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Magnetic ground state of NdB4: Interplay between anisotropic exchange interactions and hidden order on a Shastry-Sutherland lattice.

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The Shastry-Sutherland lattice, introduced as a theoretical model of a frustrated antiferromagnet [1], has been at the forefront of condensed matter research over several decades. The model has been experimentally realized for both quantum and classical spins, and one of the well-known representatives of the latter case is neodymium tetraboride NdB_4, crystallising into a tetragonal crystal structure [2]. The compound exhibits several magnetic phases and a complex multi-k ground state that has been elusive for a long time [2,3]. Here we report the solution and quantitative refinement of the magnetic ground state of NdB_4 based on neutron diffraction data. The obtained magnetic structure consists of two components; one of them is confined within the ab-plane and makes an orthogonal all-in all-out configuration maintaining translation symmetry of the crystal. Another is along the c-axis, and this component forms an anharmonic spin density wave consisting of three-up-two-down sequences with fivefold periodicity. The in-plane and out-of-plane spin structures represent distinct magnetic instabilities which normally would not coexist. Their simultaneous presence in the same phase is an interesting phenomenon associated with anisotropic exchange interactions and coupling to a symmetry breaking non-magnetic order parameter undetectable by the available diffraction data.

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