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Phase transformations in a promising Na-rich cathode material for sodium-ion batteries

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Sodium-ion batteries (SIB) are promising electrochemical devices due to the sodium availability compared to lithium. Developing efficient cathode materials is very important task for the wide distribution of SIB. One of the perspective cathode materials for SIB are hexacyanoferrates NaxM[Fe(CN)6]·nH2O (Prussian blue analogues, where M are transition metal cations), which have open framework structure and low-temperature synthesis. For successful using of the material, "y"in Na2-yFe[Fe(CN)6]·nH2O must be minimal. Ideal composition for high SIB capacity is Na2Fe[Fe(CN)6]·nH2O. In scientific research model batteries often use sodium metal anode. In this case the cathode composition can be electrochemically brought to Na2Fe[Fe(CN)6]·nH2O after first charge-discharge cycle of the battery. Real SIBs are manufactured with hard carbon as an anode. It becomes impossible to enrich electrochemically the cathode material with sodium way. Therefore, it is necessary to initially synthesize the Na-rich material.
The structural phase transitions in the commercial PW powder (Altris, Sweden) enriched with sodium, as well as in a similar synthesized Na2-yFe[Fe(CN)6]·nH2O powder during heating up to 250℃ and cooling down to -220℃ were investigated using X-ray diffraction.

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[1] W. Brant et al. Method of producing a sodium iron(II)-hexacyanoferrate(II) material // United States Patent application publication. No: 2019/0270649 A1, Sep.5 2019.

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