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Tetragonal or cotunnite, a high pressure phase of NiS_2?[1] YONGGANG G. YU, NANCY L. ROSS, Department of Geosciences, Virginia Polytechnic Institute and State University — A sequence of pressure-induced phase transitions within NiS_2 (single crystal) has been established from static LDA calculations. A dozen of AX_2 type candidate structures have been studied at high pressures including cotunnite (α-$PbCl_2$). The calculation identified that below 5 megabar, a tetragonal phase ($P4_2/n$) is more stable than the 9 bond coordinated cotunnite, which otherwise would be commonly conceived. This tetragonal structure is characterized by layers of Ni atoms in 8-fold coordination with S atoms. This phase is more stable than the vaesite phase at about 150 GPa. With further compression to about 756 GPa, the tetragonal phase transforms into a hexagonal AlB_2-type structure (P6/mmm) which is characterized by planar hexagonal layers of S intercalated by Ni atoms where each Ni atom is twelve fold coordinated by S atoms. Calculated band structures and valence charge density maps show S-S and Ni-S bonded interactions for NiS_2 under these extremely compressed conditions. The tetragonal phase may have geophysical implications if present in Earth's core.

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