Poster Presentation

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Crystal structure of a new lithium iron vanadate

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Iron vanadates and phosphates have been widely explored [1-2] as possible electrode material for Li-ion batteries. In the goal of finding new materials, our approach was to consider existing materials and to investigate the flexibility of their network for possible substitutions. Among the different materials containing iron and vanadium, Cu3Fe4(XO4)6 (X = P, V) are isostructural to Fe7(PO4)6. Lafontaine et al. [3] discussed the structural relationships between β-Cu3Fe4(VO4)6 and several other vanadates, phosphates and molybdates of general formula AxBy(VO4)6. The interesting network flexibility was then demonstrated with the existence of four different crystallographic sites, which can be partially occupied depending on the x+y value : x+y = 7 for β-Cu3Fe4(VO4)6) and x+y = 8 for NaCuFe2(VO4)3. The LixFey(VO4)6 phase was then prepared considering the substitution of Li+ and Fe3+ for Cu2+ ions in β-Cu3Fe4(VO4)6 and the existence of an extra site to accommodate the charge compensation ($7 \leq x+y \leq 8$). As expected, a new lithium iron vanadate, isotructural to mineral Howardevansite was then obtained. Single crystal diffraction data were collected at room temperature on Enraf-Nonius CAD-4 diffractometer. Structure was refined with JANA-2006 program package. Mössbauer and magnetic measurements were also used to check the oxidation state of iron ions, to support the obtained crystal structure and to consider any possible structural/magnetic transitions. All the results will be presented and discussed in this presentation.

[1] *C. Masquelier, L. Croguennec, Chem. Rev. 2013, 113, 6552-6591,* ***[2]*** *M. Dollé, S. Patoux, T.J. Richardson, J. Power Sources, 2005, 144, 208-213,* ***[3]*** *M.A. Lafontaine, J.M. Grenéche, Y. Laligant, G. Férey, J. Solid St. Chem., 1994, 108, 1-10*

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