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Structure and magnetism of the van der Waals bonded ferromagnet CrI_3[1] MICHAEL MCGUIRE, HEMANT DIXIT, VALENTINO COOPER, BRIAN SALES, Oak Ridge National Laboratory — Chromium triiodide is an easily cleavable, semiconducting ferromagnet which has received relatively little attention to date. Here we report results of our experimental investigations of the crystallographic and magnetic properties of CrI_3 single crystals. We find a first order structural phase transition at $T_S = 210$ K and strong magnetic anisotropy below the Curie temperature $T_C = 61$ K. Our findings demonstrate the interaction between structure and magnetism manifested as a magnetic anomaly at T_S and structural anomaly at T_C. Our first principles calculations incorporating the van der Waals interactions reproduce the high and low temperature structures accurately, and indicate cleavage energies comparable to materials of interest for post-silicon electronics like graphite and molybdenum dichalcogenides. Theoretical investigations of the magnetic ordering suggest ferromagnetism may persist in monolayer structures. Overall our results motivate further study of CrI_3 in few- or single-layer-thick samples.

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