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VIII International Conference
for Professionals & Young Scientists
"LOW TEMPERATURE PHYSICS"
May 29 - June 2, 2017

# Conference Program

# &

# Book of Abstracts

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## QUANTUM LIQUIDS AND QUANTUM CRYSTALS, CRYOCRYSTALS

# THERMODYNAMIC PROPERTIES OF TETRAFLUOROMETHANE IN THE SOLID PHASE I

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Thermodynamic properties of refrigerants are needed for the development of cryogenic installations and design of equipment for separation of atmospheric gases not only in the gaseous, but also in the condensed phases. This is necessary to avoid undesirable precipitation of condensed refrigerants in these cryogenic installations.

High-pressure studies of thermodynamic properties of solid halogenated methane are important in the search for new energy-intensive molecular systems based on new carbon materials suitable for the storage and easy retrieval of molecular hydrogen as a fuel.

The purpose of this paper is prediction of the thermodynamic properties of tetrafluoromethane on the melting line and in crystalline phase I in a wide range of temperatures and pressures.

Calculation of equilibrium properties of $CF_4$ was performed within the framework of thermodynamic perturbation theory applied to the crystal consisting of spherical molecules with an octupole-octupole interaction considered as a perturbation. The Helmholtz free energy calculation was based on the generalization of the Mayer group expansion applied to solids, as proposed in [1].

Theoretical equation of state previously developed on this basis, allows describing properties of the high-pressure phase of methane over a wide range of temperatures. Such an approach also was successful in predicting location of the melting line in the high-pressure region [2]. Halogenomethanes along with deuteromethane in crystalline phases adjoining melting line could be treated alike pure methane even under elevated pressures [3].

Equation of state similar to above mentioned [2] was used in this work to predict the specific volume, internal energy, enthalpy, entropy, thermal expansion coefficients, isothermal compressibility and heat capacity of tetrafluoromethane. We present the results of calculations in the temperature range (90-300 K) on the melting line and at increased pressures in the $CF_4$ crystalline phase I.

The adopted approach requires for calculating all the thermodynamic properties only the parameters of the central intermolecular interaction potential, octupole moment [4] and known dependence of the melting temperature of $CF_4$ [5] on the pressure.

The results of the thermodynamic properties calculations are compared with the available experimental data and a reasonable agreement was found. We discuss the possibility to extend the adopted approach to other halogenomethanes.

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