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The iron spin transition of deep nitrogen-bearing mineral $Fe_3N_{1.2}$ at high pressure

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Abstract

Nitrogen is an essential element for life, one of the most abundant volatiles in the atmosphere, and an important component in the Earth's interior, where iron nitride is an essential host of deep nitrogen. Here, we investigate the pressure-induced electronic spin-pairing transition of iron in siderazot ($Fe_3N_{1.2}$) at pressures up to 45.8 GPa at room temperature, using diamond-anvil cell techniques coupled with synchrotron X-ray emission spectroscopy. The integrated intensity of the satellite emission peak (K'_{β}) decreases upon compression but remains unchanged at pressures greater than 30.5 GPa. In other words, the high-spin to low-spin transition of iron in $Fe_3N_{1.2}$ starts immediately at very low pressures and completes at ~30.5 GPa. The iron spin transition completion pressures increase with the nitrogen concentration of hexagonal close-packed iron nitrides (i.e., $Fe_3N_{1.2}$, Fe_7N_3, and Fe_2N). Moreover, the identity and concentration of light elements in binary iron-rich compounds such as Fe_3N, Fe_3C, Fe_3P, Fe_3S, Fe_7C_3, and Fe_7N_3, together with their crystal structure, could affect the iron spin transition pressures. The spin transition of iron-rich alloys could alter the bonding nature and the physical properties, including the thermal and electrical conductivity, thereby influencing the thermal state and evolution of planetary interiors.

Keywords: Spin transition, X-ray emission spectroscopy, high pressure, deep nitrogen; Physics and Chemistry of Earth's Deep Mantle and Core