Interpreting Methanol ν_2-band Emission in Comets using Empirical Fluorescence g-factors

M. A. DiSanti (1), G. L. Villanueva (1,2), B. P. Bonev (1,2), M. J. Mumma (1), L. Paganini (1,3), E. L. Gibb (4), and K. Magee-Sauer (5)
(1) NASA-Goddard Space Flight Center, Maryland, USA, (2) The Catholic University of America, Washington, DC, USA, (3) NASA Postdoctoral Fellow, Maryland, USA, (4) University of Missouri – St. Louis, Missouri, USA, (5) Rowan University, New Jersey, USA (michael.a.disanti@nasa.gov / Fax: +1-301-286-1683)

Abstract

For many years we have been developing the ability, through high-resolution spectroscopy targeting ro-vibrational emission in the ~ 3 – 5 μm region, to quantify a suite of (~ 10) parent volatiles in comets using quantum mechanical fluorescence models. Our efforts are ongoing and our latest includes methanol (CH_3OH). This is unique among traditionally targeted species in having lacked sufficiently robust models for its symmetric (ν_3 band) and asymmetric (ν_2 and ν_9 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_3OH in comets.

The present study concentrates on the spectral region from ~ 2970 – 3010 cm^{-1} (3.367 – 3.322 μm), which is dominated by emission in the ν_7 band of C_2H_6 and the ν_2 band of CH_3OH, with minor contributions from CH_3OH (ν_9 band), CH_4 (ν_3), and OH prompt emissions (ν_1 and $\nu_2 - \nu_1$). Based on laboratory jet-cooled spectra (at a rotational temperature near 20 K)[1], we incorporated approximately 100 lines of the CH_3OH ν_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_3OH ν_3 band (centered at 2844 cm^{-1}, or 3.516 μm) and several hot bands of H_2O in the ~ 2.85 – 2.9 μm region, at a nominal spectral resolving power of ~ 25,000 [2]. Empirical g-factors for ν_2 lines were based on the production rate as determined from the ν_3 Q-branch intensity; application to comets spanning a range of rotational temperatures (~ 50 – 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_3OH in comets using IR spectrometers for which the ν_3 and ν_2 bands are not sampled simultaneously, for example CSHELL / NASA-IRTF or CRIRES / VLT.

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References

[1] Xu, L.-H., Wang, X., Cronin, T. J., Perry, D. S., Fraser, G. T., and Pine, A. S.: Sub-Doppler Infrared Spectra and Torsion–Rotation Energy Manifold of Methanol in the CH-Stretch Fundamental Region, *J. Mol. Sp.*, Vol. 185, 158-172, 1997.

[2] McLean, I. S., Graham, J. R., Becklin, E. E., Figer, D. F., Larkin, J. E., Levenson, N. A., and Teplitz, H. I: Performance and results with the NIRSPEC echelle spectrograph on the Keck II telescope, SPIE, Vol. 4008, 1048-1055, 2000.

[3] DiSanti, M. A., Bonev, B. P., Mumma, M. J., and Villanueva, G. L.: Highly Depleted Ethane and Slightly Depleted Methanol in Comet 21P/Giacobini-Zinner: Application of Empirical g-factors for CH_3OH near 50 K, Bull. Amer. Astron. Soc, Vol. 42, p. 946, 2010.