

CRYSTAL STRUCTURE OF 6-AMINO-4,4,5,7,8-
PENTAMETHYLDIHYDROCOUMARIN HYDROCHLORIDE

Armand Budzianowski and Andrzej Katrusiak

*Department of Crystallography, Adam Mickiewicz University,
60-780 Poznań; Grunwaldzka 6*

The crystal and molecular structure of 6-amino-4,4,5,7,8-pentamethyldihydrocoumarin hydrochloride (see Figure 1) denoted **1** was determined by X-ray diffraction. KM-4CCD single crystal diffractometer has been used. At room temperature crystals **1** are monoclinic with the space group $P2_1/c$.

This study is a continuation of our previous studies on the influence of substitutes on conformational properties and stereopopulation of coumarin derivatives. We will discuss conformation of lactone ring and the methyl groups to influence of molecular conformation. Intramolecular interaction methyl groups are often interpreted as ‘trimethyl lock’, which

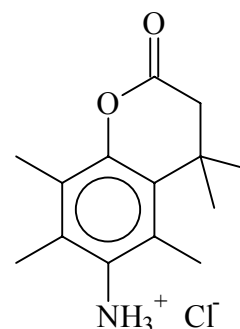


Figure 1. Structure I.

favours some conformations of molecule and promote chemical reactions of lactonization [1-3]. However our structural studies of the structures with ‘trimethyl lock’ showed that steric hindrance does not influence the conformation of molecules. Changes of conformation in this group of compounds are results from intramolecular electrostatic forces [4].

In the present study we are mainly concentrated with the thermodynamic stability of the molecular conformation of **1**.

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