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Structural characterization of high-pressure liquid water by transient infrared ultrafast spectroscopy SAMUELE FANETTI, LENS, European Laboratory for Non-linear Spectroscopy, ANDREA LAPINI, MARCO PAGLIAI, MARGHERITA CITRONI, MARIANGELA DI DONATO, LENS and "Ugo Schiff" Chemistry department, University of Florence, SANDRO SCANDOLO, Abdus Salam International Centre for Theoretical Physics (ICTP) and IOM-CNR, ROBERTO RIGHINI, ROBERTO BINI, LENS and "Ugo Schiff" Chemistry department, University of Florence — Experimental and computational studies have reported in the last years the existence of two different local structures of liquid water depending on pressure and temperature conditions, called low density (LDW) and high density water (HDW). For the first time we have combined pump-probe ultrafast spectroscopy with ultra high pressure devices to access the gigapascal range, providing new insights on the understanding of the two structures peculiarities and their interconversion, in the whole range of thermodynamic stability of liquid water, from 273 to 363 K, from ambient pressure up to 1.2 GPa. We measured the OD stretching rotational anisotropy decay time-constant and vibrational lifetime T1, in a solution of HOD in H2O, pressurized in a sapphire anvil cell, as a function of pressure at different temperatures and we performed a careful infrared linewidth study of the OD stretching mode as a function of temperature and pressure. We interpreted the pressure evolution of the measured parameters in terms of structural changes, identifying the key to correlate the structure evolution with the dynamic data that led us to define the pressure and temperature region where only HDW exists.

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