A 10¹⁰ line list for CH₄

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Methane plays an important role in atmospheric and astrophysical chemistry. Its rotation–vibration spectrum is of key importance for models of the atmospheres of bodies ranging from Titan to brown dwarfs. However the lack of precise data on methane spectra, particularly at higher temperatures, has severely limited models for atmospheres as diverse as Jupiter, exoplanets and brown dwarfs. Consequently we have embarked on a major project ExoMol [1] to fill this gap. Here we present a computationally-derived line list for methane containing almost 10^{10} transition that is sufficiently complete and accurate to be able to replicate observed spectra at temperatures up to 1500 K. This line list details transition frequencies and associated Einstein coefficients, lower energy levels and quantum numbers. It comprises ro-vibrational transitions for *J* values up to 39 and frequencies below 12,000 cm⁻¹. The line list was generated using the program TROVE and our new 9D *ab initio* potential energy and dipole moment surfaces. Hot temperature spectra of CH₄ simulated using this line list will be presented and compared to different experimental spectra of methane available in the literature as well as generated using other line lists. Our 'hot' 10^{10} line list for CH₄ will be suitable for use in modelling the spectra of planetary and stellar objects.

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[1] J. Tennyson and S. N. Yurchenko, Mon. Not. R. Astron. Soc. 2012, 425, 21.