Correction to: Performance of the DLPNO-CCSD and recent DFT methods in the calculation of isotropic and dipolar contributions to ^{14}N hyperfine coupling constants of nitroxide radicals

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The original paper contained errors in part of ^{14}N hyperfine couplings calculation using the SCAN and SCAN0 functionals. It was found that hyperfine coupling calculated using SCAN and SCAN0 functionals as implemented in the ORCA 4.2.0 program package are erroneous. For this reason, the corresponding values were recalculated using the ORCA 5.0.0 program package.

1) The correct mean absolute deviations in **Table 2** for SCAN0 are: a_{iso} v. Exp. is 6.0 G and not 12.6 G, a_{iso} v. DLPNO-CCSD is 4.0 G and not 10.7 G, corrected a_{iso} v. Exp. is 4.9 G and not 11.5 G, A_{z}^{dd} v. Exp. is 0.5 G and not 1.7 G, A_{z}^{dd} v. DLPNO-CCSD is 0.8 G and not 1.3 G, corrected A_{z}^{dd} v. Exp. is 0.7 G and not 1.4 G; for SCAN are: a_{iso} v. Exp. is 4.5 G and not 17.9 G, a_{iso} v. DLPNO-CCSD is 2.5 G and not 16.0 G, corrected a_{iso} v. Exp. is 3.4 G and not 16.8 G, A_{z}^{dd} v. Exp. is 1.5 G and not 1.6 G, A_{z}^{dd} v. DLPNO-CCSD is 1.1 G and not 1.2 G, corrected A_{z}^{dd} v. Exp. is 1.2 G and not 1.3 G;

2) In the **DFT calculation** section: “Along with MN15 functional, they bring ^{14}N a_{iso} values, which are sometimes more than 100% off from experimental values” should be

read as “as they give ^{14}N a_{iso} values that are sometimes up to 50% off from the experimental values”.

3) In the Conclusions section “The SCAN, SCAN0, and MN15 functionals were found to be the worst performers with relative errors in a_{iso} up to 100% or even more.” should be read as “For the a_{iso} calculation, the MN15 and BEEF functionals were found to be the worst performers.”

4) Corrected figures 2 and 3 are supplied along with this erratum.

These corrections do not generally affect the conclusions of the published work except for the performance of the SCAN-family of functionals.

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Fig. 2 Mean absolute deviations (MAD) for ^{14}N a_{iso} (left) and ^{14}N A_z^{dd} (right) results; a_{iso} calculations without the harmonic vibrational correction (blue shade), with the harmonic vibrational correction at 140 K (wine), and mean absolute errors versus the values calculated using the DLPNO-CCSD method (black). MAD (Mean Absolute Deviation)

$$= \frac{1}{N} \sum_i |A_{\text{calc}} - A_{\text{exp}}|$$

Fig. 3 Max. Absolute Errors for ^{14}N a_{iso} (left) and ^{14}N A_z^{dd} (right) results. a_{iso} calculations without the harmonic vibrational correction (blue shade), with the harmonic vibrational correction at 140 K (wine), and max. absolute errors versus the values calculated using the DLPNO-CCSD method (black)