

ExoMol line lists – XXIX. The rotation-vibration spectrum of methyl chloride up to 1200 K

Alec Owens,¹ A. Yachmenev, Center for Free-Electron Laser Science & Center for Ultrafast Imaging, Universität Hamburg; W. Thiel, Max-Planck-Institut für Kohlenforschung; A. Fateev, Technical University of Denmark; J. Tennyson & S. N. Yurchenko, UCL

The recent interstellar detection of methyl chloride² has undermined the possibility of CH₃Cl as a realistic biosignature gas in the search for life outside of our Solar system.³ The fact that CH₃Cl can be formed abiotically, and possibly delivered by cometary impact to young planets, means it is now far more relevant in the context of newly formed rocky exoplanets. Here, we present comprehensive rotation-vibration line lists for the two main isotopologues of methyl chloride, ¹²CH₃³⁵Cl and ¹²CH₃³⁷Cl.⁴ The line lists, OYT-35 and OYT-37, are suitable for temperatures up to $T = 1200$ K and consider transitions with rotational excitation up to $J = 85$ in the wavenumber range 0–6400 cm⁻¹ (wavelengths $\lambda > 1.56 \mu\text{m}$). Over 166 billion transitions between 10.2 million energy levels have been calculated variationally for each line list. The OYT line lists show excellent agreement with newly measured high-temperature infrared absorption cross-sections, reproducing both strong and weak intensity features across the spectrum. The line lists are available from the ExoMol database.

¹alec.owens@cfel.de

²Fayolle E. C. et al., 2017, Nat. Astron., 1, 703

³Segura A. et al., 2005, Astrobiology, 5, 706

⁴Owens A. et al., 2018, MNRAS, in press