



SEMINAIRE ISMO

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Nucleation and growth of CO₂ – combined FTIR spectroscopy and mass spectrometry study

CO₂ cluster formation can be observed in the postnozzle flow of Laval expansions below 50 K with the use of mass spectrometry and FTIR spectroscopy. The uniform Laval post-nozzle flow allows to measure mass and FTIR spectra under analogous conditions and relate information on size, shape, and phase of clusters. A wide range of cluster distributions from cluster size below 10 molecules to cluster sizes with several thousand molecules per cluster were registered. Size-dependent condensed phase CO₂ peaks can be observed in the experimental FTIR spectra. Experimental IR spectra were interpreted with the aid of exciton calculations and DFT computations. Exciton calculations were performed using information on the geometrical structure for clusters containing >55 molecules defined by shell and subshell closings and the abundances of different cluster sizes – both from mass spectrometry. For clusters below 55 molecules, the structure information was retrieved from force field and density functional theory computations.

Mardi 22 janvier 2018 à 11 h
Amphithéâtre du bât 520 (3^{ème} étage)
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