

Erratum: “Global *ab initio* ground-state potential energy surface of N₄” [J. Chem. Phys. **139**, 044309 (2013)]

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In the data used for fitting the N₄ ground-state potential energy surface (PES),¹ several CASPT2 calculations did not converge to the correct ground state. We have corrected those data points, added 14 extra data points (bringing the number of data up to 16 435), and redone the fit. The figures in the paper do not change by a noticeable amount; however, the mean errors in Table I do improve somewhat at the higher energies, and they are provided in Table I of this erratum. The complete corrected data set is contained in electronic supplementary material.² The new N₄ ground-state PES, called N4PES-GPIP-v2, has been added to the POTLIB library.^{3,4}

TABLE I. The mean unsigned errors (MUEs) and root-mean-square errors (RMSEs) of the fitted potential energy surface with respect to CASPT2/maug-cc-pVTZ results for different energy ranges (in kcal/mol).

	No. of points	MUE	RMSE
$E < 100.0$	693	1.2	1.7
$100.0 \leq E < 228.0$	1941	2.3	4.1
$228.0 \leq E < 456.0$	11 858	3.1	5.8
$456.0 \leq E < 1000.0$	1610	10.9	14.6
$E > 1000.0$	333	21.7	30.9
All data	16 435	4.1	8.2

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¹Y. Paukku, K. R. Yang, Z. Varga, and D. G. Truhlar, *J. Chem. Phys.* **139**, 044309 (2013).

²See supplementary material <http://dx.doi.org/10.1063/1.4861562> for extra information, which is given in two parts. The supplemental material replaces the entire supplemental material of the original article. Part 1 is a .pdf file containing the potential function of N₂, a longer explanation of the N₄ potential energy function than is given in the main article, Figures S1–S8, a Fortran routine to convert the internal coordinates to Cartesian coordinates, and the complete set of corrected *ab initio* data in internal coordinates. Part 2 is a .dat file with the complete set of corrected *ab initio* data in Cartesian coordinates.

³R. J. Duchovic, Y. L. Volobuev, G. C. Lynch, T. C. Allison, J. C. Corchado, D. G. Truhlar, A. F. Wagner, and B. C. Garrett, *Comput. Phys. Commun.* **144**, 169–187 (2002); Erratum **156**, 319–322 (2004).

⁴See <http://comp.chem.umn.edu/potlib/> for the latest version of POTLIB that includes the present N₄ potential energy surface.

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