Infrared probing of porous media and of molecule-surface collisions

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We present recordings of infrared transmission spectra of various gas molecules confined (but not adsorbed) within the pores of several silica-based (aerogel and xerogel) porous material samples. Their analyses show that they bring information on both the material and molecule-surface collisions. Indeed, fits of the observed lines provide, through the integrated area, the optical pathlength and thus the percentage of porosity. Furthermore, the observed line widths can be directly related to the average pore size, assuming that a single molecule-surface collisions is sufficient to change the molecule rotational state. This assumption is validated using both experiments and molecular dynamics calculations. Finally, detailed analysis of CH_4 absorptions under confined- and free-gas conditions demonstrates that very different propensity rules are associated with molecule-molecule and molecule-surface collisions.