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Molecular emission spectral line shape analysis in cometary coma using Direct Simulation Monte Carlo (DSMC) methods: What can be learned from observations of the line shapes?

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The line shape of molecular emission in a cometary coma is determined in part by the distribution of the molecular velocity and rotational level population. It is commonly believed that close to the cometary nucleus, there is a transition region in the coma, called the Knudsen layer, in which the velocity distribution of the gas is non-Maxwellian (W. Huebner and W. Markiewicz, 2000, Icarus, 148, 594-596). Similarly, in regions where molecular collisions are rare the rotational level distribution differs from the Boltzmann distribution and non-local thermal equilibrium effects determine the molecular emission line shape. We have used the Direct Simulation Monte Carlo method to determine the velocity and rotational level distributions for low-lying ground state transitions throughout the coma, and computed the resulting emission line shape for the isotopologues of H_2O with observational parameters close to those for the MIRO instrument on the Rosetta spacecraft en route to 67P/Churyumov-Gerasimenko. We will discuss the effects of heliocentric distance, diurnal and seasonal variations, and how observations of non-Maxwellian spectral line shapes in the Knudsen region and elsewhere, can be used to infer physical properties of the nucleus and coma.