ELECTRON DENSITY DISTRIBUTION IN N-OXALYL-L-ARGININE (NOLA) CRYSTAL

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Crystalline salts of L-arginine recently attracted great attention as source of promising nonlinear optical materials. Reaction of L-arginine with oxalic acid has been studied in Ref. [1], were the crystal L-Arg.$H_2C_2O_4$ with triclinic symmetry was found. In Ref. [2] the same system was studied in more detail and some new salts were prepared: 2L-Arg.$H_2C_2O_4$.2.5H_2O, L-Arg.$H_2C_2O_4$ with monoclinic symmetry and L-Arg.2$H_2C_2O_4$. Furthermore, the crystal with non-salt nature N^{α}-oxalyl-L-arginine (NOLA) with trigonal symmetry (space group $P3_221$) was found and crystal structure was determined at room temperature.

In present paper results of electron charge density distribution of NOLA at 120K will be presented. Based on the obtained X-ray diffraction data the analytical form of electron density distribution function in crystal $\rho(\mathbf{r})$ was obtained in terms of Hansen-Coppens formalism [3] using the XD program package. In order to figure out the hydrogen bonding pattern in NOLA as well as to estimate the strength of H-bonds we have carried out topological analysis of $\rho(\mathbf{r})$ function within Bader's formalisms [4]. The usage of this approach allows determining the main characteristics of all the interatomic interactions, the atomic charges and volumes as well as the energy of interatomic interactions. The later was done based on the correlation [5] between the energy of the contact with the value of the potential energy density function v(r) in the corresponding bond critical point.

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