

Abstract Submitted
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Fixed Spin Moment Study of Quantum Critical Fe₃Mo₃N BRIAN NEAL, WARREN E. PICKETT, University of California Davis — Quantum critical behavior and weak magnetism occurs in a handful of intermetallic transition metal compounds, with a recent example being Fe₃Mo₃N with the geometrically frustrated *stella quadrangula* lattice. Neutron scattering reveals antiferromagnetic ordering, but a 14 T magnetic field induces a ferromagnetic state as does substitution of 5% Co on the Fe site [1]. We present the energetics of a transition between these states with density functional based fixed spin moment studies. Our (mean field) ground state occurs with nearly equal Fe1 and Fe2 moments of 1.8 μ_B . As the total moment is reduced, a crossover occurs until at zero total moment the Fe1 moment is -1.1 μ_B (antialigned with the strong Fe2 moment). We use these results to construct scenarios for discussing the observations.

[1] T. Waki et al., J. Phys. Soc. Japan **79**, 043701 (2010).

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