

CORRECTION

[View Article Online](#)
[View Journal](#) | [View Issue](#)Cite this: *Chem. Sci.*, 2025, 16, 9029**Correction: A comprehensive approach for elucidating the interplay between $4f^{n+1}$ and $4f^n5d^1$ configurations in Ln^{2+} complexes**Maria J. Beltran-Leiva,^a William N. G. Moore,^b Tener F. Jenkins,^b William J. Evans,^{*b} Thomas E. Albrecht^{*d} and Cristian Celis-Barros^{*c}

DOI: 10.1039/d5sc90097b

rsc.li/chemical-scienceCorrection for 'A comprehensive approach for elucidating the interplay between $4f^{n+1}$ and $4f^n5d^1$ configurations in Ln^{2+} complexes' by Maria J. Beltran-Leiva et al., *Chem. Sci.*, 2025, 16, 2024–2033, <https://doi.org/10.1039/d4sc05438e>.

The original version of this manuscript contains an error in the caption for Table 1 as the incorrect computational method was referenced. The methodology given in the caption should be CASSCF/SO, rather than MC-pDFT.

The full corrected caption is as follows and replaces the original caption within the manuscript:

Table 1 Ground state Natural Spin Orbital (NSO) occupations for Ln^{3+} free ions, LnCp_3 and $[\text{LnCp}_3]^-$ complexes from the CASSCF/SO calculations. The total angular momentum quantum number (J) along with its predominant M_J are specified. In Fig. S5 a depiction of the f-orbitals and their labels are shown.

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

^aTheoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA^bDepartment of Chemistry, University of California, Irvine, California 92697-2025, USA^cRadioisotope Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA. E-mail: celisbarroca@ornl.gov^dDepartment of Chemistry, Nuclear Science & Engineering Center, Colorado School of Mines, Golden, Colorado 80401, USA