Probing NaCl at High Pressure Through Optical Studies and *Ab Initio* Calculations

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Sodium chloride, the most abundant salt on the earth, is under its solid form a transparent material, from the UV to the far infrared region, highly soluble in polar solvents such as water. Thanks to its strong ionic behaviour and these physico-chemical properties, it is a widely employed technological material for chemical, biological and optical applications. From the fundamental point of view, NaCl has been deeply studied in condensed matter physics at ambient and extreme conditions of pressure and temperature as it is the prototypical model for ionic NaCl-structured minerals, which constitute an important fraction of the earth interior [1,2]. Therefore, studying NaCl at megabar pressures is of paramount interest for geophysics.

Due to this structural stability and its simple loading in diamond anvil cells, NaCl has been exploited in several high pressure studies as pressure calibrant, hydrostatic medium electrical and thermal insulator. Indeed, electrical insulation provided by NaCl is particularly important for transport measurements in diamond anvil cells, which represent the main method to probe record high critical temperature superconductors at high pressure [3-5]. For such investigations, the characterization of NaCl infrared response at megabar pressures is a requisite. A previous optical study of this compound under pressure is available in the literature [6], however, it is limited to transmittance measured in a limited range ($P < 40$ GPa).

At Synchrotron Soleil, we have measured both the reflectivity and transmittance of NaCl in a wide pressure range 0 - 100 GPa and have combined them with *ab initio* calculations. The optical constants of sodium chloride in a wide pressure range were determined from the analysis of the spectra of a minute quantity of NaCl powder placed in diamond anvil cells. The so-called “reststrahlen band” which dominates the far infrared reflectance spectra shifts from 150 cm^{-1} up to 500 cm^{-1} at 100 GPa. For the 0 - 17.5 GPa pressure range. The data allow determining accurately both the transverse and longitudinal mode frequencies and some additional structures confirm the anharmonic character of this ionic compound. Measurements at higher pressure reveal the B1 → B2 structural transition around 30 GPa and provide values for the transverse mode frequencies. This spectroscopic signature on a sample smaller than 100 µm using light of wavelength close to this dimension was observed thanks to the high brilliance synchrotron source at the AILES beamline of synchrotron SOLEIL. In addition, *ab initio* calculations of the TO and LO frequencies for the 0 - 200 GPa range are validated by the excellent agreement with experiment.

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