Full Paper _____ *Thematic Section:* Thermodynamics.
Registration Code of Publication: 11-26-12-20 *Subsection:* Inorganic Chemistry.
Publication is available for discussion in the Internet as a material of "All-Russian Working Chemical Conference "*Butlerov's Heritage-2011*". http://butlerov.com/bh-2011/
Contributed to editorial board: July 11, 2011

Structural properties of small clusters in the Water vapor

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Keywords: *real gas, Water vapor, thermophysical properties, molecular interactions, bond energy.*

Abstract

A series expansion for a number of thermophysical properties of the Water vapor, in particular for the Joule-Thomson coefficient, contains noticeable quadratic component that reflects a large role of the four particle clusters. The phenomenology method to estimate the intermolecular bond parameters: the molecular clusters effective bond energy and volume, is developed basing on the available databases for real gases thermophysical properties. The estimates for effective intermolecular bond parameters for Water dimers, trimers and quatromers are found and used to make conclusions about the predominant types of structures for the Water vapor clusters. The Water vapor trimers are shown to exist predominantly as the open chain isomers with two hydrogen bonds and with a large mobility of links, which signal about a similarity between the trimer's and Water drop's molecular motion types. The predominant isomer of quatromers, to the contrary, possesses a rigid structure with eight hydrogen bonds and restricted freedom for molecular motion and looks like a prototype for snowflakes.