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# Possible Fe/Cu ordering schemes in the 2*a* superstructure of bornite ($Cu_5FeS_4$)

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## ABSTRACT

Based on magnetic structure and TEM studies of bornite we propose a new 2*a* Fe/Cu ordered superstructure model with symmetry $F\bar{4}3m$ and formula $Cu_8Fe_4S_8$. First principles calculations (LAPW implemented in WIEN97 code) of two Fe/Cu ordering schemes indicate that, at the ground state, the Fe atoms should fill the tetrahedral sites of sulfur atoms in the anti-fluorite cube, and the vacancies are associated with Cu atoms in the zincblende cube of the superstructure. The calculated magnetic moment of iron in the Fe/Cu-ordered structure is about 4 $\mu_\beta$, which was not expected from previous work because bornite has both covalent and metallic bonds that make crystal-field theory inappropriate for explaining the magnetic moment of Fe. High-resolution transmission electron microscopy (HRTEM) image simulations for the newly proposed structure model are much closer to experimental HRTEM images than those for the model proposed by Kanazawa et al. (1978).