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CORRECTION

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Cite this: *Phys. Chem. Chem. Phys.*, 2017, **19**, 24369

DOI: 10.1039/c7cp90197f

rsc.li/pccp

Correction: The methylsulfinyl radical CH_3SO examined

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Correction for 'The methylsulfinyl radical CH_3SO examined' by Marissa L. Estep *et al.*, *Phys. Chem. Chem. Phys.*, 2016, **18**, 22293–22299.

The molecular orbital diagram included in the original version of the article is incorrect. The correct singly-occupied molecular orbital, computed using ROHF/ANO1 with an overall doublet multiplicity for the methylsulfinyl radical, is shown in the revised Fig. 5 below. The previous version of the molecular orbital was computed using the Molpro[1] software package; the current version was computed using CFOUR, as cited in the main article. Both versions were visualized using Jmol.[2]

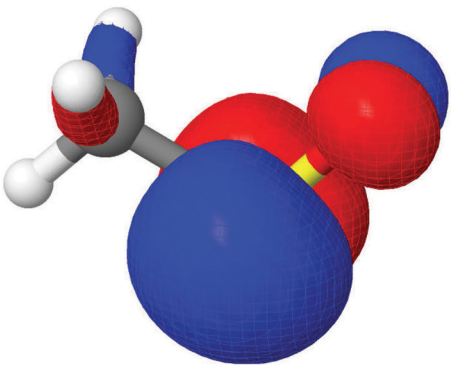

Fig. 5 Methylsulfinyl radical ground electronic state singly-occupied molecular orbital.

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

References

1 MOLPRO is a package of *ab initio* programs written by H.-J. Werner, P. J. Knowles, G. Knizia, F. R. Manby, M. Schütz, P. Celani, W. Györffy, D. Kats, T. Korona, R. Lindh, A. Mitrushenkov, G. Rauhut, K. R. Shamasundar, T. B. Adler, R. D. Amos, A. Bernhardsson, A. Berning, D. L. Cooper, M. J. O. Deegan, A. J. Dobbyn, F. Eckert, E. Goll, C. Hampel, A. Hesselmann, G. Hetzer, T. Hrenar, G. Jansen, C. Köppl, Y. Liu, A. W. Lloyd, R. A. Mata, A. J. May, S. J. McNicholas, W. Meyer, M. E. Mura, A. Nicklaß, D. P. O'Neill, P. Palmieri, D. Peng, K. Pflüger, R. Pitzer, M. Reiher, T. Shiozaki, H. Stoll, A. J. Stone, R. Tarroni, T. Thorsteinsson and M. Wang.

2 Jmol: an open-source Java viewer for chemical structures in 3D, http://www.jmol.org/.

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