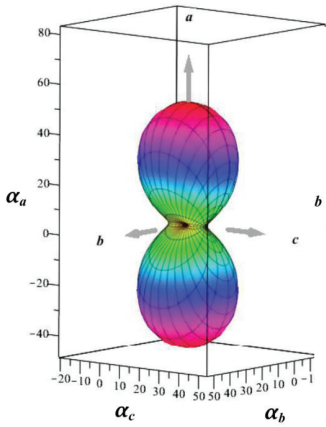


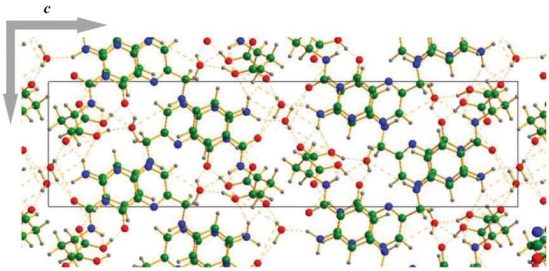
Research (What is it about?)	Thermodynamics of vitamins and hormones
UNN authors	<i>Knyazev A.V., Smirnova N.N., Markin A.V., Knyazeva S.S., Shipilova A.S., Gusarova E.V.</i>
We find (The result)	The coefficients of thermal expansion and thermodynamic functions of vitamins and hormones have been determined for the range from $T \rightarrow 0$ to 330 K
Abstract	<p>The systematic studies of bioactive compounds thermodynamic properties in a broad temperature range give one a possibility to predict its behavior in the real biological systems. In this research we have been studied these properties for three widely used compounds:</p> <p>vitamin B9 (folic acid dihydrate) which is also known as folate (the natural form in body), vitamin M, vitamin Bc (or folacin) are essential for numerous bodily functions; the human body needs folic acid to synthesizes DNA and methylates DNA as well as to act as a cofactor in certain biological reactions;</p> <p>methylprednisolone aceponate – glucocorticoid (glucocorticosteroid), which is used in medicine to treat diseases caused by an overactive immune system, such as allergies, asthma, autoimmune diseases, and sepsis;</p> <p>hydrocortisone acetate is a corticosteroid with anti-inflammatory properties; it may stimulate superoxide dismutase production as well as release antioxidants; it can be anti-allergic, antitoxin, resistance to shock action.</p> <p>The thermodynamic functions namely, the heat capacity, enthalpy, entropy and Gibbs function have been determined. Enthalpy of combustion was measured. The standard molar enthalpy of formation in the crystalline state was derived from the combustion experiments. Using a combination of the adiabatic and combustion calorimetry results, the thermodynamic functions of formation have been calculated. The coefficients of thermal expansion have been determined.</p>

Representative articles 2016-2017, quartiles	1. <i>Knyazev A.V., Emel'yanenko V.N., Smirnova N.N., Stepanova O.V., Shipilova A.S., Markin A.V., Samosudova Ya.S., Gusarova E.V., Knyazeva S.S., Verevkin S.P.</i> Thermodynamic properties of methylprednisolone aceponate. J. Chem. Thermodyn. 103 , 244–248 (2016).	Q1,Q2
	2. <i>Knyazev A.V., Emel'yanenko V.N., Shipilova A.S., Lelet M.I., Gusarova E.V., Knyazeva S.S., Verevkin S.P.</i> Thermodynamic properties of vitamin B ₉ . J. Chem. Thermodyn. 100 , 185–190 (2016).	Q1,Q2
	3. <i>Knyazev A.V., Smirnova N.N., Shipilova A.S., Larina V.N., Gusarova E.V., Knyazeva S.S.</i> Combustion calorimetry and low-temperature X-ray diffraction of steroid hormone. J Therm Anal Calorim. 123 (3), 2201-2206 (2016).	Q2,Q3,Q3
	Q-index (Qi) of the result	3.11

In collaboration	University of Rostock, Dr-Lorenz-Weg 1, D-18059 Rostock, Germany Kazan Fed Univ, Kremlevskaya Str 18, Kazan 420008, Russia Open Joint Stock Co Chemicopharmaceut Works Akrik, Kosmodamianskaya Naberezhnaya 52-5, Moscow 115054, Russia
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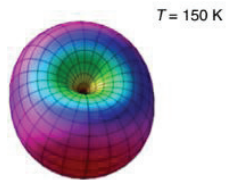
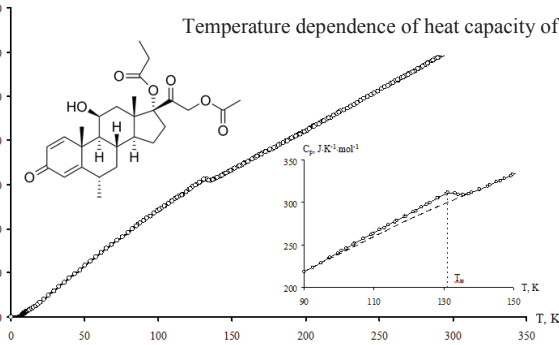


3D thermal expansion diagram and fragment of structure of *vitamin B9*.

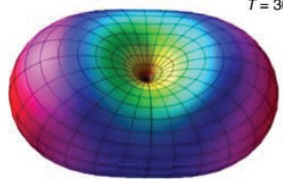


$C_p, \text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

Temperature dependence of heat capacity of *methylprednisolone aceponate*.

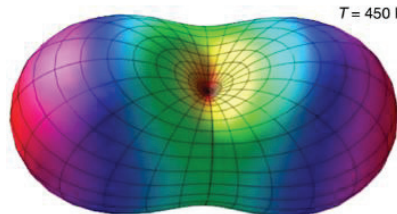


$T = 150 \text{ K}$



$T = 300 \text{ K}$

3D thermal expansion diagram of *hydrocortisone acetate*.



$T = 450 \text{ K}$