

Russian Journal of Physical Chemistry A 2014 vol.88 N9, pages 1472-1477

Thermodynamic functions of lactams in the ideal gas state

Emel'Yanenko V., Turovtsev V., Orlov Y.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Thermodynamic functions (enthalpy, entropy, free energy, and heat capacity) of azacycloalkan-2-ones with ring sizes $n = 4-8$ in the ideal gas state are calculated by means of quantum chemistry and statistical physics, using an anharmonic approximation in the range of 298-1500 K with allowance for all known conformers and optical isomers. Equilibrium structures and total energies of lactams are calculated using the B3LYP/6-311++G(3df, 3pd), B3LYP/aug-cc-pVQZ, and MP2/6-311++G(3df, 3pd) methods, and the anharmonic frequencies of the fundamental vibrations of all the investigated structures were found via B3LYP/6-311++G(3df, 3pd). © 2014 Pleiades Publishing, Ltd.

<http://dx.doi.org/10.1134/S0036024414090131>

Keywords

anharmonic frequencies, enthalpy of formation, entropy, Gibbs free energy, heat capacity, lactams, rigid rotator-anharmonic oscillator, thermodynamic properties