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MS20-O3 High pressure synthesis of bismuth disulfide, structural solution and its physical properties

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High pressure synthesis is an important method in the search for new compounds and in many cases pressure-stabilized compounds can be quenched to ambient conditions. Therefore high pressure syntheses push the boundaries of solid state chemistry. There is a large current interest in the metal dichalcogenides due to their crystal structures and electrical properties.[1,2] The most sulfur rich phase in the Bi-S phase diagram is Bi_2S_3.[3] Unlike the transition metal dichalcogenides, the Bi atoms in BiS_2 have anisotropic charge distribution and more complex structures are expected when comparing the layered structures of transition metal. The recent discovery of superconductivity in La(O,F)BiS_2 which consists of layers of insulating La(O,F) which donates electrons to superconducting layers of BiS_2 adds further motivation for studies of Bi dichalcogenides.[4] Furthermore, bismuth chalcogenides, such the compound Bi_2S_3, are known to be good thermoelectric materials.[5] The possibilities of using high pressure synthesis to discover new compounds in the Bi-S binary system were investigated as early as the 1960's.[6] The research led to discovery of a compound with BiS_2 stoichiometry, but no structure solution of BiS_2 was reported. In this research the BiS_2 compound was synthesized by a high pressure and high temperature method using a multi-anvil large volume press and the structure was solved by single crystal x-ray diffraction. The structure contains Bi atoms in distorted square-based pyramidal coordination to five surrounding sulfur atoms. The structure, physical properties and theoretical calculations will be discussed and compared to other metal dichalcogenide compounds.

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