Interpreting Methanol \( \nu_2 \)-band Emission in Comets using Empirical Fluorescence g-factors

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Abstract

For many years we have been developing the ability, through high-resolution spectroscopy targeting ro-vibrational emission in the \( \sim 3 \sim 5 \) \( \mu \)m region, to quantify a suite of \( \sim 10 \) parent volatiles in comets using quantum mechanical fluorescence models. Our efforts are ongoing and our latest includes methanol (CH\(_3\)OH). This is unique among traditionally targeted species in having lacked sufficiently robust models for its symmetric \( (\nu_1 \) band) and asymmetric \( (\nu_2 \) and \( \nu_8 \) bands) C-H\(_3\) stretching modes, required to provide accurate predicted intensities for individual spectral lines and hence rotational temperatures and production rates. This has provided the driver for undertaking a detailed empirical study of line intensities, and has led to substantial progress regarding our ability to interpret CH\(_3\)OH in comets.

The present study concentrates on the spectral region from \( \sim 2970 \sim 3010 \) cm\(^{-1}\) (3.367 \sim 3.322 \( \mu \)m), which is dominated by emission in the \( \nu_1 \) band of C\(_2\)H\(_2\) and the \( \nu_2 \) band of CH\(_3\)OH, with minor contributions from CH\(_3\)OH \( (\nu_6 \) band), CH\(_4 \) \( (\nu_3 \) band), and OH prompt emissions (\( \nu_1 \) and \( \nu_2 \sim \nu_1 \)). Based on laboratory jet-cooled spectra (at a rotational temperature near 20 K)[1], we incorporated approximately 100 lines of the CH\(_3\)OH \( \nu_2 \) band, having known frequencies and lower state rotational energies, into our model. Line intensities were determined through comparison with several comets we observed with NIRSPEC at Keck 2, after removal of continuum and additional molecular emissions and correcting for atmospheric extinction. In addition to the above spectral region, NIRSPEC allows simultaneous sampling of the CH\(_3\)OH \( \nu_1 \) band (centered at 2844 cm\(^{-1}\), or 3.516 \( \mu \)m) and several hot bands of H\(_2\)O in the \( \sim 2.85 \sim 2.9 \) \( \mu \)m region, at a nominal spectral resolving power of \( \sim 25,000 \) [2]. Empirical g-factors for \( \nu_2 \) lines were based on the production rate as determined from the \( \nu_2 \) Q-branch intensity; application to comets spanning a range of rotational temperatures (\( \sim 50 \sim 90 \) K) will be reported. This work represents an extension of that presented for comet 21P/Giacobini-Zinner at the 2010 Division for Planetary Sciences meeting [3]. Our empirical study also allows for quantifying CH\(_3\)OH in comets using IR spectrometers for which the \( \nu_1 \) and \( \nu_2 \) bands are not sampled simultaneously, for example CSHELL / NASA-IRTF or CRIRES / VLT.

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References

