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Lattice and magnetic instabilities in CaFe₂As₂ SHIBABRATA NANDI, ALAN GOLDMAN, Ames Loboratory, US DOE and Iowa State University, DIMITRI ARGYRIOU, Helmholtz-Zentrum Berlin fur Materialien und Energie, BACHIR OULADDIAF, Institute Laue-Langevin, TAPAN CHAT-TERJI, Forschungszentrum Julich Outstation at Institute Laue-Langevin, AN-DREAS KREYSSIG, NI NI, SERGEY BUD'KO, PAUL CANFIELD, ROBERT MCQUEENEY, Ames Loboratory, US DOE and Iowa State University — Neutron diffraction measurements of a high quality single crystal of CaFe₂As₂ are reported. A sharp transition was observed between the high temperature tetragonal and low temperature orthorhombic structures at $T_S=172.5$ K (on cooling) and 173.5 K (on warming). Concomitant with the structural transition we observe a rapid, but apparently continuous, ordering of the Fe moments, in a commensurate antiferromagnetic structure, with a saturated moment of 0.80(5) μ_B /Fe directed along the orthorhombic a-axis. The hysteresis of the structural transition is 1 K between cooling and warming and is consistent with previous thermodynamic, transport and single crystal x-ray studies. The temperature onset of magnetic ordering shifts rigidly with the structural transition providing clearest evidence to date of the coupling between the structural and magnetic transitions in this material and the broader class of arsenides.

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