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Mössbauer studies of structural properties and electrochemical characteristics of LiFePO₄

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Abstract

The valency state and local coordination of Fe ions of four industrial samples and a sample of cathodic materials for rechargeable lithium ion batteries obtained using an original technology of St. Petersburg State Technological Institute (Technological University) were studied using the Mössbauer effect on the ⁵⁷Fe isotope. It was found that the main valency state for more than 90% of iron ions was Fe²⁺. The values of isomer shift $\delta = 0.96\text{-}0.98$ mm/s and quadrupole splitting $\sigma = 2.88\text{-}2.93$ mm/s for Fe²⁺ ions coincide with the values for compounds with the structure of olivine LiFePO₄ and occupy positions in highly distorted FeO₆ octahedrons. Fe³⁺ ions are in octahedral and/or tetrahedral local positions. © 2012 Pleiades Publishing, Ltd.

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