

The phenomenon of polymorphism in the atomic structure of the methylprednisolone aceponate

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Scientists at Lobachevsky University (UNN) in Nizhny Novgorod are studying physico-chemical properties of steroid hormone crystals. Steroid hormones are a group of physiologically active substances that regulate the processes of vital activity in animals and humans. These include, for example, sex hormones and corticosteroids. In particular, corticosteroids are a subclass of steroid hormones that are produced exclusively by the adrenal cortex. They are characterized by their glucocorticoid or mineralocorticoid activity.

Provided by Lobachevsky University

UNN researchers have discovered the phenomenon of polymorphism in the atomic structure of the methylprednisolone aceponate crystal. They synthesized a single crystal of corticosteroid [hormone](#) methylprednisolone aceponate of sufficient size for X-ray diffraction studies. As a result, they obtained a three-dimensional model of the [atomic structure](#) of methylprednisolone aceponate at different temperatures for the first time.

In particular, the researchers found that at a temperature of 131 K (-142°C), the methylprednisolone aceponate crystal experiences a second-order phase transition. It is manifested in the fact that with a decrease in temperature, chaotically located methyl groups are ordered and exhibit a strict spatial periodicity. In this case, one of the parameters of the unit cell increases by a factor of three compared with the high-temperature phase.

In-depth study of physicochemical properties of steroid hormone crystals is important for the synthesis of new medicines. It is also of great practical value for the modern pharmaceutical industry: to create a new medicine, not only an appropriate active substance is required, but also an effective method for storing it.

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