Erratum: "New investigation of the v_3 C–H stretching region of 12 CH₄ through the analysis of high temperature infrared emission spectra" [J. Chem. Phys. 148, 134306 (2018)]

Badr Amyay,¹ Aline Gardez,² Robert Georges,² Ludovic Biennier,² Jean Vander Auwera,³ Cyril Richard,¹ and Vincent Boudon^{1,a)} ¹Laboratoire Interdisciplinaire Carnot de Bourgogne (ICB), UMR 6303 CNRS, Université Bourgogne Franche-Comté, 9 Avenue A. Savary, BP 47870, 21078 Dijon Cedex, France ²Institut de Physique de Rennes, UMR 6251, Campus de Beaulieu, Université de Rennes I/CNRS, F-35042 Rennes Cedex, France ³Service de Chimie Quantique et Photophysique, C.P. 160/09, Université Libre de Bruxelles, 50 Avenue F. D. Roosevelt, B-1050 Brussels, Belgium

https://doi.org/10.1063/1.5034108

In our recent article,¹ Fig. 9 compares a methane spectrum recorded at 1404 K with spectra calculated at the same conditions using the Theoretical Reims-Tomsk Spectral (TheoReTS) data line list, in addition to predictions from our work. Unfortunately, an older version of the TheoReTS line list was used, instead of the latest version,² which accounts for corrections on the line positions. The new Fig. 9 reproduced below corrects this mistake. Its inspection shows the very good agreement between the TheoReTS predictions and the emission spectrum recorded at 1404 K.

We wish to thank Dr. Michaël Rey for indicating us this new version of TheoReTS.

¹B. Amyay, A. Gardez, R. Georges, L. Biennier, J. Vander Auwera, C. Richard *et al.*, "New investigation of the ν_3 C–H stretching region of ¹²CH₄ through the analysis of the high temperature infrared emission spectra," J. Chem. Phys. **148**, 134306 (2018).

²M. Rey, A. V. Nikitin, and V. G. Tyuterev, "Accurate theoretical methane line lists in the infrared up to 3000 K and quasi-continuum absorption/emission modeling for astrophysical applications," Astrophys. J. 847, 105 (2017).

^{a)}Author to whom correspondence should be addressed: Vincent.Boudon@u-bourgogne.fr



FIG. 9. Comparison between the observed spectrum of 12 CH₄ at 1404 K (red) and the calculated spectrum (gray) in the spectral region 2600-3300 cm⁻¹. The contribution of the cold band (blue) and related hot bands (green and magenta) is highlighted separately at the bottom of each sub-figure. Also a comparison with the TheoReTS calculated database (brown curve) is given for both low and high *J* transitions at the bottom of each sub-figure.