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Title:Water dynamics as affected by interaction with biomolecules and change of thermodynamic state: a neutron scattering study

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Abstract:The dynamics of water as subtly perturbed by both the interaction with biomolecules and the variation of temperature and pressure has been investigated via neutron scattering spectroscopy. A measurement of inelastic neutron scattering devoted to the study of the coherent THz dynamics of water in a water-rich mixture with DNA (hydration level of 1 g DNA/15 g D<sub>2</sub>O) at room temperature is reported. The DNA hydration water coherent dynamics is characterised by the presence of collective modes, whose dispersion relations are similar to those observed in bulk water. These dispersion relations are well described by the interaction model developed in the case of bulk water, and the existence of a fast sound is experimentally demonstrated. The behaviour of the collective water dynamics was complemented by studying the single-particle dynamics of bulk water along the isotherm  $T = 298$  K in the pressure range 0.1-350 MPa by means of incoherent scattering. This experiment is an attempt to simulate the change of the water molecular arrangement due to the interaction with DNA, by increasing the pressure as the presence of the biomolecule produces an increase in the density. An anomaly is found in the behaviour of the relaxation time derived from the quasi-elastic scattering signal, which can be related to the hypothetical second critical point in water. This anomaly and the transition from slow to fast sound take place in the same Q range, thus suggesting that the two phenomena could be related at some microscopic level.

Number of references:34

Inspected controlled terms:dispersion relations - DNA - macromolecules - molecular biophysics - neutron diffraction - solvation - water

Uncontrolled terms:hypothetic second critical point - quasielastic scattering signal - relaxation time - incoherent scattering - single-particle dynamics - dispersion relations - collective modes - DNA - water-rich mixture - coherent THz dynamics - inelastic neutron scattering -

thermodynamic state - biomolecules - water dynamics - temperature 298 K - pressure 0.1 MPa to 350 MPa - H<sub>2</sub>O

Inspec classification codes:A8230N Association, addition, and insertion - A8715K Biomolecular interactions, charge transfer complexes

Numerical data indexing:temperature 2.98E+02 K;pressure 1.0E+05 3.5E+08 Pa

Chemical indexing:H2O/bin H2/bin H/bin O/bin

Treatment:Experimental (EXP)

Discipline:Physics (A)

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