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Highly responsive ground state of PbTaSe<sub>2</sub>: structural phase transition and evolution of superconductivity under pressure S. L. BUDKO, U. S. KALUARACHCHI, Y. DENG, M. F. BESSER, K. SUN, L. ZHOU, M. C. NGUYEN, C. ZHANG, J. S. SCHILLING, M. J. KRAMER, S. JIA, C. Z. WANG, K. M. HO, P. C. CANFIELD, Ames Laboratory, Dept. of Physics, ISU, Dept. of Physics, Washington University, St. Louis, ICQM, School of Physics, Peking University — Thermodynamic and transport studies of PbTaSe<sub>2</sub> under pressure suggest existence of two superconducting phases with the phase boundary at ~ 0.25 GPa at low temperatures that is defined by a very steep, first order, structural, phase transition. The structural phase transition line extends to ~ 425 K at ambient pressure as evidenced by transmission electron microscopy and x-ray diffraction at elevated temperatures. The new, high temperature / high pressure phase has similar crystal structure and slightly lower unit cell volume. The details of this new structute were identified based on first-principles total energy calculations.

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