

The nickel battery positive electrode revisited: stability and structure of the β -NiOOH phase†

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The crystal structure of the nickel battery positive electrode material, β -NiOOH, is analyzed through a joint approach involving NMR and FTIR spectroscopies, powder neutron diffraction and DFT calculations. The obtained results confirm that structural changes occur during the β -Ni(OH)₂/ β -NiOOH transformation leading to a metastable crystal structure with a TP2 host lattice. This structure involves two types of hydrogen atoms both forming primary and secondary hydrogen bonds. The formation of TP2 NiOOH as opposed to the more stable P3 host type during β -Ni(OH)₂/ β -NiOOH transformation has a kinetic origin that can be understood by a lower strain penalty involved in the transformation.

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