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# Publisher Correction: Optical clumped isotope thermometry of carbon dioxide

Ivan Prokhorov , Tobias Kluge &amp; Christof Janssen

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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  $^{13}\text{C}^{16}\text{O}_2$  from  $^{12}\text{C}^{16}\text{O}^{17}\text{O}$  at  $m/z = 45$  or  $^{13}\text{C}^{16}\text{O}^{18}\text{O}$  from  $^{12}\text{C}^{17}\text{O}^{18}\text{O}$  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  $^{13}\text{C}^{16}\text{O}_2$  from  $^{12}\text{C}^{16}\text{O}^{17}\text{O}$  at  $m/z = 45$  or  $^{13}\text{C}^{16}\text{O}^{18}\text{O}$  from  $^{12}\text{C}^{17}\text{O}^{18}\text{O}$  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<sup>22,33,36</sup> 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<sup>34</sup>, 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<sup>22,36</sup> 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<sup>34</sup>, indicate that the error at that temperature is about 5 ppm.”

In Table 2 the column heading,

“CL2012<sup>36</sup>”

now reads:

“CL2012<sup>54</sup>”

Additionally in Table 2 the column heading,

“CBRZ2014<sup>54</sup>”

now reads:

“CBRZ2014<sup>36</sup>”

Finally, the Table 2 legend,

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

now reads:

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

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



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