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Multi-k magnetic order in Ca3CuNi2(PO4)4: irrep approach and Shubnikov symmetry

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The multi-k magnetic structures with propagation vectors k being the arms of the propagation vector star rarely can be justified experimentally. We show that the antiferromagnetic structure in the low dimensional quantum spin trimer system Ca3CuNi2(PO4)4 is based on the full star of propagation vector k=[1/2,1/2,0] of the paramagnetic space group C2/c. The relation between representation analysis in the propagation vector formalism and Shubnikov magnetic space group (MSG) symmetry is examined in details. A symmetry restrictive MSG that excellently fits the experimental data can be constructed only with the use of the full star. The magnetic structure is further supported by the calculations of the spin expectation values of the isolated Ni-Cu-Ni trimer with realistic Hamiltonian.

Keywords: magnetic structure, representation analysis, Shubnikov symmetry