207
Accession number:20120814795451
Title:Vibrational features of water at the low-density/high-density liquid structural transformations
Authors:Khusnutdinoff, Ramil M. (1); Mokshin, Anatolii V. (1)
Author affiliation:(1) Department of Physics, Kazan (Volga Region) Federal University, Kremlevskaya Street 18, 420008 Kazan, Russia
Corresponding author:Khusnutdinoff, R.M.(khrm@mail.ru)
Source title:Physica A: Statistical Mechanics and its Applications
Abbreviated source title:Phys A Stat Mech Appl
Volume:391
Issue:9
Issue date:May 1, 2012
Publication year:2012
Pages:2842-2847
Language:English
ISSN:03784371
CODEN:PHYADX
Document type:Journal article (JA)
Publisher:Elsevier, P.O. Box 211, Amsterdam, 1000 AE, Netherlands
Abstract:A structural transformation in water upon compression was recently observed at the temperature T=277K in the vicinity of the pressure p≈2000atm [R.M. Khusnutdinoff, A.V. Mokshin, J. Non-Cryst. Solids 357 (2011) 1677]. It was found that the transformations are related with the principal structural changes within the first two coordination shells as well as the deformation of the hydrogen-bond network. In this work, we study in detail the influence of these structural transformations on the vibrational molecular dynamics of water by means of molecular dynamics simulations on the basis of the model Amoeba potential (T=290K, p=1.0÷10000atm). The equation of state and the isothermal compressibility are found for the considered (p, T)-range. The vibrational density of states extracted for THz-frequency range manifests two distinct modes, where the high-frequency mode is independent of pressure whereas the low-frequency one has the strong, non-monotonic pressure-dependence and exhibits a step-like behavior at the pressure p≈2000atm. The extended analysis of the local structural and vibrational properties discovers that there is a strong correlation between the primary structural and vibrational aspects of the liquidliquid structural transformation related with the molecular rearrangement within the range of the second coordination shell. 
Number of references:42
Main heading:Molecular dynamics
Controlled terms:Equations of state - Hydrogen - Internet protocols
Uncontrolled terms:Coordination shells - Equation of state - Extended analysis - High-frequency mode - Hydrogen bond networks - Isothermal compressibility - Liquid-liquids - Low frequency - Molecular dynamics simulations - Molecular rearrangement - Pressure dependence - Strong correlation - Structural change - Structural transformation - Vibrational density of state - Vibrational features - Vibrational properties - Water models
Classification code:723 Computer Software, Data Handling and Applications - 801.4 Physical

Chemistry - 804 Chemical Products Generally - 921 Mathematics
DOI:10.1016/j.physa.2011.12.037
Database:Compendex