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Erratum

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Erratum: Method for Visualizing and Quantifying the Nonvalence Character of Excess Electrons

Thomas Sommerfeld*

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Our previous article[1] introduces an analysis scheme for characterizing excess electrons, which is based on plotting the density as a function of the distance to the nearest atom. For comparison, other characterizations, which had been used in this field, were provided, in particular, the expectation value of the distance to the center of mass, $\langle r \rangle = \langle |\hat{r}| \rangle$, and the so-called radius of gyration, $r_{gy} = (\langle \hat{r}^2 \rangle - \langle \hat{r} \rangle^2)^{1/2}$ of the excess electron. The values reported for the latter quantity, r_{gy}, listed in Table 1 of the original article[1] and plotted in Figures 2 and 3 of the original article[1] are wrong. The corrected table and figures are provided in this Erratum; as most of the comparisons made use $\langle r \rangle$ rather than r_{gy}, none of the discussion and conclusion in the original article[1] is affected.

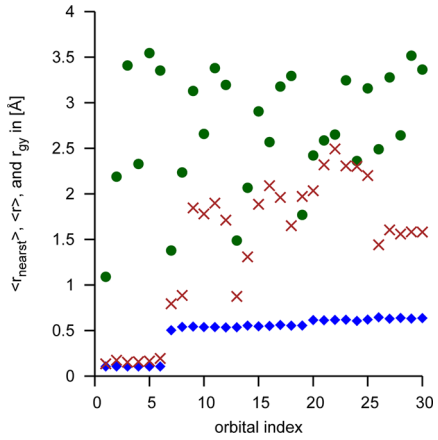

Figure 2. Expectations values $\langle r_{nearest} \rangle$ (blue diamonds) and $\langle r \rangle$ (green circles) as well as radii of gyration, r_{gy}, (brown crosses) for the 30 occupied orbitals of the AA-isomer of the water hexamer.

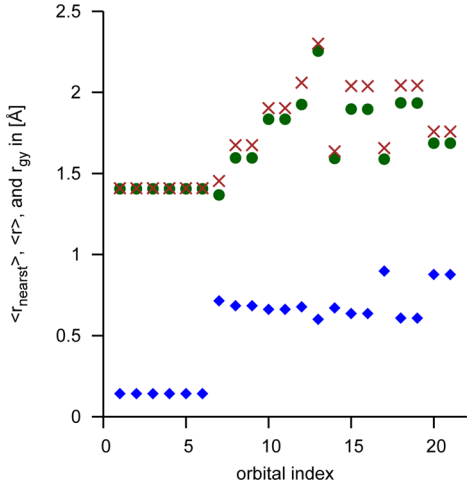

Figure 3. Expectations values $\langle r_{nearest} \rangle$ (blue diamonds) and $\langle r \rangle$ (green circles) as well as radii of gyration, r_{gy}, (brown crosses) for the 21 occupied orbitals of the benzene molecule.

Table 1. Expectations Values $\langle r_{nearest} \rangle$, $\langle r \rangle$, and the Radius of Gyration, r_{gy}, for the Five Occupied SCF Orbitals of the H_2O Monomer

	$\langle r \rangle$ [Å]	$\langle r_{nearest} \rangle$ [Å]	r_{gy} [Å]
$1a_1$	0.124	0.105	0.122
$2a_1$	0.648	0.536	0.707
$1b_2$	0.793	0.538	0.871
$3a_1$	0.759	0.630	0.849
$1b_1$	0.719	0.673	0.821

REFERENCES

(1) Sommerfeld, T. *J. Chem. Theory Comput.* **2013**, *9*, 4866.

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