

High pressure/high temperature infrared transmittance spectra of carbon dioxide; measured and simulated data

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The modelling of the transmittance of gases at extreme conditions, in particular high pressure and high temperature, in some cases is not satisfactory as it would need for an accurate determination of the physical-chemical parameters in deep atmospheres. To better interpret the data coming from the remote sensing instruments flying in space, like Venus Express, we have built up a set-up in our laboratory to measure the optical properties of gases at high pressure and/or high temperature. A Fourier Transform InfraRed (FT-IR) interferometer has been integrated with a special customized high pressure-high temperature (HP-HT) gas cell and the system has been employed to measure CO₂ transmittance at the conditions typically found in the deep atmosphere of Venus. This set-up is able to work in a wide spectral range, from 350 to 25000 cm⁻¹ (0.4 to 29 μm), with a relatively high spectral resolution, from 10 to 0.07 cm⁻¹. The HP-HT gas cell is able to work at a pressure up to about 50 bar (real limitation being the CO₂ source) and a temperature up to 350°C. Measurements were done varying the pressure from 1 to 50 bar and the temperature from 298 to 550K.

Measurements have been compared with synthetic spectra obtained using two different models: one consist in a custom code called “ARS” which implements a line by line calculation; another one called “Solution”, taking into account mechanisms thought to be responsible of the shape of the spectral lines. The latter in particular models the “line mixing”, or interference of rotational states where individual rotational lines overlap, and the dense, short-path lengths intermolecular collisions, which yields to effect produced by far wings of spectral lines. A preliminary comparison leads us to conclude that in the real gases under pressure higher than only a few bars, the shape of the spectral lines no longer follows the conventional Voigt form. In particular, the absorption in the far wings of strong ro-vibrational bands at a few hundred cm⁻¹ from band cores, is 10³-10⁴ times higher than predicted by the Lorentz profile. Another aspect under study is the “Collision Induced Absorption” (CIA). This effect is due to the dipole moment induced by collision processes. We discuss here the comparison between data and models.