

Cine: Line excitation by infrared fluorescence in cometary atmospheres

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Summary

CINE is a Python module for calculating infrared pumping efficiencies that can be applied to the most common molecules found in cometary comae such as water, hydrogen cyanide or methanol. Excitation by solar radiation of vibrational bands followed by radiative decay to the ground vibrational state is one of the main mechanisms for molecular excitation in comets. This code calculates the effective pumping rates for rotational levels in the ground vibrational state scaled by the heliocentric distance of the comet as detailed in Bensch and Bergin (2004) and Crovisier and Encrenaz (1983). Line transitions are queried from the latest version of the HITRAN spectroscopic repository (Rothman et al. 2013) using the astroquery affiliated package of astropy (Ginsburg et al. 2016). Molecular data are obtained from the LAMDA database (Schöier et al. 2005).

These coefficients are useful for modeling rotational emission lines observed in cometary spectra at sub-millimeter wavelengths. Combined with computational methods to solve the radiative transfer equations based, e.g., on the Monte Carlo algorithm (de Val-Borro and Wilson 2016), this model can retrieve production rates and rotational temperatures from the observed emission spectrum.

The code and issue tracker of *CINE* are available on GitHub (de Val-Borro 2017) and any questions or bug reports can be raised there. The source code for *CINE* is also available from the Python Package Index (PyPI).

References

- Bensch, F., and E. A. Bergin. 2004. “The Pure Rotational Line Emission of Ortho-Water Vapor in Comets. I. Radiative Transfer Model” 615 (November): 531–44. doi:10.1086/424439.
- Crovisier, J., and T. Encrenaz. 1983. “Infrared fluorescence of molecules in comets - The general synthetic spectrum” 126 (September): 170–82.
- de Val-Borro, M. 2017. “CINE on Github.” <https://github.com/migueldvb/cine>.
- de Val-Borro, M., and T. G. Wilson. 2016. “CRETE: Comet RadiativE Transfer and Excitation.” *Astrophysics*

Source Code Library.

Ginsburg, Adam, Madhura Parikh, Julien Woillez, Brigitta Sipocz, Austen Groener, Simon Liedtke, Thomas Robitaille, et al. 2016. “Astropy/Astroquery: ESASKY.” doi:10.5281/zenodo.160246.

Rothman, L. S., I. E. Gordon, Y. Babikov, A. Barbe, D. Chris Benner, P. F. Bernath, M. Birk, et al. 2013. “The HITRAN2012 molecular spectroscopic database” 130 (November): 4–50. doi:10.1016/j.jqsrt.2013.07.002.

Schöier, F. L., F. F. S. van der Tak, E. F. van Dishoeck, and J. H. Black. 2005. “An atomic and molecular database for analysis of submillimetre line observations” 432 (March): 369–79. doi:10.1051/0004-6361:20041729.