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攀枝花钒钛磁铁矿主要成矿元素地球化学特征的能量因子

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摘要: 攀枝花钒钛磁铁矿矿床为富集钒、钛、铁等过渡元素的典型岩浆矿床。运用量子地球化学的理论和方法研究了该矿床的元素组合、分配及变化特征, 并用量子地球化学的 *ab initio* Hartree Fock 分子轨道法对钛磁铁矿和钛铁矿晶体结构进行了模拟计算。结果表明: 在其结晶过程中, V, Ti, Fe 等成矿元素富集于钛磁铁矿和钛铁矿中而形成钒钛磁铁矿, 矿床受其晶体结构形成过程的能量最低原则控制。

关键字: 量子地球化学; *ab initio* Hartree Fock 分子轨道; 钛磁铁矿; 钛铁矿

Energy factors of primary ore forming elements in Panzhihua vanadic titanomagnetite ore deposit and their geochemical characterization

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Abstract: Panzhihua vanadic titanomagnetite ore deposit is characterized by high concentration of transition elements V, Ti and Fe etc. The theory and method of quantum geochemistry were applied to study the energy factors of primary ore forming elements and their geochemical characterizations. The crystal structure models of titanomagnetite and ilmenite were calculated by *ab initio* Hartree Fock molecular orbital method. The results show that the primary ore forming elements are controlled by the principle of energy minimization during the crystallization processes, and V, Ti, Fe and other ore forming elements are re-concentrated in titanomagnetite and ilmenite.

Key words: quantum geochemistry; *ab initio* Hartree Fock molecular orbital; titanomagnetite; ilmenite

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