Publisher Correction: Optical clumped isotope thermometry of carbon dioxide

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Correction to: *Scientific Reports* https://doi.org/10.1038/s41598-019-40750-z, published online 18 March 2019

The original version of this Article contained errors.

References 6-9 were incorrectly listed as references 11-14. References 10-12 were listed as references 7-9. References 13 and 14 were listed as references 15 and 10 respectively. References 15-16 were listed as references 16-17. References 17-23 were listed as references 19-25. References 24–27 were listed as references 28, 26, 30 and 29 respectively. References 28-33 were listed as references 31-36.

Reference 34 was listed as reference 27. References 35-36 were listed as references 37 and 39 respectively. References 37-40 were listed as references 40-43. Reference 41 was listed as reference 18. References 42-52 were listed as references 44-54. Reference 53 was listed as reference 6. Reference 54 was listed as reference 38.

Furthermore, in the Introduction,

"Typical operation conditions are around $\Delta M/M \sim 40000$ or lower, which is insufficient to separate $^{13}C^{16}O_2$ from $^{12}C^{16}O^{17}O$ at m/z = 45 or $^{13}C^{16}O^{18}O$ from $^{12}C^{17}O^{18}O$ at m/z = 47, for example."

now reads:

"Typical operation conditions are around $M/\Delta M \sim 40000$ or lower, which is insufficient to separate $^{13}C^{16}O_2$ from $^{12}C^{16}O^{17}O$ at m/z = 45 or $^{13}C^{16}O^{18}O$ from $^{12}C^{17}O^{18}O$ at m/z = 47, for example."

In the lower inset of Figure 1 the two labels P(9) and P(17) were inadvertently switched.

In the Operating Principles and Instrumental Approach section,

"The uncertainty of this calibration is very small: different calculations at 1000 K are given in the literature[22,33,36] and our calculation based on partition functions evaluated as direct sums of energy levels provided by ab initio calculations that were refined by spectroscopic measurements[34], indicate that the error at that temperature is about 5 ppm."

now reads:

"The uncertainty of this calibration is very small: different calculations at 1000 K are given in the literature[22,36] and our calculation based on partition functions evaluated as direct sums of energy levels provided by ab initio calculations that were refined by spectroscopic measurements[34], indicate that the error at that temperature is about 5 ppm."

In Table 2 the column heading,

"CL2012[36]"

now reads:

"CL2012[54]"

Additionally in Table 2 the column heading,

"CBRZ2014[54]"

now reads:

"CBRZ2014[36]"

Finally, the Table 2 legend,

"Different theories are employed: BMU approach using harmonic frequencies for application of the Teller-Redlich[28] rule and anharmonic correction to the ZPEs – WSE2004[22]. The same approach using harmonic frequencies from another level of theory – CL2012[36]. Path-Integral Monte Carlo (PIMC) evaluation of partition sums – WM2014[33]. Approximate direct sum partition functions from a refined potential surface – CBRZ2014[54]. Direct sum calculation of partition functions (this work) using state energies from new spectroscopic data generated from experimentally refined ab initio calculations[34]. aValues at temperatures other than 200, 300 and 1000 K were recalculated from molecular constants in Table 3 of Wang *et al.*[22]."

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"Different theories are employed: BMU approach using harmonic frequencies for application of the Teller-Redlich[28] rule and anharmonic correction to the ZPEs – WSE2004[22]. The same approach using harmonic frequencies from another level of theory – CL2012[54]. Path-Integral Monte Carlo (PIMC) evaluation of partition sums – WM2014[33]. Approximate direct sum partition functions from a refined potential surface – CBRZ2014[36]. Direct sum calculation of partition functions (this work) using state energies from new spectroscopic data generated from experimentally refined ab initio calculations[34]. aValues at temperatures other than 200, 300 and 1000 K were recalculated from molecular constants in Table 3 of Wang *et al.*[22]."

These errors have now been corrected in the PDF and HTML versions of the Article.