Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Giant pressure-induced volume collapse in the pyrite mineral MnS2 SIMON KIMBER, European Synchrotron Radiation Facility, ASHKAN SALAMAT, Lyman Laboratory of Physics, Harvard University, SHAUN EVANS, University of Bern, HARALD JESCHKE, KALIAPPAN MUTHUKUMAR, MILAN TOMIC, FRANCESC SALVAT-PUJOL, ROSER VALENTI, Institute for Theoretical Physics, Goethe University, Frankfurt, MARIA KAISHEVA, Formerly at the University of Edinburgh, IVO ZIZAK, Helmholtz-Zentrum Berlin, TAPAN CHATTERJI, Institute Laue-Langevin — Dramatic volume collapses under pressure are fundamental to geochemistry and of increasing importance to fields as diverse as hydrogen storage and high temperature superconductivity. In transition metal materials, collapses are usually driven by so-called "spin state" transitions- the interplay between the single-ion crystal field and the size of the magnetic moment. Here we show that the classical S= 5/2 mineral Hauerite (MnS2) undergoes an unprecedented 22% volume collapse driven by a conceptually new magnetic mechanism. Using synchrotron x-ray diffraction we show that cold compression induces the formation of a disordered intermediate. However, using an evolutionary algorithm we predict a new structure with edge-sharing chains. This is confirmed as the thermodynamic ground state using in-situ laser heating. We show that magnetism is globally absent in the new phase, as low-spin quantum S= 1/2 moments are quenched by dimerisation. Our results show how the emergence of metal-metal bonding can stabilise giant spin-lattice coupling in Earth's minerals.

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Date submitted: 14 Nov 2013 Electronic form version 1.4