Methane Spectra Assignment with the MM line list and Marvel Update

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The ExoMolHD (ExoMol in High Definition) project delivers accurate molecular line lists tailored for the studies of exoplanetary atmospheres in the current era of high-resolution (R=100 000) observations. ExoMolHD combines theoretical predictions with large-scale experimental datasets to refine line positions and enhance the applicability of molecular line lists for high-resolution studies.

Methane (CH_4) is a key molecule in astrochemistry due to its presence in various astrophysical environments. We use the recently developed ExoMol MM (MARVELous Methane) line list (Yurchenko et al. 2024 MNRAS, Kefala et al. 2024 JQSRT), which combines variational calculations from the TROVE program with empirical refinement via the MARVEL methodology, as a reference to assign previously unassigned experimental transitions. Serving as a high-accuracy spectral fingerprint, the MM line list includes over one million line positions with experimental precision.

This work presents a significant update to the methane MARVEL compilation. We incorporated approximately $11,000$ transitions from 11 literature sources spanning 1000–9100 cm^{-1} which we assigned using the MM line list, as well as about $2,700$ transitions from five recently published experimental studies.

The expanded MARVEL dataset now includes gives us $29,800$ energy levels, of which approximately $6,500$ are newly derived in this update. Among these new levels, 31% are confirmed with combination differences (i.e., defined by more than one transition). These additions primarily improve coverage in the icosad and triacontad (polyads 5 and 6), which were previously under-represented in the MARVEL compilation.

The resulting updated MARVEL energy levels feed back into the MM line list, enhancing its accuracy by enabling further refinement of the potential energy surface (PES) and replacing theoretical energies with empirical ones where available. This iterative process leads to continuous improvement of the line list's accuracy.