Erratum to: Chemical bond between Cu(II) and Rn: ab initio study of CuRn_n^{2+} ($n = 1\text{--}6$) by coupled cluster method

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In L. Belpassi and co-workers' paper (*J. Am. Chem. Soc.*, 2008, 130 (3), 1048–1060), the authors have first introduced the charge displacement function, which is today a well established and successful tool for chemical bond analysis in a wide variety of contexts.

In our recent paper, we named the “charge displacement function” as “integrated charge transfer”, without the citation of the source paper (*J. Am. Chem. Soc.*, 2008, 130 (3), 1048–1060). Professor F. Tarantelli pointed out our fault. We take this opportunity to thank professor F. Tarantelli and co-workers for checking and correcting. We learned much from the paper and work of his group, we should have given a proper credit to the reported valuable results and methods, and this erratum aims to correct our paper and apologize to the authors of the original work.

The list of corrections is

1. For the paper, The “integrated charge transfer” should read as “charge displacement”.
2. Reference [20] (Belpassi L, Infante I, Tarantelli F, Visscher L (2008) *J Am Chem Soc* 130:1048) of the paper should be cited.

Page 262 (left panel):

The sentence, “Topological analysis of the Laplacian, electron density deformation, integrated charge transfer, bond critical point (BCP) properties and reduced density gradient (RDG) are performed on CuRn_n^{2+} to explore the nature of the interaction.” should read as “Topological analysis of the Laplacian, electron density deformation, charge displacement [20], bond critical point (BCP) properties and reduced density gradient (RDG) are performed on CuRn_n^{2+} to explore the nature of the interaction.”

Page 262 (right panel):

The sentence, “as it moves along the inter-nuclear axis (from $-\infty$ to z) and is defined as follows:” should read as “as it moves along the inter-nuclear axis (from $-\infty$ to z) and is defined as follows [20]:”

Equation 11 should be as below

$$Q(z) = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^z \Delta\rho(x, y, z') dz' \quad (11)$$

Numerical results and discussions are not affected by these corrections.

The online version of the original article can be found under doi:[10.1007/s11224-013-0285-2](https://doi.org/10.1007/s11224-013-0285-2).

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