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Phase diagram of Na1-xCaxV2O4 compounds synthesized at high pressure TAMAS VARGA, JOHN MITCHELL, Argonne Natl Lab, KAZUNARI YAMAURA, DAVID MANDRUS, Oak Ridge Natl Lab, JUN WANG, Argonnne Natl Lab — Ambient pressure CaV2O4 and high-pressure NaV2O4 crystallize in the CaFe2O4 structure type containing double chains of edge-sharing VO6 octahedra. Recent measurements on NaV2O4 reveal low-dimensional metallicity and evidence of half-metallic ferromagnetism. In contrast, CaV2O4 is an antiferromagnetic insulator. To explore the evolution of these ground-state behaviors, we have prepared a series of Ca-doped NaV2O4 compounds with the formula Na1-xCaxV2O4 (x=0-1) using high-pressure synthesis. The lattice parameters of Na1-xCaxV2O4 samples change with nominal x according to Vegard's law. The metallic state in NaV2O4 is dramatically altered by Ca doping. Samples with higher Ca concentrations (x=0.6-0.8) exhibit a metal-insulator transition around 150 K. Samples at the Na end (x=0-0.2) show a broad antiferromagnetic transition in the 120-160 K range in accordance with earlier reports. With increased Ca doping, the antiferromagnetic transition is suppressed to ∼70 K at the Ca-endmember. Transport measurements show an insulator-metal transition at x∼0.4. Comparison to existing studies at the Ca- and Na-rich ends will be discussed along with a schematic (T-x) phase diagram for the Na1-xCaxV2O4.

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