# Comment on "Analytic value of the atomic three-electron correlation integral with Slater wave functions"

James S. Sims
*National Institute of Standards and Technology, Gaithersburg, Maryland 20899-8911, USA*

Stanley A. Hagstrom
*Department of Chemistry, Indiana University, Bloomington, Indiana 47405, USA*

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Reference is made to the paper by Remiddi [Phys. Rev. A **44**, 5492 (1991)]. In this Comment we point out two misprints in the paper. We provide further verification of the corrections with a short table comparing 30 significant digit results using Remiddi's formula (with our corrections) and the output of our recently developed triangle integral package.

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Reference is made to the paper by Remiddi [1], where misprints occur in two important equations.

In Eq. (33) of Ref. [1], the sum of the ln[···]ln[···] type terms should be

$$\ln\left[\frac{w_1+w_2}{w_3}\right]\ln\left[\frac{w_1+w_2+w_3}{w_1+w_2}\right]+\ln\left[\frac{w_1+w_3}{w_2}\right]\ln\left[\frac{w_1+w_2+w_3}{w_1+w_3}\right]+\ln\left[\frac{w_2+w_3}{w_1}\right]\ln\left[\frac{w_1+w_2+w_3}{w_2+w_3}\right], \tag{1}$$

while in Eq. (42) of Ref. [1], line 8 should be $(w_1-w_2+w_3)$ instead of $(w_1-w_2+w_3)^2$. With these two changes, both equations are now invariant under interchange of the nonlinear parameters $w_1$ and $w_3$, as is required by the symmetry of the electron interaction operator.

Harris [2] has shown that the formulas of Remiddi are equivalent to the older, more general formulas of Fromm and Hill [3] in their common region of applicability [Remiddi's Eq. (33) only]. However, he failed to point out the misprints.

We provide further verification of the correctness of the modified Eq. (42) of Ref. [1] for several values of the nonlinear parameters with a short table comparing 30 significant digit results using Remiddi's formula (with the above corrections) and the output of our recently developed triangle integral package (details to be published).

We calculate, for various values of $w_1$, $w_2$, and $w_3$,

$$\mathbf{Z}(w_1,w_2,w_3)=\int r_{12}r_{23}r_{13}^{-1}e^{-w_1r_1-w_2r_2-w_3r_3}d\mathbf{r}_1d\mathbf{r}_2d\mathbf{r}_3. \tag{2}$$

Table I shows the results of the usual expansion technique [4] (18 terms) followed by a Levin $u$ transform ($k_{\max}=17$) [5] and compared with Remiddi's formula results. (The $64\pi^3$ factor in Remiddi's Eq. (42) is *not* included in these numbers.) The Remiddi results are accurate to 30 digits and therefore indicate an accuracy of 20 to 23 places for our Levin extrapolated values (details to be published).

TABLE I. $\mathbf{Z}(w_1,w_2,w_3)$ results for various $w_1$, $w_2$, and $w_3$.

| $w_1$ | $w_2$ | $w_3$ | Direct+Levin $u$-transform | Remiddi |
|---|---|---|---|---|
| 1.50 | 1.00 | 1.00 | 8.7835058015481861493257 | 8.7835058015481861493249653496 1 |
| 1.50 | 1.00 | 1.50 | 2.5395646052604153330274 5 | 2.5395646052604153330274924249 5 |
| 1.50 | 1.00 | 2.00 | 1.0539103665078177677 7 | 1.0539103665078177678353934304 3 |
| 1.50 | 1.50 | 1.00 | 2.5395646052604153330274 5 | 2.5395646052604153330274924249 5 |
| 1.50 | 2.00 | 1.50 | 3.5112601509772735423 7 | 3.5112601509772735423091622241 9 |
| 2.00 | 1.00 | 1.00 | 2.98667298227213234381 | 2.9866729822721323437564708827 8 |
| 2.00 | 2.00 | 1.00 | 3.24350301286034626758 6 | 3.2435030128603462675830985414 0 |

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