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SHORT COMMENT

Erratum and answer to the comment by Harris on: Numerical treatment of two-center overlap integrals (J Mol Mod, 12,213–220, 2006)

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Abstract In the present contribution, we present two numerical tables for overlap integrals over Slater type functions and over B functions using the method present in the paper (J Mol Model, 12:213–220, 2006) where there were typos in the data that led Harris to conclude that our method is flawed and not useful for serious work. The typos are corrected and the numerical tables are listed as well as values from the literature and values obtained using ACJU code in order to perform comparisons with regards to accuracy.

Keywords Convergence accelerator · Exponential type functions · Nonlin-ear transformations · Numerical integration · Two-center molecular integrals

First, we would like to thank Harris for his comment [1] on our paper [2], where he pointed out discrepancies in some numerical results that we presented for the overlap integrals over Slater type functions (STFs). These discrepancies, which are due to typos in the data, might led to the conclusion that the method presented in the paper is flawed. In lines 15–17 of Table 3 in [2], the values of ζ_2 should be 2.5, 1.5, 6, and 1.5 and the values of R should be 10, 30, 10, and 10 respectively. In his comment, Harris performed the calculations corresponding to these entries (lines 15–17) and changed the values of ζ_1 to the respective values 10, 30, 10, 10. We would like to notice that the values of ζ_1 in Table 3 in the paper [2] are correct.

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We corrected the typos and we performed the same calculations and the values are listed in Table 1 (corresponds to Table 3 in [2]) to show that our method is highly efficient for the treatment of overlap integrals over B functions. We performed the same calculations using the ACJU code developed by Homeier et al. [3] for the overlap integrals over B functions, to which we added a subroutine expressing overlap over STFs as linear combinations of overlap integrals over B functions. The same calculations were presented in: first set from Table 1 in [4], second set from Table 1 in [5], third set from Table 2 in [6] and the last set from Table 1 in [7]. We listed these values in order to perform comparisons with our numerical results. Note that we listed our values with 15 digits, to avoid misinterpretations of the round of errors.

From the first set in Table 1, one can notice that our values are in a complete agreement (13 to 14 similar 1 digits) with those obtained using ACJU code and the values obtained by Talman, with the exception of the line 8, where our value .107 437 341 689 547(−1) agrees to 10 digits with Talman's value and only to 7 digits with ACJU's value. From the second set, one can notice that our values are in complete agreement with those obtained using ACJU and those obtained by Guseinov et al., with the exception of the third and fourth lines of the second set, where our values are in complete agreement with the value obtained by Guseinov et al. and shares 10 (third entry) and 12 (fourth entry) similar digits with ACJU's values. From the third set, we notice an exception occurring in the last entry, where our value and ACJU's value have only 3 similar digits, but our value agrees to 11 digits with the value obtained by Guseinov et al. In the last set, we have an exception occurring in the line 7, where our value agrees with the value obtained by Guseinov et al. to 12 digits, but only to 4 digits with ACJU's value. In the last two entries of the

Table 1 Evaluation of two-center overlap integrals over STFs given by Eq. 15

n_1	l_1	m_1	ζ_1	n_2	l_2	m_2	ζ_2	R	Values $\overline{D}$	Values$^{\mathrm{ACJU}}$	Values [4–7]
5	4	0	1.0	5	4	0	1.0	1.	.768 617 015 567 111(0)	.768 617 015 567 176(0)	.768 617 015 6(0)
5	4	4	1.0	5	4	4	1.0	1.	.955 778 746 293 132(0)	.955 778 746 293 192(0)	.955 778 746 3(0)
5	4	0	5.0	5	4	0	1.0	1.	.900 262 309 241 791(−2)	.900 262 309 241 891(−2)	.900 262 309 2(−2)
5	4	4	5.0	5	4	4	1.0	1.	.318 003 745 748 137(−1)	.318 003 745 748 142(−1)	.318 003 745 7(−1)
5	4	0	5.0	5	4	0	5.0	1.	−.138 257 011 551 862(0)	−.138 257 011 551 886(0)	−.138 257 011 6(0)
5	4	4	5.0	5	4	4	5.0	1.	.356 825 986 845 748(0)	.356 825 986 845 726(0)	.356 825 986 8(0)
8	0	0	1.0	8	0	0	1.0	1.	.989 015 721 319 447(0)	.989 015 721 332 468(0)	.989 015 721 3(0)
8	0	0	5.0	8	0	0	1.0	1.	.107 437 341 689 547(−1)	.107 437 034 156 233(−1)	.107 437 341 7(−1)
8	0	0	5.0	8	0	0	5.0	1.	.785 230 850 010 521(0)	.785 230 850 009 304(0)	.785 230 850 0(0)
4	3	0	1.9	6	5	0	0.1	100.	−.534 413 558 059 944(−5)	−.534 413 558 059 944(−5)	−.534 413 558 059 942(−5)
6	3	2	1.4	8	5	2	0.6	40.	−.321 391 598 543 043(−4)	−.321 391 598 542 944(−4)	−.321 391 598 542 938(−4)
12	7	3	1.3	12	7	3	0.7	15.	.229 354 178 100 624(−1)	.229 354 177 505 829(−1)	.229 354 178 100 625(−1)
17	8	4	1.8	14	6	4	0.2	30.	.913 905 848 808 478(−6)	.913 905 775 241 321(−6)	.913 905 848 808 666(−6)
10	7	1	2.5	8	1	1	2.5	10.	.152 138 456 890 817(−1)	.152 138 456 890 819(−1)	.152 138 456 890 819(−1)
18	12	6	1.5	18	12	6	1.5	30.	.948 615 868 693 123(−2)	.948 615 858 501 109(−2)	.948 615 878 639 653(−2)
21	10	5	6.0	9	6	5	6.0	10.	−.293 153 644 937 242(−7)	−.293 153 644 747 095(−7)	−.293 153 644 789 973(−7)
30	10	8	1.5	14	8	8	1.5	10.	.122 376 276 853 106(0)	.122 875 676 594 157(0)	.122 376 276 855 421(0)
3	2	1	8.0	3	2	1	2.0	5.	−.442 287 766 988 262(−3)	−.442 287 766 988 261(−3)	−.442 287 766 988 261(−3)
9	5	3	6.0	8	4	3	4.0	9.	−.546 510 242 850 746(−7)	−.546 510 243 022 673(−7)	−.546 510 243 022 855(−7)
10	7	1	14.4	8	2	1	9.6	5.	−.184 189 014 015 193(−9)	−.184 189 026 173 202(−9)	−.184 189 026 173 207(−9)
10	9	9	4.8	10	9	9	1.2	5.	.623 122 318 191 125(−3)	.623 122 318 196 602(−3)	.623 122 318 196 866(−3)
17	8	4	11.0	8	7	4	9.0	5.	−.100 640 064 142 575(−5)	−.100 640 064 117 530(−5)	−.100 623 367 113 747(−5)
21	10	6	9.0	9	8	6	9.0	5.	.538 980 685 338 283(−4)	.538 980 685 685 899(−4)	.538 980 685 350 612(−4)
30	10	8	7.0	14	10	8	7.0	5.	.135 074 709 591 440(−1)	.135 554 467 261 784(−1)	.135 074 709 592 800(−1)
40	4	3	4.8	12	4	3	1.2	5.	.948 359 636 822 715(−1)		.948 379 265 599 810(−1)
43	10	6	7.2	18	8	6	16.8	5.	−.115 825 616 305 187(−3)		−.115 907 687 123 104(−3)

$\theta = \phi = 0^o$

Table 2 Evaluation of two-center overlap integrals given by Eq. (13)

n_1	l_1	m_1	n_2	l_2	m_2	ζ_2	Values $\overline{D}$	Values $W-\overline{D}$	Values [8] and [9]
1	0	0	1	0	0	2.2	.241222730889281(−2)	.241222730889278(−2)	.241222730889277(−2)
1	0	0	1	0	0	5.5	.155947042412085(−3)	.155947042412480(−3)	.155947042412479(−3)
1	0	0	1	0	0	9.9	.260333516751945(−4)	.260333516751267(−4)	.260333516751266(−4)
3	1	1	1	1	0	2.2	.113546037053703(−3)	.113546037053703(−3)	.113546037053703(−3)
3	1	1	1	1	0	5.5	.656024309177995(−5)	.656024309177992(−5)	.656024309177991(−5)
1	1	0	3	1	1	2.2	.191855872151891(−3)	.191855872151892(−3)	.191855872151891(−3)
1	1	0	3	1	1	5.5	.229394207154353(−4)	.229394207154353(−4)	.229394207154352(−4)
5	0	0	5	0	0	2.2	.883967476162948(−3)	.883967476162948(−3)	.883967476162948(−3)
5	0	0	5	0	0	5.5	.839121794539345(−4)	.839121794539339(−4)	.839121794539339(−4)
5	5	5	1	0	0	2.0	−.508703856032153(−7)	−.508703856032153(−7)	−.508703856100857(−7)
4	4	4	3	3	3	2.0	−.156368843560451(−5)	−.156368843560451(−5)	−.156368843564954(−5)
3	3	3	4	4	4	2.0	.167067525481025(−5)	.167067525481025(−5)	.167067525482610(−5)
1	0	0	5	5	5	2.0	.131799234942743(−6)	.131799234942743(−6)	.131799234952278(−6)

ζ_1=1.5 and $\overrightarrow{R} = (2.0, 45.0^o, 0.0^o)$

Values $\overline{D}$ were obtained using the nonlinear $\overline{D}$ transformation. Values $W-\overline{D}$ were obtained using the W algorithm [10] and $\overline{D}$ transformation. These values are in complete accordance with those listed in Table 3 in Ref. [8] and in Table 3 in Ref. [9].

fourth set corresponding to considerably large values of quantum numbers, our values agrees with the values obtained by Guseinov et al. only to 4 and 6 digits respectively. For the last line of this set, we obtained −.115 825 534 109 604(−3), which agrees to 9 digits with the value given by Harris in his comment (−.115 825 653(−3)).

For the entry on line 22, we obtained −.100 640 064 117 699(−5), which is in complete agreement with the value obtained by Harris (−.100 640 064(−5) as given in his comment [1]).

We also performed the same calculations presented in Table 1 in [2] and we listed the values obtained by Weniger et al. [8] (first set) and by Grotendorst et al. [9] (second set). We also perform the calculations using the recursive algorithm W [10] for the computation of the approximations $\overline{D}_n^{(2)}$ in order to show that the method can also be computed recursively for a better control of the degree of accuracy. From Table 2 (corresponds to Table 1 in [2]), one can easily notice that our results are in complete agreement with those listed in [8, 9] (15 similar digits at the worst case scenario).

As can be seen from the numerical tables, our method is highly accurate for overlap integrals. It is able to reproduce values from the literature even for considerably large values of the quantum numbers and our values are in agreement with those obtained using the ACJU code.

We do agree with Harris that there exist methods for overlap integrals over Slater type functions (STFs), which are more efficient than expressing STFs in terms of B functions. Overlap integrals over STFs can be obtained using direct space methods [11–13]. In our paper [2], we added Table 3 with values for the overlap integrals over STFs because it was requested by the referee as well as calculations with large values of quantum numbers. In our approach, we do not use STFs except when we need to compare our numerical results with existing values from the literature, where most of them are obtained using STFs.

In the calculations presented in Table 1, the finite integrals occurring in Eq. (41) (as listed in [2]) were evaluated using Gauss-Legendre of order 48. In the calculations presented in Table 2, the finite integrals occurring in Eq. (41) (as listed in [2]) were evaluated using Gauss-Legendre of order 24. The finite integrals involved in the infinite series in Eq. (17) (as listed in [2]), were evaluated using Gauss-Legendre of order 96. In all tables, the numbers in parentheses represent powers of 10.

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