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CORRECTION

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Correction: Deciphering the molecular origin of the 19.3 eV electronic excitation energy of H_3^+

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Correction for 'Deciphering the molecular origin of the 19.3 eV electronic excitation energy of H_3^+' by Josene M. Toldo *et al.*, *Chem. Sci.*, 2026, https://doi.org/10.1039/d5sc09067a.

The authors regret that panel A of Fig. 4 in the original article was not complete as its right part, with results for the excited state labelled 1^1B_2, was accidently omitted. The missing part, with the topological analysis of the electron density, the 2D Laplacian of the electron density, and the natural orbitals of the 1^1B_2 state, is contained in the new Fig. 4 shown as follows.

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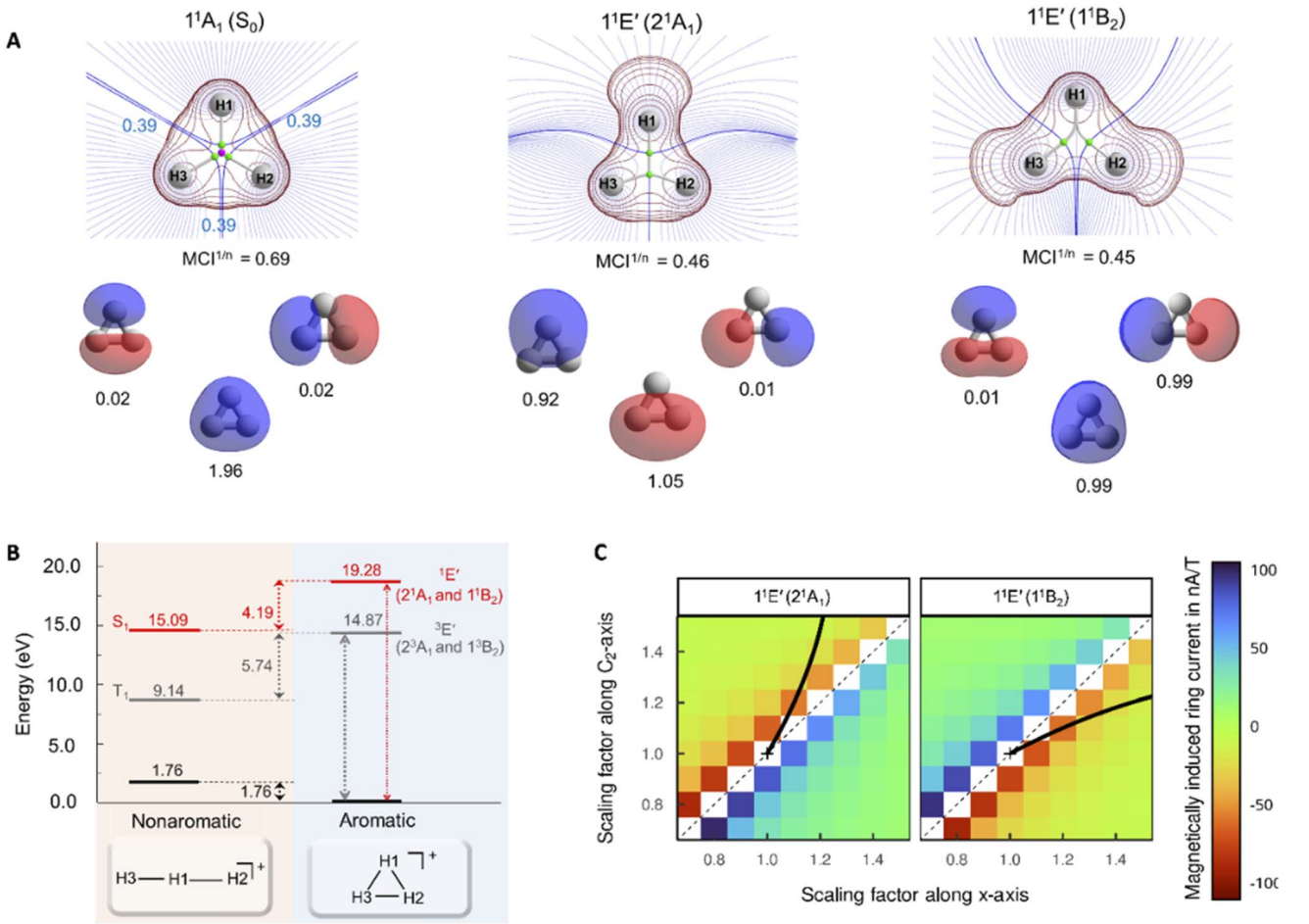

Fig. 4 (A) Topological analysis of the electron density, 2D Laplacian of the electron density (in red), and natural orbitals (with populations) for the S_0 and $1^1E'$ states, the latter labelled as 2^1A_1 and 1^1B_2 in C_{2v} symmetry. The rays of the basins drawn in blue and density gradient lines in purple. MCI$^{1/n}$ values (computed using Becke-rho's partition)[56] are given below the Laplacian plots of the electron density. (B) Vertical excitation energies and relative energies of H_3^+ at, respectively, $D_{\infty h}$ and D_{3h} symmetries. (C) Magnetically induced ring currents for the 2^1A_1 and 1^1B_2 states which stem from the $1^1E'$ states upon geometric distortions to C_{2v} symmetric structures. The scaling factors reflect how large this distortion was (the value 1.0 represents the H–H bond lengths of the S_0 equilibrium geometry). The C_2-axis indicates distortions in the direction of forming an acute isosceles triangle (moving H1 atom) and the x-axis distortions along an obtuse isosceles triangle formation (increasing the separation between H2 and H3).

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