# Crystal Structure of Nickel Picolinate Tetrahydrate

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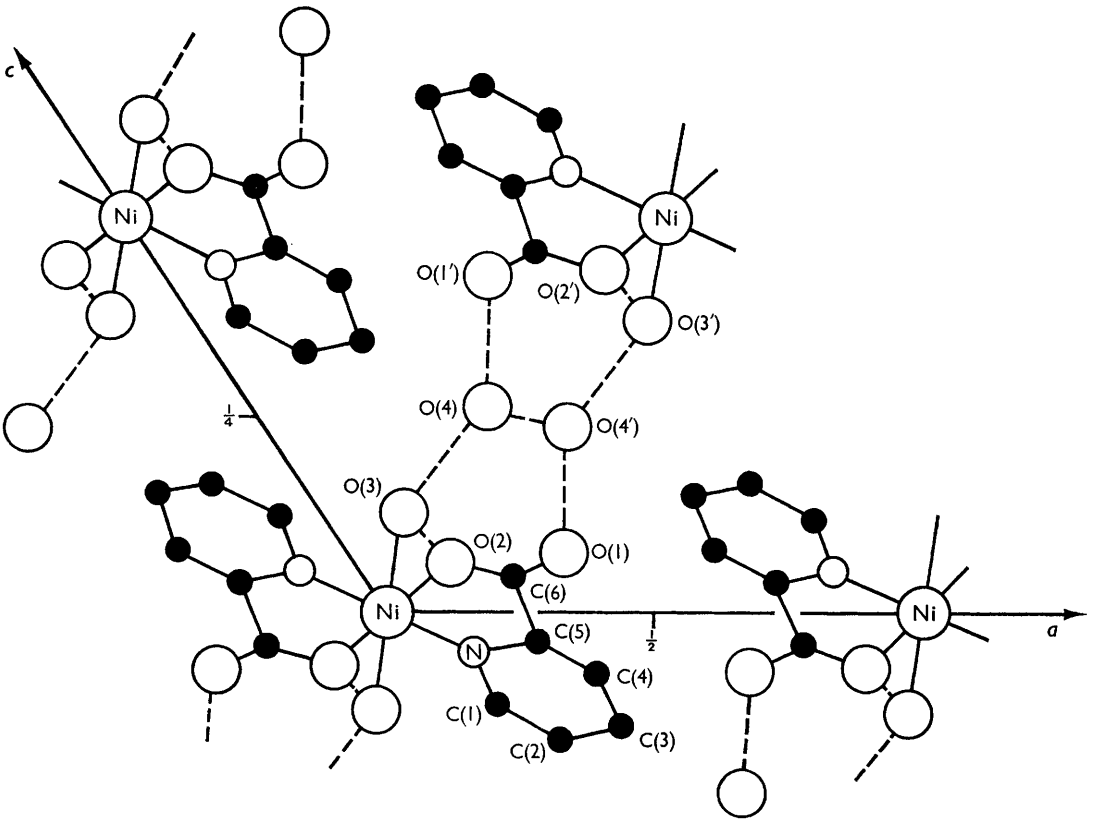
THE nickel picolinate tetrahydrate $(C_5H_4NCO_2)_2Ni,4H_2O$ crystallizes in the monoclinic system with the space group $P2_1/c$: $a = 9{\cdot}727 \pm 0{\cdot}012$, $b = 5{\cdot}2342 \pm 0{\cdot}0017$, $c = 17{\cdot}463 \pm 0{\cdot}023$ Å; $\beta = 123°46' \pm 05'$; $Z = 2$.

Intensity data were recorded on multiple-film Weissenberg photographs for a cylindrical crystal of 0·3 mm. diameter rotating around the *b*-axis (Cu-$K_\alpha$:$\lambda = 1{\cdot}5418$ Å; 772 non-zero reflexions).

The special Ni position (centre) was chosen as origin and the co-ordinates $x$ and $z$ of all other atoms apart from hydrogen were found easily by the Patterson projection $P(u, w)$; the third co-ordinate $y$ was estimated by the trial and error method.

The structure was refined by three cycles of isotropic least-squares calculations on a CDC 3600; the final $R$-value was 0·106.

The Figure shows the molecules projected on the (010) plane. The Ni atom is surrounded by an octahedral arrangement of two N atoms, two chelating carboxylic oxygens O(2) and another two aqueous oxygens O(3). The oxygen atoms O(4) are not bonded to the nickel. The intermolecular contacts are formed by hydrogen bonds between the oxygen atoms (dotted lines on the Figure).




FIGURE

This work is being continued by the localisation of hydrogen atoms and by a three-dimensional refinement with anisotropic thermal corrections.

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