Infrared absorption by molecular gases as a probe of nanoporous xerogel and molecule-surface collisions

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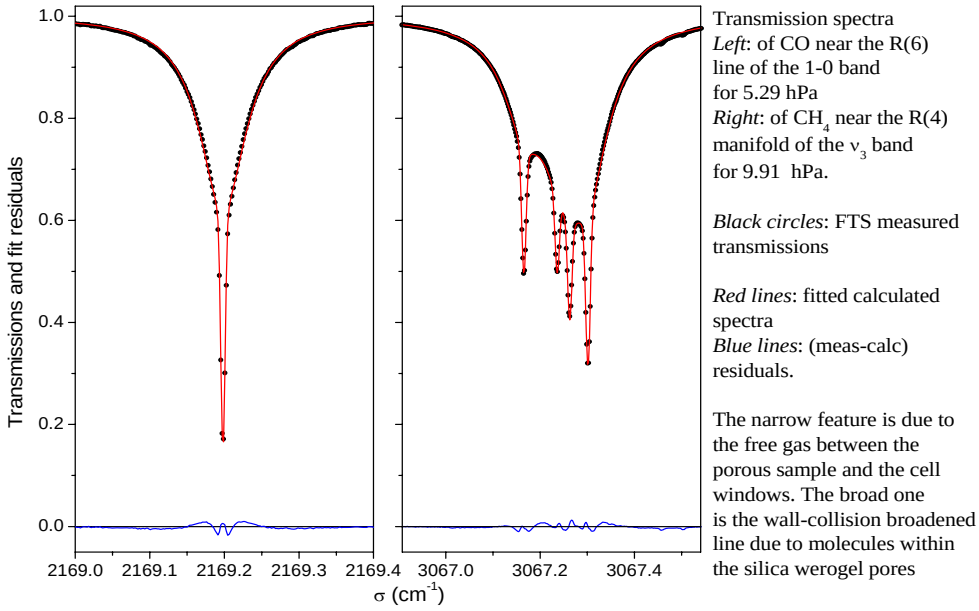
Transmission spectra of gases confined (but not adsorbed) within the pores of a silica xerogel sample have been recorded between 2.5 and 5 μm using a high resolution Fourier transform spectrometer. This was done for pure CO, CO_2, N_2O, H_2O and CH_4 at room temperature and pressures of a few hPa. Least squares fits of measured absorption lines (eg Fig. below) provide the optical-path lengths within the confined (L^C) and free (L^F) gas inside the absorption cell, and the half width at half maximum Γ^C of the lines of the confined gases. The values of L^C and L^F retrieved using numerous transitions of all studied species are very consistent and in good agreement with those determined from independent measurements. Reliable information on the open porosity volume can thus be obtained from an optical experiment. The values of Γ^C, here entirely due to collisions of the molecules with the inner surfaces of the xerogel pores, are practically independent of the line for each gas and inversely proportional to the square-root of the probed-molecule molar mass. This is a strong indication that, for the transitions studied, a single collision of a molecule with a pore surface is sufficient to change its rotational state. A previously proposed simple model is then used for the prediction of the line shape that leads to satisfactory agreement with the observations. Furthermore, it also enables a determination of the average pore size, bringing information complementary to that obtained from nitrogen adsorption porosimetry.



Transmission spectra
Left: of CO near the R(6) line of the 1-0 band for 5.29 hPa
Right: of CH_4 near the R(4) manifold of the ν_3 band for 9.91 hPa.

Black circles: FTS measured transmissions

Red lines: fitted calculated spectra
Blue lines: (meas-calc) residuals.

The narrow feature is due to the free gas between the porous sample and the cell windows. The broad one is the wall-collision broadened line due to molecules within the silica werogel pores

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