Supporting information for:

Anion-ordered chains in a d^1 perovskite oxynitride; $NdVO_2N$ by Judith Oró-Solé et al.

Experimental Details

NdVO₂N was prepared by ammonolysis at 700 °C of NdVO₄. The oxide precursor was prepared by solid state reaction in air between Nd₂O₃ (Aldrich, 99.9 %) and V₂O₅ (Aldrich, 99.99 %). Nd₂O₃ was previously treated at 900 °C for 12 hours. The binary oxides were mixed in the stoichiometric proportions, pelletized and treated at 900 °C for 15 hours. NdVO₄ was nitrided by two 40 hours treatments in flowing NH₃ (Carburos Metálicos, 99.9%) at a rate of 600 cm³/min, with slow cooling to room temperature in the ammonia atmosphere and intermediate regrinding.

N contents were determined by combustion analysis using a Thermo Fisher Scientific instrument. X-ray diffraction data were collected on a Siemens D5000 diffractometer using Cu ka radiation (l= 1.5418 Å) (Figure S-1).

Electron diffraction patterns from individual microcrystallites of $NdVO_2N$ were obtained using a JEOL 1210 transmission electron microscope operating at 120 kV equipped with a side entry 60/308 double-tilt GATHAN 646 specimen holder. The samples were prepared by dispersing the powders in hexane and depositing a droplet of this suspension on a carbon-coatedholey film supported on a copper grid.

Magnetic measurements were performed between 2 and 300 K in fields of 0.0025 and 1 T using a Quantum Design SQUID magnetometer.

Supplementary figure S-1. X-ray diffraction pattern of NdVO₂N.

