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Erratum: “MARVEL Analysis of the Measured High-Resolution Rovibronic Spectra and Definitive Ideal-Gas Thermochemistry of the $^{16}\text{O}_2$ Molecule” [J. Phys. Chem. Ref. Data 48, 023101 (2019)] **FREE**

Tibor Furtenbacher ; Mátyás Horváth; Dávid Koller; Panna Sólyom; Anna Balogh; István Balogh; Attila G. Császár 



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CONTENTS

References 1

In Ref. 1, the direct summation technique was used to obtain accurate, temperature-dependent, ideal-gas thermochemical functions for $^{16}\text{O}_2$ from the nearly complete set of its (mostly empirical) rovibronic energy levels. To obtain expanded uncertainties, U_{ULB} , for these thermochemical functions, the method of upper-and-lower-bounds (ULB) was used.

While working on the results presented in Ref. 2, two of the authors of this Erratum, T. F. and A. G. C., checked the results given in Ref. 1, and found a programming mistake. The miscalculation affected some of the uncertainties given for $C_p(T)$, the isobaric heat capacity, of $^{16}\text{O}_2$ in Ref. 1, resulting in incorrect U_{ULB} values. A clear symptom of the problem is that the uncertainty unphysically went to zero at a temperature near 3500 K.

In Ref. 2, the ULB method was correctly applied to estimate the uncertainties of the calculated functions. The Supplementary Material of Ref. 2 provides the correctly calculated U_{ULB} uncertainties of $C_p(T)$ of $^{16}\text{O}_2$. It is also important to point out that even though the thermochemical functions themselves were calculated correctly in Ref. 1, they are superseded, in fact not only for $^{16}\text{O}_2$ but also for H_2^{16}O (see Ref. 3), by the values given in Ref. 2, that were obtained using the latest values of the physical constants.

References

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