Thematic Section: Theoretical Chemistry	A	Analytical	Stud	y
---	---	------------	------	---

Subsection: Physical Chemistry. Registration Code of Publication: 12-30-4-37

Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*". http://butlerov.com/readings/

Contributed: March 2, 2012.

## *pVT*-properties of crystalline polymers. Theory.

## © Vladimir F. Skorodumov

Department of Physics. A.N. Kosygin Moscow State Textile University. Malaya Kaluzhskaya St., 1. Moscow, GSP-1. 119991. Russia. Phone: +7 (495) 955-37-54. E-mail: SVF1950@yandex.ru

**Keywords:** polymers, pVT-properties, cell model, the intermolecular forces, the quantum harmonic oscillator.

## **Abstract**

On the basis of the cell model "harmonic oscillator" we obtained the thermal equation of state, the expressions for the force constant, vibrational frequencies and Grüneisen parameter in the case of crystalline polymers. The classical and the quantum cases were discussed. The limits of applicability of the model were defined.