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# Structure Transformations in Nickel Oxalate Dihydrate $\text{NiC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$ and Nickel Formate Dihydrate $\text{Ni}(\text{HCO}_2)_2 \cdot 2\text{H}_2\text{O}$ during Thermal Decomposition

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## Abstract

Structure and thermolysis of  $\text{NiC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$  (**I**) and  $\text{Ni}(\text{HCO}_2)_2 \cdot 2\text{H}_2\text{O}$  (**II**) were studied for the precipitated powders from the water solutions of precursors. The compound (**I**) has a disordered structure ( $C2/c$ ,  $a=11.7916(5)$ ,  $b=5.31798(14)$ ,  $c=9.7806(7)$  Å,  $\beta=127.014(6)^\circ$ ,  $V=489.73(4)\text{Å}^3$ ) which is described *via* the displacement vector applied to the basis atoms and the part of the shifted atoms. Thermal dehydration of (**I**) leads to formation of the disordered  $\beta\text{-NiC}_2\text{O}_4$  (**III**), the structure of which ( $P2_1/n$ ,  $a=5.8294(9)$ ,  $b=5.1685(13)$ ,  $c=5.2712(4)$  Å,  $\beta=117.793(12)^\circ$ ,  $V=140.50(5)\text{Å}^3$ ) was refined from the powder diffraction. Oxalates (**I**) and (**III**) are both characterized by the essential part of the shifted atoms causing the extinction of some lines in XRPD pattern. The final product of thermal decomposition of (**I**) in air is NiO, whereas thermolysis of (**II**) leads to formation of Ni/NiO mixture. The content of Ni in the latter depends on the thickness of the decaying layer in the sample because the gaseous products of the reaction prevent the oxidation of the nickel formed initially.

**Keywords:** Nickel Oxalate dihydrate, Nickel Oxalate, Nickel Formate dihydrate, Crystal structure, Powder diffraction, thermal decomposition

## Introduction

Nickel oxalate and Nickel formate attract the stable interest of researchers because of their low thermal stability which allows to obtain the metal and/or metal oxide system for various applications and theoretical study. In particular, thermal decomposition of nickel oxalate [1,2] produces the nanocrystalline NiO powder which may be used as catalyst [3,4] including the coating on the ceramic carrier [5], nanofibers [6] or as nanoparticles working in the liquid medium [7]. A lot of published

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