

CONFORMATIONAL TRANSFORMATION IN NH--N BONDED FERROELECTRIC 1,4-DIAZABICYCLO[2.2.2]OCTANE PERCHLORATE

Armand Budzianowski i Andrzej Katrusiak

*Dep. of Crystallography, Adam Mickiewicz University,
Grunwaldzka 6; 60-780 Poznań; Poland.*

This report continues our studies on the thermodynamics and transformations of NH--N bonded structures [1]. Crystals of 1,4-diazabicyclo[2.2.2]octane perchlorate (**1**) were reported to exhibit ferroelectricity related to the transformation of the NH--N hydrogen bonds [2,3]. The paraelectric-ferroelectric phase transition at $T_{12}=377$ K changes the crystal symmetry from $P4/mmm$ to $Pm2_1n$ [4]. We have found a second phase transition in this substance at $T_{23}=220$ K, and investigated the low temperature phase. The crystal symmetry is further lowered to $Pa2_1n$, and the unit-cell parameter c doubles. The phase transition at T_{23} is connected with the conformation change of the octane rings. The ethylene moieties become twisted, which breaks the mirror symmetry of the cations. The structural dimensions of structure **1** in the function of temperature will be discussed in relation to the intriguing properties of these crystals.

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Literatura

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