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A new crystal phase of ammonium nitrate: a monoclinic distortion of AN-IV IVAN OLEYNIK, BRAD STEELE, University of South Florida — Ammonium nitrate (AN) is a major component of the energetic material ANFO. It is important to understand the high-pressure crystal phases and corresponding phase transitions of AN as its structural polymorphism might affect the energetic performance, including crystal density, detonation velocity and shock initiation of chemical reactions. A new crystal phase of AN is found using first principles evolutionary crystal structure search. It is a monoclinic distortion of phase IV of AN (AN-IV) in the $P2_1/m$ space group (AN-$P2_1$ /m). The calculated Raman spectrum of this new phase is consistent with the recently reported experimental Raman spectrum that contains two peaks at high pressures associated with the phase transition. The new phase is calculated to have lower free energy than AN-IV above 11.2 GPa, a pressure close to the experimentally reported phase transition pressure of 17 GPa. The calculated Raman spectra of both AN-$P2_1$ /m and AN-IV as a function of pressure display good agreement with experiment up to 40 GPa.

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