14)$		STO-20G $\varepsilon^a = 1.2(-14)$	
α_i	c_i	α_i	c_i
0.1541972558E+05	-0.4772248864E-02	0.2657973404E+05	-0.3634920018E-02
0.2828589380E+04	-0.7551926479E-02	0.4875781996E+04	-0.5752657548E-02
0.7922996438E+03	-0.1151923151E-01	0.1365729337E+04	-0.8777233728E-02
0.2730479755E+03	-0.1688770930E-01	0.4706688272E+03	-0.1287752504E-01
0.1071382784E+03	-0.2395701308E-01	0.1846809908E+03	-0.1830094211E-01
0.4605330333E+02	-0.3300383374E-01	0.7938436608E+02	-0.2531192708E-01
0.2120425083E+02	-0.4412923411E-01	0.3654888101E+02	-0.3412641398E-01
0.1030836509E+02	-0.5692007677E-01	0.1776447645E+02	-0.4476266061E-01
0.5240720981E+01	-0.6976617596E-01	0.9025753924E+01	-0.5671998830E-01
0.2768741245E+01	-0.7872832352E-01	0.4760750694E+01	-0.6836367592E-01
0.1514444429E+01	-0.7637363878E-01	0.2594749692E+01	-0.7596024286E-01
0.8562083030E+00	-0.5247236574E-01	0.1457134036E+01	-0.7275139533E-01
0.3012676665E+00	0.7269482807E-01	0.8418759738E+00	-0.4960311183E-01
0.1868346162E+00	0.1333206894E+00	0.3048852805E+00	0.6942847954E-01
0.1187939635E+00	0.1415043291E+00	0.1904575230E+00	0.1298818803E+00
0.7705045957E-01	0.9241690309E-01	0.1215008409E+00	0.1418125027E+00
0.5064910346E-01	0.3320997063E-01	0.7883442862E-01	0.9587261667E-01
0.3339778144E-01	0.5089861175E-02	0.5173782054E-01	0.3580034614E-01
0.2155235949E-01	0.1835280626E-03	0.3402046743E-01	0.5713055894E-02
		0.2187792900E-01	0.2148358286E-03

[a] Squared error in the norm of the expansion.

TABLE IV (cont.)

α- and c-parameters for the STO-NG expansions of the STO-2S with exponent equal to one. (N = 21 to 24).

STO-21G $\varepsilon^a = 4.1(-15)$		STO-22G $\varepsilon^a = 1.9(-15)$	
α_i	c_i	α_i	c_i
0.4530072752E+05	-0.2784342094E-02	0.7673959300E+05	-0.2139283532E-02
0.8309962189E+04	-0.4406751036E-02	0.1407710962E+05	-0.3385924081E-02
0.2327661810E+04	-0.6724779756E-02	0.3943071084E+04	-0.5167466923E-02
0.8021794061E+03	-0.9870508007E-02	0.1358897638E+04	-0.7586608010E-02
0.3147598267E+03	-0.1404183444E-01	0.5332062888E+03	-0.1079914394E-01
0.1352981503E+03	-0.1946483775E-01	0.2291966293E+03	-0.1498929518E-01
0.6229074524E+02	-0.2636614455E-01	0.1055206421E+03	-0.2035865178E-01
0.3027388201E+02	-0.3490886706E-01	0.5128236820E+02	-0.2710000524E-01
0.1537754538E+02	-0.4504824154E-01	0.2604575491E+02	-0.3533539949E-01
0.8105223782E+01	-0.5623477746E-01	0.1372356905E+02	-0.4498283951E-01
0.4409817231E+01	-0.6686873938E-01	0.7460036820E+01	-0.5549147701E-01
0.2467189808E+01	-0.7346621210E-01	0.4165340589E+01	-0.6535872469E-01
0.1415731678E+01	-0.6984025114E-01	0.2380503968E+01	-0.7136445034E-01
0.8318597651E+00	-0.4753032399E-01	0.1388791323E+01	-0.6771722390E-01
0.3071417331E+00	0.6752651092E-01	0.8257136399E+00	-0.4620742028E-01
0.1925665380E+00	0.1281190938E+00	0.3083529534E+00	0.6655959731E-01
0.1229739754E+00	0.1421574469E+00	0.1936334225E+00	0.1273146780E+00
0.7974862391E-01	0.9773989679E-01	0.1236842188E+00	0.1423828350E+00
0.5226832576E-01	0.3712275303E-01	0.8017362133E-01	0.9863494141E-01
0.3431180630E-01	0.6024724761E-02	0.5250850441E-01	0.3773508684E-01
0.2202532892E-01	0.2304291059E-03	0.3444122419E-01	0.6167401012E-02
		0.2208989827E-01	0.2375531112E-03

STO-23G $\varepsilon^a = 1.3(-15)$		STO-24G $\varepsilon^a = 3.1(-16)$	
α_i	c_i	α_i	c_i
0.1297556734E+06	-0.1645192157E-02	0.1196765641E+06	-0.1713069737E-02
0.2380238268E+05	-0.2603952874E-02	0.2195347033E+05	-0.2711381325E-02
0.6667172826E+04	-0.3974273114E-02	0.6149282624E+04	-0.4138207112E-02
0.2297704393E+04	-0.5835680488E-02	0.2119224360E+04	-0.6076283869E-02
0.9015776188E+03	-0.8309685381E-02	0.8315459436E+03	-0.8651905578E-02
0.3875398766E+03	-0.1154272946E-01	0.3574383806E+03	-0.1201687148E-01
0.1784203575E+03	-0.1570232573E-01	0.1645643132E+03	-0.1634364950E-01
0.8670969676E+02	-0.2096756304E-01	0.7997990517E+02	-0.2181328102E-01
0.4403615311E+02	-0.2750460932E-01	0.4062462817E+02	-0.2858414934E-01
0.2319839528E+02	-0.3541162156E-01	0.2141027331E+02	-0.3672102611E-01
0.1260427560E+02	-0.4460371126E-01	0.1164512120E+02	-0.4604818608E-01
0.7029532662E+01	-0.5458107796E-01	0.6510310689E+01	-0.5587167245E-01
0.4007682001E+01	-0.6397829919E-01	0.3730039921E+01	-0.6451638599E-01
0.2327491928E+01	-0.6978139498E-01	0.2185872901E+01	-0.6871680081E-01
0.1373387123E+01	-0.6636234367E-01	0.1308822983E+01	-0.6322915360E-01
0.8224460641E+00	-0.4547610576E-01	0.8004589519E+00	-0.4166615919E-01
0.3089203227E+00	0.6612389856E-01	0.3188566460E+00	0.5699015800E-01
0.1941116065E+00	0.1269802049E+00	0.2073513908E+00	0.1102818986E+00
0.1239927148E+00	0.1424975425E+00	0.1372278215E+00	0.1318102053E+00
0.8035432034E-01	0.9902242192E-01	0.9218070796E-01	0.1068593006E+00
0.5260918111E-01	0.3799460403E-01	0.6263455177E-01	0.5556346669E-01
0.3449495996E-01	0.6227436032E-02	0.4284009934E-01	0.1609938922E-01
0.2211653189E-01	0.2405452167E-03	0.2923889886E-01	0.1995239176E-02
		0.1946489210E-01	0.5787073350E-04

[a]Squared error in the norm of the expansion.

TABLE IV (cont.)

α- and c-parameters for the STO-NG expansions of the STO-2S with exponent equal to one. (N = 25 to 27).

STO-25G $\varepsilon^a = 1.0(-16)$		STO-26G $\varepsilon^a = 4.0(-17)$		STO-27G $\varepsilon^a = 2.1(-17)$	
α_i	c_i	α_i	c_i	α_i	c_i
0.1933277897E+06	-0.1347824918E-02	0.3102466583E+06	-0.1063965867E-02	0.4961466479E+06	-0.8413498275E-03
0.3546405578E+05	-0.2133308162E-02	0.5691166037E+05	-0.1684033006E-02	0.9101316615E+05	-0.1331684185E-02
0.9933671065E+04	-0.3256039162E-02	0.1594126173E+05	-0.2570368810E-02	0.2549327893E+05	-0.2032598257E-02
0.3423437914E+04	-0.4781383645E-02	0.5493833534E+04	-0.3774702811E-02	0.8785744675E+04	-0.2985061859E-02
0.1343297213E+04	-0.6809537624E-02	0.2155685367E+04	-0.5376530001E-02	0.3447375532E+04	-0.4252133404E-02
0.5774143337E+03	-0.9462261596E-02	0.9266189344E+03	-0.7473091865E-02	0.1481851281E+04	-0.5911259161E-02
0.2658413439E+03	-0.1288132501E-01	0.4266154349E+03	-0.1017923646E-01	0.6822449416E+03	-0.8054695890E-02
0.1292014073E+03	-0.1722412208E-01	0.2073392008E+03	-0.1362644458E-01	0.3315777736E+03	-0.1078996138E-01
0.6562525784E+02	-0.2265026546E-01	0.1053134004E+03	-0.1795768870E-01	0.1684174576E+03	-0.1423844893E-01
0.3458483022E+02	-0.2928884959E-01	0.5549972041E+02	-0.2331299996E-01	0.8875460574E+02	-0.1852967711E-01
0.1880843067E+02	-0.3716752834E-01	0.3018097459E+02	-0.2979626357E-01	0.4826379334E+02	-0.2378653957E-01
0.1051153157E+02	-0.4607135015E-01	0.1686470995E+02	-0.3740629951E-01	0.2696700029E+02	-0.3009311366E-01
0.6017801329E+01	-0.5528520546E-01	0.9651226764E+01	-0.4590433274E-01	0.1542936295E+02	-0.3743027898E-01
0.3520689450E+01	-0.6317877640E-01	0.5641484726E+01	-0.5457868512E-01	0.9014729596E+01	-0.4555483523E-01
0.2101416812E+01	-0.6667655408E-01	0.3361256777E+01	-0.6187138240E-01	0.5365612923E+01	-0.5378600795E-01
0.1278375499E+01	-0.6092836340E-01	0.2038041557E+01	-0.6489670144E-01	0.3246871489E+01	-0.6065916202E-01
0.7922362708E+00	-0.4001869787E-01	0.1256142071E+01	-0.5910543494E-01	0.1994113777E+01	-0.6345160186E-01
0.3212047200E+00	0.5520784676E-01	0.7864642029E+00	-0.3883028193E-01	0.1241427124E+01	-0.5779023981E-01
0.2098264657E+00	0.1081156469E+00	0.3226896308E+00	0.5413759633E-01	0.7828462311E+00	-0.3806202129E-01
0.1391681911E+00	0.1312873919E+00	0.2113074052E+00	0.1069330658E+00	0.3235223600E+00	0.5356150659E-01
0.9352308433E-01	0.1084317454E+00	0.1402714294E+00	0.1310916935E+00	0.2120998524E+00	0.1063447974E+00
0.6349872414E-01	0.5753360109E-01	0.9425363157E-01	0.1093448758E+00	0.1408399187E+00	0.1310277864E+00
0.4336833216E-01	0.1702568580E-01	0.6395260272E-01	0.5860014783E-01	0.9461943839E-01	0.1098211524E+00
0.2954587493E-01	0.2155926629E-02	0.4363815462E-01	0.1751516265E-01	0.6417515476E-01	0.5913208303E-01
0.1962960068E-01	0.6393471590E-04	0.2969934639E-01	0.2240096835E-02	0.4376847937E-01	0.1775567508E-01
		0.1971056234E-01	0.6710975512E-04	0.2977267447E-01	0.2281239006E-02
				0.1974893434E-01	0.6866102788E-04

[a] Squared error in the norm of the expansion.

TABLE V
Three-center nuclear attraction integrals.

N	Integral I	Integral II	Integral III
13	0.0075741015	0.04116619724	0.07173271572
14	0.0075742296	0.04116638702	0.07173283686
15	0.0075742268	0.04116645735	0.07173288410
16	0.0075742644	0.04116649508	0.07173292406
17	0.0075742647	0.04116651127	0.07173294232
18	0.0075742761	0.04116651828	0.07173294893
19	0.0075742768	0.04116652325	0.07173295327
20	0.0075742802	0.04116652611	0.07173295525
21	0.0075742809	0.04116652750	0.07173295599
22	0.0075742818	0.04116652837	0.07173295669
23	0.0075742822	0.04116652886	0.07173295715
24	0.0075742824	0.04116652905	0.07173295732
25	0.0075742827	0.04116652914	0.07173295739
26	0.0075742827	0.04116652920	0.07173295745
27	0.0075742828	0.04116652923	0.07173295748
Other authors'[15]	0.0075742801	0.041166529	0.071732965

All integrals are of the form $< 1s^A \mid r_C^{-1} \mid 1s^B >$

Integral I
A: (0, 0, 0)
B: (2, 0, 0)
C: (1, 1.73205, 0)
$\zeta^A = 0.2$
$\zeta^B = 10.0$

Integral II
A: (0, 0, 0)
B: (2, 0, 0)
C: (-0.5, 0, 0)
$\zeta^A = 1.0$
$\zeta^B = 5.0$

Integral III
A: (0, 0, 0)
B: (2, 0, 0)
C: (0.5, 0, 0)
$\zeta^A = 1.0$
$\zeta^B = 5.0$

TABLE VI
Many-center electron repulsion integrals.

N	Integral I	Integral II	Integral III	Integral IV
13	0.1944688677192	0.000128167676	0.3455378141237	0.0021169819938
14	0.1944688666269	0.000128156646	0.3455378154938	0.0021169834517
15	0.1944688680287	0.000128156025	0.3455378149214	0.0021169831262
16	0.1944688676775	0.000128159857	0.3455378150222	0.0021169827234
17	0.1944688674944	0.000128162562	0.3455378150930	0.0021169826839
18	0.1944688676478	0.000128163168	0.3455378150180	0.0021169827699
19	0.1944688676386	0.000128162871	0.3455378150506	0.0021169828080
20	0.1944688676033	0.000128162650	0.3455378150489	0.0021169827983
21	0.1944688676161	0.000128162703	0.3455378150411	0.0021169827843
22	0.1944688676217	0.000128162857	0.3455378150461	0.0021169827818
23	0.1944688676170	0.000128162959	0.3455378150452	0.0021169827849
24	0.1944688676164	0.000128162984	0.3455378150440	0.0021169827870
25	0.1944688676178	0.000128162976	0.3455378150446	0.0021169827869
26	0.1944688676177	0.000128162968	0.3455378150444	0.0021169827862
27	0.1944688676172	0.000128162972	0.3455378150441	0.0021169827859
Other authors'[16]	0.0194469	0.0001281719	0.3455	0.0021

Integral I	A: (0, 0, 0)	$1s^A$ (1.2)
	B: (2, 0, 0)	$1s^B$ (1.2)
	C: (0, 0, 0)	$1s^C$ (1.2)
	D: (1, 1, 0)	$1s^D$ (1.2)
Integral II	A: (0, 0, 0)	$1s^A$ (5.7)
	B: (0, 7.5, 0)	$1s^B$ (1.0)
	C: (0, 2.5, 0)	$2s^C$ (2.6)
	D: (0, 2.5, 0)	$1s^D$ (1.0)
Integral III	A: (0, 0, 0)	$1s^A$ (1.0)
	B: (1, 0, 0)	$1s^B$ (1.0)
	C: (0, 1, 0)	$1s^C$ (1.0)
	D: (0, 0, 1)	$1s^D$ (1.0)
Integral IV	A: (0, 0, 0)	$1s^A$ (6.0)
	B: (1, 0, 0)	$1s^B$ (6.0)
	C: (0, 1, 0)	$1s^C$ (6.0)
	D: (1, 1, 0)	$1s^D$ (6.0)

TABLE VII
Many-center electron repulsion integrals with high quantum numbers.

N	Integral I	Integral II	Integral III	Integral IV
13	-0.0141752422071	0.0152948544673	0.0245956549957	-0.0070857513990
14	-0.0141752422033	0.0152948553564	0.0245956564199	-0.0070857443050
15	-0.0141752424622	0.0152948556922	0.0245956570091	-0.0070857411709
16	-0.0141752425362	0.0152948555417	0.0245956567835	-0.0070857396973
17	-0.0141752424959	0.0152948554718	0.0245956566653	-0.0070857393590
18	-0.0141752424810	0.0152948555080	0.0245956567262	-0.0070857393254
19	-0.0141752425014	0.0152948555307	0.0245956567688	-0.0070857392704
20	-0.0141752425074	0.0152948555229	0.0245956567579	-0.0070857392250
21	-0.0141752425052	0.0152948555162	0.0245956567459	-0.0070857392156
22	-0.0141752425034	0.0152948555170	0.0245956567463	-0.0070857392192
23	-0.0141752425038	0.0152948555187	0.0245956567492	-0.0070857392196
24	-0.0141752425049	0.0152948555189	0.0245956567498	-0.0070857392176
25	-0.0141752425049	0.0152948555183	0.0245956567489	-0.0070857392167
26	-0.0141752425046	0.0152948555182	0.0245956567487	-0.0070857392169
27	-0.0141752425046	0.0152948555183	0.0245956567488	-0.0070857392171

Integral I $[\,2s^A\, 2s^B \mid 2p_x^C\, 2s^D\,]$

Integral II $[\,2s^A\, 2s^B \mid 2p_x^C\, 2p_x^D\,]$

Integral III $[\,2s^A\, 2s^B \mid 2p_x^C\, 3d_{xy}^D\,]$

Integral IV $[\,2s^A\, 2s^B \mid 2d_{xy}^C\, 3d_{xy}^D\,]$

For all the integrals:

A: (2.64, 0, 0)
B: (1.32, 2.286, 0)
C: (-1.32, 2.286, 0)
D: (-2.64, 0, 0)

All the exponents equal to 1.56788.

many-center integrals as those reported in the previous work[1]. As no other results of higher accuracy were available in the literature, the accuracy was estimated by testing the convergence of the integral values as the expansions were extended. The results obtained in the selected three-center nuclear attraction integrals are presented in Table V.

An interesting feature of these results (confirmed by other calculations that we have carried out with this aim) is that the absolute error remains almost constant for a given expansion, independently of the exponents of the STO's and distances between the centers. For instance, in case of the STO-27G expansion, this error is about 10^{-10}.

In Tables VI and VII the corresponding results for some three- and four-center electron repulsion integrals are collected. For a given expansion, the accuracy achieved in these integrals is higher than that obtained in the three-center nuclear attraction integrals. An absolute error of about 10^{-12} is attained with the STO-27G expansion, while the STO-12G yields, for the same case, only four correct figures and an absolute error of about 10^{-8}.*

As it was previously suggested, the fact that better results are obtained for electron repulsion integrals than for three-center nuclear attraction integrals may be explained by the different nature of the two types of integrals: the former depend on the potential throughout the whole space, whereas the latter depend on point values of the potential.

The above results clearly show that the STO-27G expansion provides a means accurate enough for testing other algorithms and procedures designed for the calculation of many-center molecular integrals with Slater basis functions.

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* It should be noticed that there is a misprint in some of our previously reported results (Table VI of ref.[1]) where the integral values are incorrectly multiplied by a factor of 10.