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CORRECTION

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Correction: Anisotropy of the vorticity tensor as a magnetic indicator of aromaticity

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Correction for 'Anisotropy of the vorticity tensor as a magnetic indicator of aromaticity' by S. Pelloni *et al.*, *Phys. Chem. Chem. Phys.*, 2020, **22**, 1299–1305, DOI: 10.1039/C9CP05563K.

An error was detected,[1] and is hereby corrected, in the computation of the paramagnetic contribution to the vorticity tensor, correctly defined by eqn (15) in the published article. The computer code was incorrect by a factor of −2, which caused an overestimation of its magnitude. The correct isosurface maps are reported here for the collective threshold 0.031 a.u., which was determined *via* some preliminary tests. This value overrides the 0.5 a.u. value in the published article. Although the shapes of the isosurfaces are somewhat different from those in the published article, the general conclusions arrived at previously regarding the reliability of the anisotropy of the vorticity tensor as a criterion of magnetotropicity are confirmed. In particular, the revised maps show the absence of unequal vorticity in the regions of C–H bonds in planar conjugated hydrocarbons, as well as B–H and N–H bonds in borazine. A domain of enhanced anisotropy of the vorticity tensor is observed in Fig. 6 about the centre of the cyclopropane molecule, whereas the hollow regions appearing in the isosurface, in the proximity of the midpoint of C–C bonds, confirm the absence of σ-diatropicity.

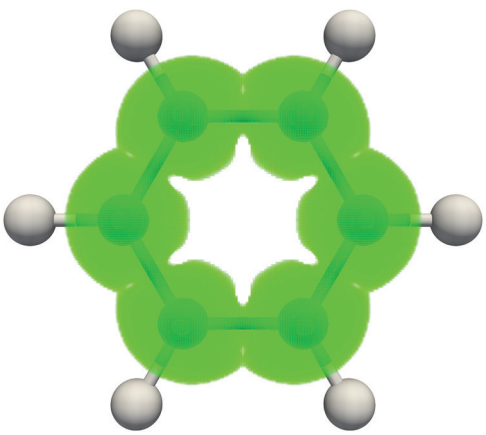

Fig. 1 Isosurface with value 0.031 a.u. of the anisotropy of the vorticity tensor in benzene. From the CODATA compilation,[2] the conversion factor to SI units is $eE_h/(a^3\hbar)$ = 4.469839112 × 10^{26} A m^{-3}.

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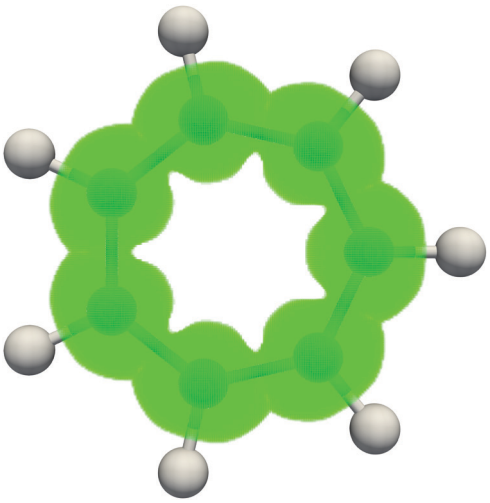

Fig. 2 Isosurface with value 0.031 a.u. of the anisotropy of the vorticity tensor in cycloheptatriene cation.

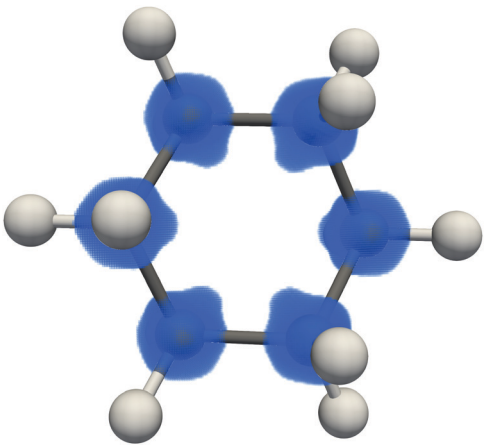

Fig. 3 Isosurface with value 0.031 a.u. of the anisotropy of the vorticity tensor in cyclohexane.

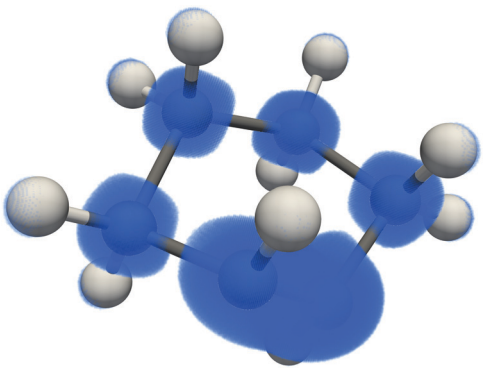

Fig. 4 Isosurface with value 0.031 a.u. of the anisotropy of the vorticity tensor in cyclohexene.

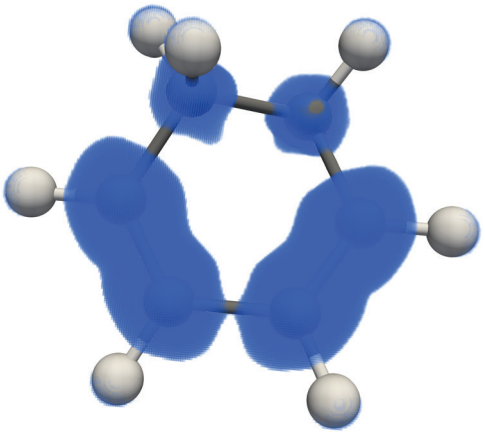

Fig. 5 Isosurface with value 0.031 a.u. of the anisotropy of the vorticity tensor in 1,3-cyclohexadiene.

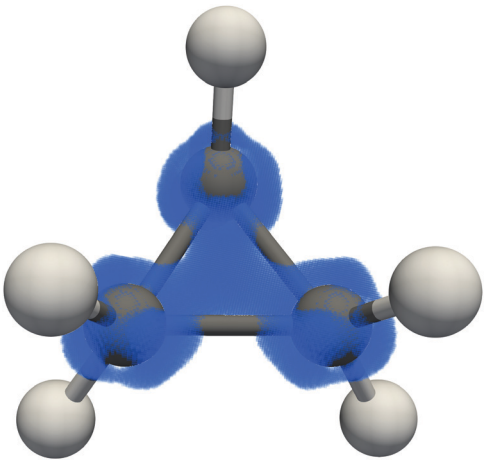

Fig. 6 Isosurface with value 0.031 a.u. of the anisotropy of the vorticity tensor in cyclopropane.

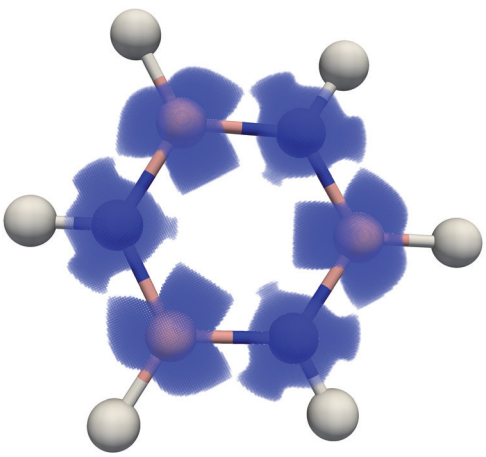

Fig. 7 Isosurface with value 0.031 a.u. of the anisotropy of the vorticity tensor in borazine.

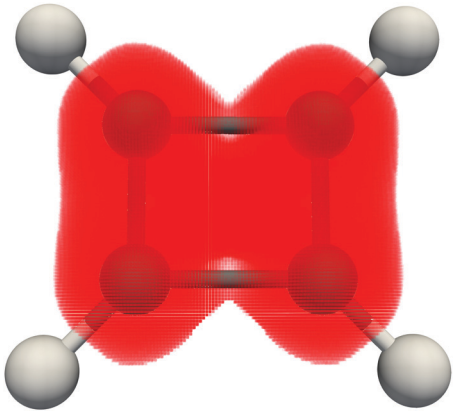

Fig. 8 Isosurface with value 0.031 a.u. of the anisotropy of the vorticity tensor in cyclobutadiene.

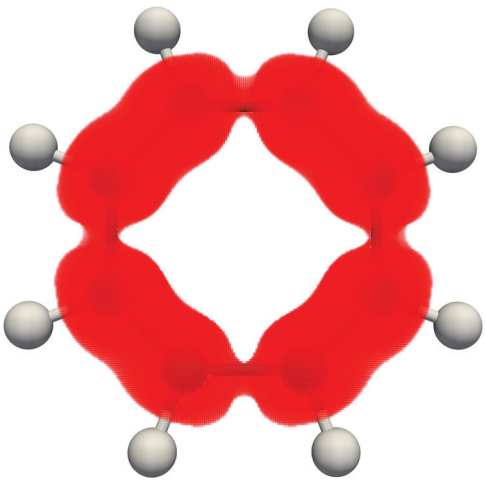

Fig. 9 Isosurface with value 0.031 a.u. of the anisotropy of the vorticity tensor in cyclo-octatetraene.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

Acknowledgements

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References

1 R. Zanasi, private communication.
2 P. J. Mohr, D. B. Newell and B. N. Taylor, *Rev. Mod. Phys.*, 2016, **88**, 035009.

