



Corrigendum to “The importance of suppressing spin diffusion effects in the accurate determination of the spatial structure of a flexible molecule by nuclear Overhauser effect spectroscopy” [J. Mol. Struct. 1106 (2016) 373–381]



I.A. Khodov^{a, b, *}, S.V. Efimov^b, M.G. Kiselev^a, L.A.E. Batista de Carvalho^c, V.V. Klochkov^b

^a Laboratory of NMR-spectroscopy and Numerical Investigation Methods of Liquids, G.A. Krestov Institute of Solution Chemistry, Russian Academy of Sciences, Akademicheskaya St. 1, Ivanovo, 153045, Russia

^b Institute of Physics, Kazan Federal University, Kremlevskaya St. 18, Kazan, 420008, Russia

^c Molecular Physical Chemistry R&D Unit, University of Coimbra, 3004-535, Coimbra, Portugal

The original article to which this erratum refers was published in Journal of Molecular Structure, vol. 1106 (2016) [1]. In the original version of this article, Table 1 contained an error in column 10 (interatom distance averaging following the (r^6) -algorithm, proton pairs H9–H5 and H7–H9). Analogous mistype was also present in Table 2 in Ref. [2] for distances H7–H9. Values present in Refs. [1,2] were far too small, but they were presented only for the sake of comparison of different averaging methods and did not influence the final conformer distribution. The Table 1 is reproduced below with the error corrected.

Moreover, the original article [1] contained a minor analytical mistake that we have corrected below. The results and conclusions of our work are not affected by these mistake. The authors apologize for the mistake. Equation (10) in Ref. [1], and same equation (3) in Ref. [2] should read:

$$r_i^{eff} = \left[\left(\frac{1}{n_I n_S} \sum_i \frac{1}{r_i^3} \right)^2 \right]^{-1/6}$$

We thank Dr Craig Butts (School of Chemistry, Bristol University) for noticing this error.

DOI of original article: <http://dx.doi.org/10.1016/j.molstruc.2015.10.055>.

* Corresponding author. Laboratory of NMR-spectroscopy and Numerical Investigation Methods of Liquids, G.A. Krestov Institute of Solution Chemistry, Russian Academy of Sciences, Akademicheskaya St. 1, Ivanovo, 153045, Russia.

E-mail address: Ilya.Khodov@gmail.com (I.A. Khodov).

<http://dx.doi.org/10.1016/j.molstruc.2016.02.072>

0022-2860/© 2016 Elsevier B.V. All rights reserved.